



**7th International Conference
on Multiscale Materials
Modeling**

**6–10 October 2014
Berkeley, California**

mmm2014berkeley.iop.org

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Dislocation patterns

Ladislas P. Kubin

LEM, CNRS-ONERA, 92322 Châtillon Cedex FRANCE

In the long march that leads from the elastic and core properties of individual dislocations to the mechanical response of real materials, one finds collective dislocation processes. In spite of many efforts, the spontaneous formation of dislocation patterns under stress has not yet been convincingly modeled. A short historical sketch shows how the physical content of successive models evolved through the importation of new concepts borrowed from thermodynamics, the dynamics of non linear dissipative systems, statistical mechanics and the continuum theory of dislocations.

Among the various types of patterns found in deformed single crystals, the dislocation cell structures that emerge during unidirectional deformation in stage III have attracted most of the attention. Because of their almost periodic ladder structure, the persistent slip bands formed in fcc metals during cyclic deformation under low plastic strain amplitudes also drew some attention. Although a few confusions are sometimes found in the current literature, the basic dislocation mechanisms that lead to these two types of patterns are now better understood. In the context of modeling, two of their properties are worth being mentioned. When there is no lattice resistance dislocation microstructures follow two scaling laws, which are experimentally well documented. One of them, the dislocation strengthening relation is understood and reasonably well modeled, whereas the physical origin of the second one, the similitude relation, still remains unclear. The state of the art in the simulation of dislocation cell structures will be illustrated by a few examples. Simulating other types of microstructures, in particular the ones obtained at very large strains, still remains a challenge.

The seminal article by M. Carmen-Miguel *et al.* [1] on dislocation avalanches uncovered a new vision of the elementary event that leads to macroscopic plastic flow. This suggests basing the next generation of models for dislocation patterning on the spatio-temporal evolution of the dislocation density stored by avalanches.

[1] M.-Carmen-Miguel *et al.*, Nature, **410**, 667 (2001).

Rethinking the Meaning of Defect Structure

David J. Srolovitz, Jian Han, Vaclav Vitek

University of Pennsylvania, USA

We often think of defects such as grain boundaries, dislocation cores, surfaces,... as a specific, well-defined structure. There is considerable evidence that in fact the structure of individual defects is not well-defined and is statistically distributed. I will discuss some recent work on grain boundaries that shows the extremely wide range of metastable states that are possible and the structural origin of this multiplicity of states. This plethora of states has profound influence on the statistical mechanics of such structures - this puts bounds rather than values on defect properties. Perhaps, more importantly, defect kinetics necessarily explore these variety of states - e.g., grain boundary point defect sink/source behavior, migration, sliding.

Modeling of neutron irradiation embrittlement of reactor pressure vessel steels

Naoki Soneda

Director, Materials Science Research Laboratory Central Research Institute of Electric Power Industry Japan

Reactor pressure vessels (RPVs) of nuclear power plants are exposed to the fast neutron irradiation during plant operation, which causes reduction in fracture toughness of the RPV steels. This phenomenon is known as neutron irradiation embrittlement of RPV steels, and is a primary concern for the structural integrity analyses of the RPVs. The estimation of the reduction in fracture toughness, which is normally evaluated in terms of a shift in ductile-to-brittle transition temperature, is a key technology for the safe operation of nuclear power plants.

The initial process of the embrittlement is a displacement cascade of lattice atoms due to neutron bombardment. The lattice defects produced diffuse to cause structural changes of materials in a nano-meter scale such as precipitation, segregation and formation of point-defect clusters. Such nano-features affect the mobility of dislocations in a micron-meter scale, which results in the change in the fracture toughness of the materials in a centimeter scale. The whole process is a time-evolving multi-scale phenomenon, and the understanding and modeling of the whole process is essential for the development of an accurate and predictive method to estimate the amount of neutron irradiation embrittlement.

CRIEPI has been working on understanding the microstructural changes of neutron irradiated RPV steels as well as analyzing the mechanical property data of the Japanese surveillance materials from all the commercial nuclear power plants in Japan. Based on these results, a mechanism-guided embrittlement correlation method to estimate the amount of embrittlement was developed, which is now adopted in the Code of the Japan Electric Association to determine the plant operation conditions of the Japanese nuclear power plants. In this talk, the findings obtained by nano & micro scale experiments and computer simulations will be presented, followed by the modelling of microstructural changes and the link of micro- and macro- properties regarding the neutron irradiation embrittlement of RPV steels.

**Over a Decade of Folding@home: how citizen science has lead to key new advances
in biophysics and fighting disease**

Vijay Pande

Stanford University, USA

On October 1, 2000, my group and I publicly released the Folding@home Distributed Computing Project, which has enabled us to build a tremendous computational resource – now more powerful than any traditional supercomputer — by rallying together the efforts of millions of computers throughout the world. Now, almost 15 years later, we have achieved many of the goals we set out to accomplish at that time, including key new advances in biophysics (especially in the areas of protein folding, misfolding, and conformational change) as well as new small molecule drugs candidates (especially in new areas of drug repurposing to rapidly develop small molecule drugs in an academic setting). Moreover, this new approach of bringing citizen scientists into cutting edge research has had its own impacts in many ways. Finally, I will conclude by talking about the future of Folding@home and where we hope to be in the next 15 years.

Comparisons of 3D Experiments and Simulations on Plastic Deformation of Metals

A.D. Rollett

Dept. of Materials Sci. & Eng. Carnegie Mellon University

The aim of this presentation is to point out that the current state of comparisons between experiments and simulations of deformation of polycrystalline materials reveals some interesting challenges. Addressing first the experimental sources of data, High Energy Diffraction Microscopy (HEDM) takes advantage of the high energy monochromatic x-rays available at third generation sources. Computer simulation of plastic deformation experiments has been accomplished almost entirely with the finite element method. In the past few years, however, an image-based approach that relies on the Fast Fourier Transform (FFT) offers a more efficient solution of the same equations (e.g. mechanical equilibrium) as the finite element approach. Thus one can, for example, take a measured 3D image from HEDM with thousands of grains and import it directly into the FFT simulation code. Such image-based simulations enable substantially more complex microstructures to be simulated than has been standard practice.

Turning to the underlying scientific issues, polycrystal plasticity is akin to deformation of a composite in which each grain has different properties by virtue of its anisotropic response to loading. It is important to demonstrate that we can validate crystal plasticity simulations in order to relate damage initiation such as cracks and voids to extreme values in stress, for example, as they relate to microstructural features such as triple lines. Specific examples of the use of HEDM will be given for tensile tests on pure copper and zirconium, and fatigued nickel-based superalloy. In general, both experiments and simulations show that hot spots in stress or elastic energy density occur close to grain boundaries, triple lines and quadruple points. Whether strain or orientation is used, however, comparisons of the full fields show significant differences despite at the good agreement found at the statistical level. This suggests that all aspects of the simulations will require attention.

Returning to the multiscale aspects of the problem, at the engineering scale, there is a need to develop accurate, physically-based constitutive models for mechanical behavior. Especially for problems such as initiation of cracks and voids, there is an obvious need for accurate full field modeling so that extremes in stress, slip, strain etc. are understood. In the other direction, the uncertainty around the capability of mesoscopic crystal plasticity modeling provides motivation for validation with molecular dynamics (MD) and dislocation dynamics (DD) simulations of polycrystals. An introduction will be given to application of the FFT method for accelerating the DD method and enabling anisotropic polycrystals modeling.

Role of Multiscale Materials Modeling in Integrated Computational Materials Engineering

Mark Asta

Department of Materials Science & Engineering,
University of California, Berkeley, USA

The past five years have witnessed the emergence of the field of Integrated Computational Materials Engineering (ICME) as a subdiscipline of materials engineering aimed at the use of multiscale materials modeling as a framework for accelerating the timescale and reducing the cost of materials development and manufacturing. Progress in the development of the scientific and algorithmic frameworks underlying multiscale modeling of materials remains critical to advancing the goals of ICME. This talk will provide a basic introduction to the goals of ICME, as defined in the original National Academies report, and review outstanding challenges as identified in the recent implementation study by TMS. The synergistic relationship between ICME and the Materials Genome Initiative will also be discussed.

Contact and Friction of Rough Adhesive Surfaces

Lars Pastewka^{1,2}, Tristan A. Sharp¹, Mark O. Robbins^{1,3}

¹Department of Physics and Astronomy, Johns Hopkins University, 3400 N. Charles St., Baltimore, MD 21218

²MikroTribologie Centrum µTC, Fraunhofer-Institut für Werkstoffmechanik IWM, 79108 Freiburg, Germany

³Department of Mechanical Engineering, Johns Hopkins University, 3400 N. Charles St., Baltimore, MD 21218

Experimental surfaces typically have roughness on a wide range of length scales. This roughness greatly reduces the fraction of the area that is in intimate molecular contact and thus can contribute to friction and adhesion. The talk will first describe recent numerical calculations of elastic contact between rough surfaces with nominally flat or spherical geometries on large scales. An efficient Greens function approach allows calculations for systems with roughness on nanometer to micrometer scales to be performed with atomic resolution in the contact. Results for a wide range of geometries can be collapsed using simple scaling relations that depend on the root mean squared surface slope, sphere radius, elastic modulus, and work of adhesion. The scaling relations explain why adhesive interactions have little effect unless the surfaces are extremely smooth or soft. The traditional Fuller-Tabor model for adhesion of rough surfaces is shown to be qualitatively inconsistent with the simulations. The effect of atomic scale plasticity on contact and adhesion is surprisingly small. The talk will conclude by considering how forces in the contact area give rise to friction. Friction shows strong scale effects and the partial slip assumed in many contact models is not found in contacts with dimensions of nanometers to micrometers.

Multiscale Modeling in Mesoscale Materials

George Crabtree

Argonne National Laboratory
University of Illinois at Chicago

Mesoscale science embraces the bottom-up manipulation of interactions among atomic, molecular and nanoscale components to produce new behavior not found in the constituents, a rich opportunity not only for new materials and phenomena, but also for multiscale modeling at the descriptive and predictive levels. New features that emerge at the mesoscale include interacting degrees of freedom, statistical variation, defects and collective behavior. A general introduction to mesoscale science will be followed by materials challenges that are ripe for multiscale modeling solutions drawn from solvation in organic liquids, fractures and other defects in solid materials, and heterogeneous and amorphous materials.

Transformation induced inhomogeneity and its effects on creep, fatigue and deformation of titanium alloys

Rui Yang

Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China

The nature and pattern of inhomogeneity determine the mechanical behavior of alloys to a large extent, and design of structural materials usually centers on optimizing the size and distribution of these inhomogeneities so as to control the critical stress and pace of plastic deformation under load. Understanding how these inhomogeneities form and evolve is part of the microstructural frontier. The theme of this talk is how plastic deformation interacts with and is interrupted by inhomogeneities that are already present or formed during loading, drawing examples from titanium alloys.

Gamma titanium aluminides are beginning to be used to make aircraft engine blades and future engines require increased creep strength. Nb addition is very effective in strengthening TiAl but for a long time the predominant mechanism is not clear. Recent first principles computation suggests the switch of sublattice occupancy of Nb, with increasing content, from the Ti- to Al-sublattice, forming short range order in addition, thus improving creep resistance. The sublattice short range order also provided embryos for a range of omega type transformations. Electronic modeling helps to clarify the relative stability of these phases and to understand why the addition of Mo hinders their formation, thus playing an important role in the design and optimization of next generation, creep resistant titanium aluminide alloys.

Near alpha titanium alloys for high temperature application experience significant drop in fatigue life under cold dwell condition. It has long been known that microstructure, microtexture and stress level are the main factors influencing dwell sensitivity, but it was revealed only recently how the microtexture was influenced by microstructure and why two commercial alloys, which differ only by 4 wt.% Mo, exhibited drastically different dwell sensitivity. While several crystal plasticity modeling investigations have been conducted on this subject, the atomistic mechanisms of crack initiation are still elusive. A first attempt at molecular dynamics simulation of the crack nucleation at twin boundaries will be presented and its relevance to dwell fatigue discussed.

In beta type titanium alloys several metastable phases, often stress-induced and therefore reversible, may compete to form and grow during loading, markedly changing elastic properties and modifying stress-strain behavior. The stability of these phases can be estimated by first principles computation. By ignoring the nucleation of multiple martensitic phases at the nano scale and by employing the mean field concept and the embedded-atom method, an interatomic potential was constructed for a typical alloy. Molecular dynamics simulations showed that the potential is capable of reproducing various manners of plastic deformation, e.g., dislocation nucleation and propagation, deformation twinning, and phase transformation. Regarding high strain rate deformation, a new mechanism of twin nucleation, facilitated by the reversible transformation from the omega to the bcc phase in beta titanium alloys, was proposed and supported by both experimental observation and results of first principles computation.

The Materials Genome: Overview, Success Stories and Outlook

Kristin A. Persson

Lawrence Berkeley National Laboratory

The Materials Genome Initiative (MGI) aims to develop an infrastructure to discover, develop, manufacture, and deploy advanced materials at least twice as fast as possible today, at a fraction of the cost. The exponential growth of computer-processing power, combined with the laws of physics expressed through quantum mechanics, has made it possible to design new materials from scratch using supercomputers and first-principle physics. Concurrently, high-throughput (HT) synthesis and measurement experimental techniques are being developed which enable rapid validation and benchmarking.

This presentation will give an overview of goals of the Initiative and exemplify the materials genomic approach by describing singular efforts that have used it to optimize and discover novel materials from computations and experimental efforts as well as the data and tools emerging from these efforts. Among these examples are innovative novel materials and electrolytes in energy storage and energy production, the broad searchable dissemination of phase stability, solid-aqueous stability, elastic properties and electronic structure information across structure and chemical space. Finally it will be recognized that the information age has finally reached the materials science field and that the infrastructure tools being prevalently utilized in other fields should be leveraged for accelerating materials research.

Toward mastery of microstructural degrees of freedom in engineering design

Dennis M. Dimiduk, Michael A. Groeber, Michael D. Uchic

Air Force Research Laboratory, Materials and Manufacturing Directorate
AFRL/RXC Bldg 655, 2230 10th Street, Wright-Patterson AFB, OH 45433-7817, USA

Having “The Microstructural Frontier” theme for the present MMM conference, it is fitting to examine the means for using microstructural information as an integral part of the design-materials-manufacturing enterprise. During the 1980’s and early 1990’s process-modeling frameworks introduced formal linkages between manufacturing and engineering design systems. Extensions of these now treat primarily empirical or mean-field representations of microstructure influences. Common design practices optimize materials structure, as represented via spatiotemporal fields of continuum state variables gleaned from process models of selected manufacturing operations (i.e. casting, forming, etc.) Selectively, those continuum methods are coupled to microstructure evolution and performance models, but only for mean-field representations. Thus, the methods implicitly represent materials structure, or treat it in only a homogenized fashion. Looking further, computational linkages between materials structure descriptions and manufacturing processes or, between materials structure descriptions and engineering performance are more tenuous, even from an implicit perspective. The MMM challenge is to devise schemes for explicitly and objectively operating with microstructural degrees of freedom while minimizing needs for measured information.

In this work we describe a growing software environment that permits objective and quantitative descriptions of hierarchical materials microstructure information and, management of its linkages to both materials performance simulations and experimental validation tools. The environment, which is called “DREAM.3D” [1], is an open source software base that evolved from more than a decade of community wide efforts toward mastering the machine representation of microstructure information. Recent and current developments show the multi-scale applicability of the framework and its formal ties to destructive and non-destructive materials characterization. Further, selected linkages to simulations at multiple scales are also shown. These and future prospects for MMM are discussed.

This work was performed under funding from the Air Force Research Laboratory. The authors acknowledge community wide contributions, especially those from Profs. A. Rollett, S. Ghosh and G. Rohrer and Dr. D. Rowenhorst. We also acknowledge key contributors toward the integrated simulation-experimental framework including Drs. C. Woodward, P. Shade, J. Schuren and T.J. Turner, and Mr. M. Jackson.

[1] <http://dream3d.bluequartz.net/>

Image Based Crystal Plasticity FE Models for Predicting Fatigue in Polycrystalline Metals and Alloys: Addressing the ICMSE Initiative

Somnath Ghosh

Departments of Civil Engineering and Mechanical Engineering
Johns Hopkins University, Baltimore, MD 21218, USA

The Integrated Computational Materials Science & Engineering or *ICMSE* initiative entails integration of information across length and time scales for relevant materials phenomena and enables concurrent analysis of manufacturing, design, and materials. Computational Mechanics plays an important role in this integration. This talk will present various ICMSE approaches in the development of a microstructure based modeling of fatigue crack initiation in polycrystalline alloys. The model implements crystal plasticity theory with explicit grain structures and the mechanical response of polycrystalline aggregates are deduced from the behavior of constituent crystal grains. These calculations provide a platform for the implementation of physics-based crack evolution criterion that accounts for the effects of microstructural inhomogeneity. Systematic development of a crystal plasticity-based fatigue crack nucleation model is conducted. The presentation will also discuss a wavelet transformation based multi-time scaling (WATMUS) algorithm for accelerated crystal plasticity finite element simulations. The WATMUS algorithm does not require any scale-separation and naturally transforms the coarse time scale response into a monotonic cycle scale without the requirement of sub-cycle resolution. The method significantly enhances computational efficiency in comparison with conventional single time scale integration methods. Adaptivity conditions are also developed for this algorithm to improve accuracy and efficiency. Finally the talk will discuss an approach to evaluate coupled crystal plasticity-damage evolution relations based on molecular dynamics simulations of a crystalline material with an embedded crack.

Impact of Spatially Non-Random Solute on the Strength of Aluminum Alloys

Alban de Vaucorbeil, Chad W Sinclair, Warren J Poole

Dept of Materials Engineering, University of British Columbia,
Vancouver, BC V6T 1Z1, Canada

For many aluminum alloys natural aging leads to solute redistribution and solute clustering. The significance of this process on yield strength is well illustrated by alloy AA6111 where the yield strength increase can be >200% upon room temperature aging [1]. The microstructural evolution during this period is complex as the composition, size, shape and spatial distribution of the resulting solute clusters is difficult to define (fig. 1). How one should physically incorporate detailed information coming from atomic scale measurements into mean-field engineering models for yield strength becomes a question since such models do not, by definition, naturally include effects arising from distributions in obstacle size, strength and spatial distribution.

Motivated by a desire to predict the macroscopic yield strength during low temperature aging of aluminum alloys, we have examined the influence of obstacle strength and spatial distribution in the glide plane using meso-scale two-dimensional areal glide models [2,3]. We have also investigated an addition law appropriate for obtaining the macroscopic yield strength when a set of two or more obstacles (e.g. solute, clusters, precipitates and dislocations) is present on the glide plane [3]. Such meso-scale models require ad-hoc assumptions to be made about the correlation between an obstacle and its strength. To investigate this further, particularly for the case of solute clusters, we have performed fully atomistic molecular dynamics/molecular statics simulations to investigate how a dislocation samples different spatially distributed sets of solute atoms for model alloy systems. The challenges and successes of integrating the approaches used in this work will be discussed.

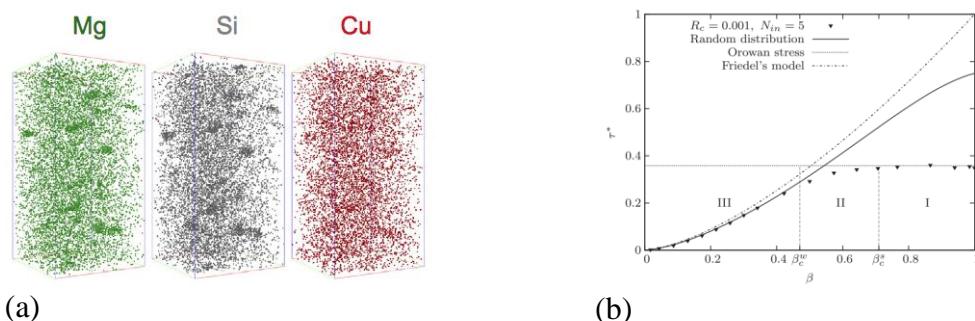


Figure 1: a) The early stages of cluster formation in AA6111 held at 180°C for 4 minutes [1] b) Prediction from an areal glide model of the effect of obstacle clustering in the glide plane on the normalized critical resolved shear stress for dislocation motion [2].

[1] R.K.W. Marceau, A. de Vaucorbeil, G. Sha, S.P. Ringer, W.J. Poole, *Acta Mater.* **61** (2013) 7285–7303.

[2] A. de Vaucorbeil, C.W. Sinclair, W.J. Poole, *Phil. Mag.*, **93** (2013) 3664–3679.

[3] A. de Vaucorbeil, W.J. Poole, C.W. Sinclair *Mater. Sci. Eng. A*, **582** (2013) 147–154.

Hierarchical crystal plasticity model for nickel-based superalloys: sub-grain microstructures to polycrystalline aggregates

Shahriyar Keshavarz, Somnath Ghosh

Department of Civil Engineering, Johns Hopkins University, Baltimore, MD 21218

A hierarchical crystal plasticity model for Ni-based superalloys is developed for three scales in this study. In order to establish a hierarchical constitutive model, behaviors at different length scales have to be formulated to capture desired phenomena corresponding to the application. Such formulations include all dominated mechanisms. APB-shearing and Micro-twinning are two activated mechanisms in this temperature ranges. In the lowest scale, explicit dependencies on sub-grain scale morphological characteristics are attributed. An essential ingredient for this development is a sub-grain scale crystal plasticity FEM model scale for micromechanical RVE analysis with explicit depiction of the $\gamma - \gamma'$ morphology. The model numerically implements a size-dependent dislocation density-based crystal plasticity model with a representation of APB shearing of γ' precipitates by γ -matrix dislocations. It is computationally expensive to incorporate the explicit models of the $\gamma - \gamma'$ microstructure in a crystal plasticity based model to simulate the response of the crystalline microstructure of these alloys. Thus to retrieve the morphology features into the next scale, the lowest scale model is homogenized as a function of various microstructural parameters and the activation-based homogenized model is used at the next level (i.e., single crystal grain scale) of crystal plasticity model. In the next ascending scale, a polycrystalline microstructure of Ni-based superalloys is modeled using the homogenized CPFE model for single crystal scale analysis. Different grain features are incorporated to simulate the polycrystalline microstructure by augmentation and incorporation of the homogenized activation energy-based crystal plasticity constitutive model for this scale. The results of each scale are compared with experimental data at corresponding scales with good agreement.

Vi(CA)₂T – Virtual Cement & Concrete Aging Analysis Toolbox

Yann Le-Pape, Julien Sanahuja, Nanthilde Reviron, Nhu-Cuong Tran

EDF R&D, département MMC, av. des Renardières, Ecuisses, 77818 Moret-sur-Loing Cédex,
France

For managing the long term operation of nuclear power plants and preparing the construction of new ones, the assessment of the aging of cement and concrete materials play a significant role. It permits electricity utilities to control civil works' degradation and optimize their maintenance in order to ensure plants' safety. At EDF, the biggest nuclear operator in the world (owner of 73 reactors in UK and France, joint-owner of 5 reactors in USA), this assessment primarily relies on an extensive set of periodic monitoring data and experimental tests. EDF approach being turned towards continuous improvement of safety, EDF research and development service (EDF R&D) is currently developing, in a combined effort with EDF engineering services, a numerical tool aimed at predicting cementitious materials ageing, called Vi(CA)₂T (Virtual Cement and Concrete Ageing Analysis Toolbox). This contribution presents the version 2.1 of this tool suite.

To be predictive and to avoid relying on both empirical models and a huge database of tests, Vi(CA)₂T takes advantage of recent progresses in physics-based material modelling. More precisely, it is made up of

- a physico-chemical computation module to predict the evolution with respect to time of cement phases' volume fractions,
- mechanical computation modules in order to estimate the evolution of material parameters like Young modulus, compression strength and creep.

In the physico-chemical computation, hydration kinetics are predicted based on the laws of Avrami [1] and of Fuji & Kondo [2]. The effect of silica fume is also taken into account. The mechanical computations are based on mean field micromechanical models developed in literature [3, 4] and at EDF R&D [5, 6]. In the objective of building a professional tool suite for engineering services, the development of Vi(CA)₂T considers the user experience as a first priority. Usage is very simple: the user needs to enter only cement and concrete formulations and the computation results are available within less than 60 seconds.

Prospects for version 3 include the estimation of transport properties, such as resistivity or permeabilities. As these properties are expected to be highly dependent on the composite morphology, this might require to switch to full field (3D) micromechanical tools.

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Decoding Cement Hydrate: Hierarchical Modeling from Electrons to Microstructures

Rouzbeh Shahsavari^{1,2}

¹Department of Civil and Environmental Engineering, Rice University, Houston, TX 77005

²Department of Material Science and NanoEngineering, Rice University, Houston, TX 77005

Despite the omnipresence of concrete as the world's dominating manufacturing material, which accounts for 5-10% of the total anthropogenic CO₂ emissions worldwide, the interplay between structure, morphology and chemical composition of its smallest building block, Calcium-Silicate-Hydrate (C-S-H), is essentially unexplored. Together these characteristics of this "liquid stone" gel define cement hydrate and enable modulation of its physical and mechanical properties with the ultimate goal of reducing concrete environmental footprint. Here, we propose a bottom-up multi-scale approach developed with the focus of unraveling the hierarchical structure of C-S-H, which is the principal source of strength and durability in all Portland cement concretes (**Figure 1**). First, by using statistical mechanics coupled to a combinatorial defect optimization approach, we decode the basic molecular structure of hundreds of amorphous C-S-H gels, corresponding to different chemical compositions. By allowing for short silica chains distributed as monomers, dimers, and pentamers, these C-S-H archetypes of molecular descriptions of interacting CaO, SiO₂, and H₂O units provide not only realistic values of calcium to silicon (C/S) ratios but the

densities, which are computed by a unique combination of grand canonical Monte Carlo simulation of water adsorption and molecular dynamics at 300 K. We found that the C-S-H gel structure includes glass-like short-range order features at large C/S, and crystalline features of the mineral tobermorite at low C/S. Second, we show that upon applying strain-controlled tension to the decoded C-S-H polymorphs, rupture occurs mostly around the silica-rich and defected regions. These weak regions enable identifying particle boundaries for various C-S-H particles, which together form the C-S-H microstructure. The latter is modeled using meso-scale

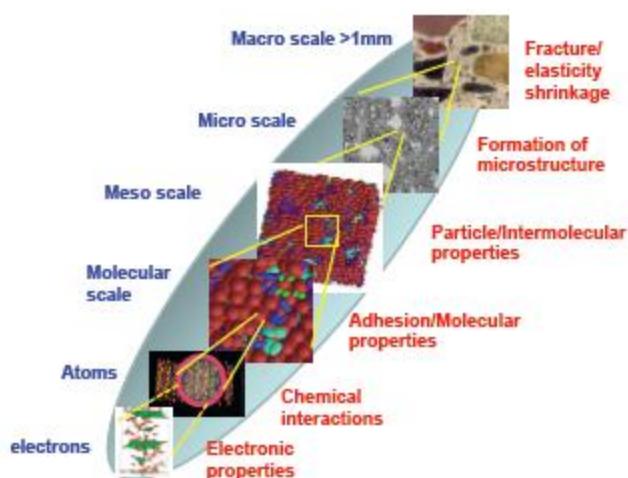


Figure 1. Hierarchical Structure of concrete across scales.

Monte-Carlo simulations with inter-particle interactions based on parameters directly obtained from partial atomic charges computed by *ab-initio* calculations. Finally, we probe the mechanical stiffness, strength, and matrix morphology of the microstructural model, and compare the results with experimentally measured properties of C-S-H. In view of this MMM conference theme on "Microstructural Frontiers", this bottom-up approach, motivated by combinatorial atomistic modeling, introduces innovative paradigms for acknowledge-based modulation of the cement chemistry at the micro scale to answer the global needs for greening construction materials.

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FTMP-based Continuum Description of 4D Discrete Dislocation Systems

Tadashi Hasebe¹, Takuya Naito², Motoki Uematsu²

¹Kobe University, Nada, Kobe 657-8501, Japan

²Graduate School of Kobe University, Nada, Kobe 657-8501, Japan

A sophisticated method for expressing three-dimensionally evolving discrete dislocation ensembles is proposed based on Field Theory of Multiscale Plasticity (FTMP)[1] coupled with a working hypothesis called flow-evolutionary law[2]. The law can be visualized by “duality diagram,” where the spatial trace of the incompatibility tensor for the targeted system is plotted against fluctuation part of the elastic strain energy. Collapsing walls made of mixed dislocation networks, screw networks, and that mimicking lath wall, are simulated by using dislocation dynamics, respectively. The duality diagram representation for them is demonstrated to provide a number of valuable pieces of information characterizing the evolutionary aspects of the system. It visually tells us how the targeted system tries to store/release the strain energy, resulting in the configurational changes, while the ratios at each point on the diagram, referred to as duality coefficient κ , can quantitatively capture the “stability/instability” of the system, as summarized in Fig.1, where the standard deviation of the dislocation segments from the original configurations is used for characterizing the degree of collapse of the walls. The mixed walls tend to yield larger slope than the lath wall, implying less stability characteristics, whereas the lath wall is regarded as most stable among others as the smaller slope result

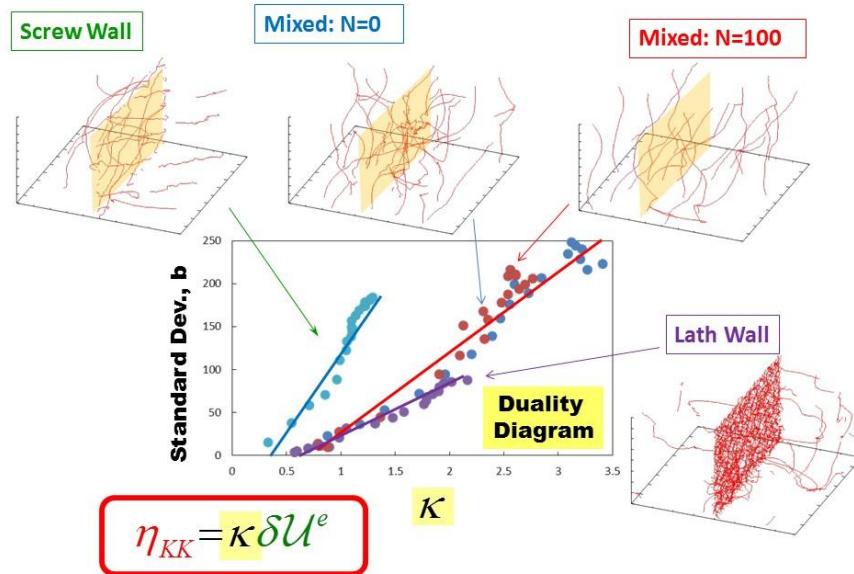


Figure 1: Quantitative evaluation of collapsing dislocation walls by duality coefficient, i.e., ratio of incompatibility to fluctuating strain energy, in terms of structural stability/instability, comparing three distinct cases.

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Hot-working Multiscale Simulations Using Multi-phase-field Finite Element Dynamic Recrystallization Model

Tomohiro Takaki, Yoshimoto Chihiro

Mechanical and System Engineering, Kyoto Institute of Technology, Matsugasaki,
Sakyo, Kyoto 606-8585, Japan

During hot-working of low-to-medium stacking fault energy material, dynamic recrystallization (DRX) with plastic deformation and recrystallization occurs. Therefore, in order to evaluate macroscopic mechanical behaviors during hot-working of the DRX material, it is important to take the microstructure evolution into account.

In our previous study [1], we have developed a hot-working multiscale model where macroscopic mechanical behaviors are evaluated by elastic-plastic large deformation finite element (FE) simulations and microstructure evolutions are simulated by multi-phase-field (MPF) method [2]. We call the model as multi-phase-field finite element dynamic recrystallization (MPFFE-DRX) model.

In this study, we show realistic hot-working simulations using the MPFFE-DRX model. Figure 1 shows a compression simulation of truncated cone with 16 mm height. The simulation was performed as an axisymmetric problem with 100 triangular elements. Although not shown here, the microstructure evolutions are simulated in every triangular element using MPF. The detail results will be presented in the conference.

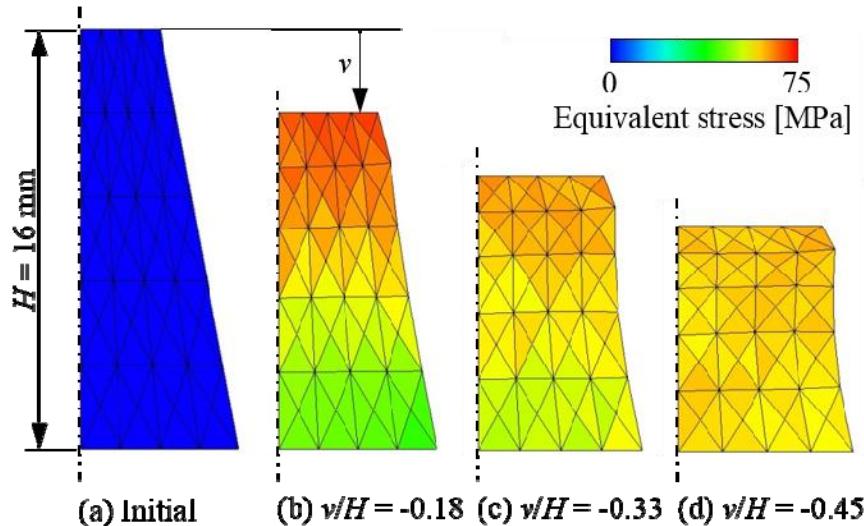


Figure 1 Compression simulation of truncated cone using MPFFE-DRX model.

This work was supported by JSPS KAKENHI Grant Number 25630011.

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Search for substitutes of critical materials with targeted properties by scale-bridging and high-throughput modelling and simulation

Christian Elsässer

Fraunhofer IWM, Freiburg, Germany

In this lecture I will address three case studies on how sustainable substitutes for such materials, which have outstanding functionalities but also constraining criticalities, can be discovered and developed efficiently by employing multi-scale-coupling and high-throughput-screening concepts of ICME.

In the first case, a multi-scale chain from atomic-level first-principles theory to microstructure-level phase-field theory for ferroelectric piezoelectrics is set up for the still best material $\text{Pb}(\text{Zr},\text{Ti})\text{O}_3$ (PZT), which contains the biomedically health-critical element Pb, and then transferred to $(\text{K}, \text{Na})\text{NbO}_3$ (KNN), which is a potential substitute for PZT. [1]

The second case is on the modelling of structure-property relationships for transparent and conductive oxides (TCO), which are free of the geologically ressource-limited element Indium and therefore potential substitutes for the still best TCO material Indium Tin Oxide (ITO) for front electrodes on, e.g., smart phones or solar cells. [2]

In the third case, a combinatorial high-throughput-screening approach is employed to search for crystal structures and chemical compositions of intermetallic phases of transition-metal (TM) and rare-earth (RE) elements, which have sufficiently good intrinsic ferromagnetic properties for permanent magnets but contain less amounts of the geopolitically supply-critical RE elements than, e.g., the still best permanent magnets based on $(\text{Nd},\text{Dy})_2\text{Fe}_{14}\text{B}$. [3]

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Modeling the Behavior of Cellular Silicone Pads in the Structure-Continuum Transition

Chris I. Hammetter, Wei-Yang Lu, Terry D. Hinnerichs

Sandia National Laboratory, Albuquerque, New Mexico 87123, USA

Cellular silicone pads have properties that make them excellent materials for applications where components must be protected from the effects of high temperature, intense mechanical loading, and other extremes. These pads can be engineered to have a controlled distribution of pore sizes through a process of adding spherical particles to silicone, curing the mixture, and then washing out the inclusions to form pores. Experiments have shown that when these pads are thin (1-2 pores through the thickness) they are drastically stronger in compression than thicker pads, which exhibit a continuum-like response that is independent of thickness. The goal of this work is to develop models for this behavior to guide material characterization experiments and improve the continuum-based material models. The results of FE simulations, in which pads of varied thickness and with randomly placed pores of uniform size are compressed under periodic boundary conditions, confirm the trend of increasing strength with decreasing thickness (see Figure 1). This behavior is consistent with the stretching and bending of struts/walls in foams, as quantified by Alkhader et al [1], and a similar behavior is seen in periodic structures [2]. The presentation will further explore the underlying mechanics leading to this behavior and compare results with an accompanying experimental study to better predict the behavior of these materials.

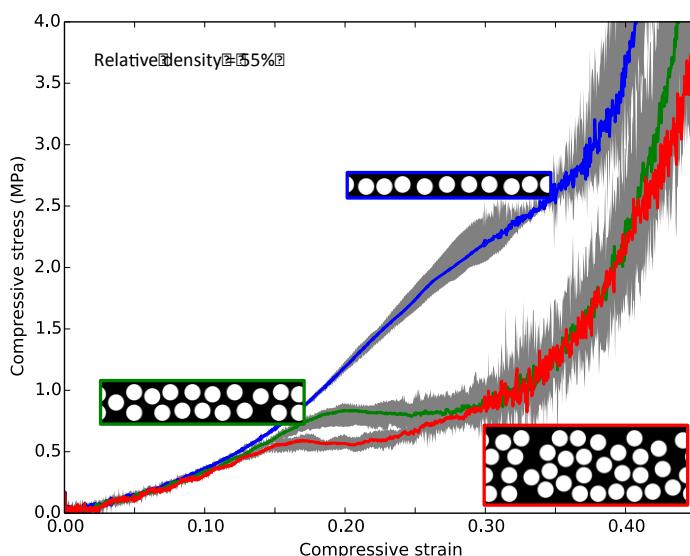


Figure 1: Finite Element modeling shows thinner cellular silicone pads exhibit a stronger stress-strain response than thicker pads. Each curve is the averaged response of several foams of equal thickness with the shaded region representing the maximum and minimum response. Representative images of the foams are shown for each thickness.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Analysis of electronic subgap states in amorphous semiconductor oxides on the example of Zn-Sn-O systems

Wolfgang Körner¹, Daniel F. Urban¹, Peter Gumbsch^{1,2}, Christian Elsässer^{1,2}

¹Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstr. 11, 79108 Freiburg, Germany

²Institute for Applied Materials, Karlsruhe Institute of Technology, Kaiserstr. 12, 76131 Karlsruhe, Germany

A molecular dynamics (MD) and density-functional-theory (DFT) study of amorphous Zn-Sn-O (ZTO) with focus on the use as transparent conducting oxides materials is presented. The amorphous structures generated by MD are in the following relaxed using the local-density-approximation (LDA) of DFT. The Zn/Sn ratio, the oxygen content and individual point defects are investigated concerning their thermodynamic and electronic properties and compared to data of crystalline structures. Defect levels in the electronic band structure of ZnO are analysed in terms of densities of states, which are calculated by means of the LDA and with a self-interaction-correction (SIC).

In our study we connect the electronic subgap states, which were observed recently by Nomura et al.[1] and Erslev et al.[2] with structural features of the amorphous samples. According to our analysis the valence band tail, caused by the disordered O 2p orbitals, is superimposed by deep defect states that can be assigned to undercoordinated O atoms which is not in line with the assignment of those states to oxygen vacancies by Kamiya et al.[3]. Our alternative is further supported by the fact that doping with H atoms suppresses these states by creating O--H bonds, which improves the transparency and is consistent with experimental findings [1].

The deep levels below the conduction band arise mainly from undercoordinated Sn atoms or Zn--Sn pairs. The addition of oxygen can be a possible route to reduce such defect levels.

In a similar study on In-Ga-Zn-O (IGZO) we have found essentially the same characteristics. Defect levels due to undercoordinated oxygen atoms create defect levels in the lower half of the band gap whereas metal--metal (In--Zn e.g.) related defects lead to defect levels in the upper half of the band gap. Our work is published in

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Materials Design and Discovery: Role of Atomic-Scale Modeling

Susan B. Sinnott

Department of Materials Science and Engineering, University of Florida, Gainesville,
Florida, 32611-6400

A driving force for much of the research that takes place in many disciplines is the discovery and design of new materials to improve existing technologies or enable new applications. Material modeling methods are now widely applied and show promise for fulfilling the ultimate goal contained within the phrase “materials by design”. This presentation will review the evolution of some common material modeling methods and their integration with cutting-edge experimental methods as well as data informatics. Illustrative applications will be discussed within the context of metal/piezoelectric interfacial systems for electronic devices, new metal alloy design, and the role of strain and dopants in the design of multifunctional materials. A future outlook of materials modeling within the context of material design and discovery will also be provided.

Thermodynamics of α -Fe solid solution: interplay between vacancies and interstitial solutes (C, N and O)

Thomas Schuler, Maylise Nastar

CEA, DEN, Service de Recherches de Métallurgie Physique, F-91191 Gif-sur-Yvette,
France

Carbon (C), nitrogen (N) and oxygen (O) atoms are always present in α -iron (Fe), either as impurities or as alloying elements. Even the so-called pure Fe usually contains at least 0.1 appm of each impurity.

In this work we show that, despite low solute concentrations and even lower equilibrium vacancy concentrations, their interplay has an important impact on some thermodynamic properties of α -Fe solid solutions, e.g. vacancy formation energies and solute solubility limits.

For each solute, a generalized Hamiltonian is derived on the perfect body-centered cubic lattice including substitutional and octahedral interstitial sites. It is composed of 2-, 3- and 4-body interactions between vacancies and solutes, up to the 8th nearest-neighbour. Interactions are fitted to a whole set of DFT calculations of small vacancy-solute clusters binding energies, and the predictive capability of the Hamiltonian is checked against another set of clusters. The interaction model is included into a Low Temperature Expansion formalism (validated by comparison with Atomic Monte Carlo simulations) from which the free energy of the solid solution is obtained. First, it is shown how solutes (mostly N and O) strongly decrease the vacancy formation energy, even at concentrations below 1 appm. This observation could as well explain the frequent disagreement between experimental and DFT decomposition of Fe self-diffusion activation energy. Then, the Fe-rich part of Fe-X (X = C, N or O) phase diagrams is computed, using a semi-empirical method for the estimation of solute solution entropies. Vacancies are predicted to play a non-negligible role in the phase diagram of Fe-O.

This work was supported by the joint program "CPR ODISSEE" funded by AREVA, CEA, CNRS, EDF and Mécachrome under contract n°070551.

OpenKIM.org: Ensuring reliability, reproducibility and transferability in multiscale and atomistic simulations

Ellad Tadmor¹, Ryan Elliott¹, James Sethna²

¹University of Minnesota, ²Cornell University

Multiscale and atomistic simulations using empirical interatomic potentials play a key role in realistic scientific and industrial applications. This talk describes a current NSF-CDI funded effort to develop an open source online tool for promoting the use and reliability of interatomic models. The open Knowledgebase of Interatomic Models (<https://OpenKIM.org>) allows users to compare model predictions and reference data using a visualization system, to generate new predictions by uploading simulation test codes, and to download models conforming to an application programming interface (API) standard that has been developed in collaboration with atomistic simulation community. An overview of the KIM project will be given along with recent developments related to the KIM API, a new data structure for representing arbitrary material properties, and metrics for interatomic model transferability.

Grain boundary segregation as a route to stabilize nanocrystalline alloys: A phase field study

Fadi F. Abdeljawad, Stephen M. Foiles

Computational Materials and Data Science,
Sandia National Laboratories, Albuquerque, NM, 87185 USA

Owing to their nanometer characteristic length scale, nanostructured alloys exhibit a unique combination of properties, which render them an attractive material of choice in many technological sectors. On the other hand, these systems are often unstable against grain growth and coarsening processes even at low service temperatures and/or modest processing schedules. The development of nanostructured materials with increased stability against microstructural evolution processes is necessary in order to increase their competitiveness *viz-à-viz* other materials systems, especially in applications with harsh operating environments and elevated temperatures.

Recent experimental findings suggest that stable nanostructured alloys can be formed. In such systems, a heterogeneous distribution of solute is reached when the alloying elements preferentially occupy grain boundary regions; a state where bonding preferences are satisfied and a reduction in grain boundary energy is achieved. The design parameters here are the choice of solute and host atoms and their respective compositions, such that the resulting alloy is stable against grain growth and long-range chemical ordering.

In this talk, we present a diffuse-interface model for grain boundary segregation in binary nanostructured alloys and the accompanying solute drag affecting grain growth and phase separation. The model accounts for bulk thermodynamics, interface-driven processes and solute-grain boundary interaction, and is linked with atomistic models through several input parameters, such as diffusivity, boundary mobility and interfacial energy.

Simulation results highlight the role of high solute content in grain boundaries on grain growth in these systems. Furthermore, scaling laws for growth dynamics and their dependence on solute concentration, which are extracted from the modeling results, provide further avenues to explore as far as the stability of these systems.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000. FFA and SMF would like to acknowledge the financial support from the US department of Energy, Office of Basic Energy Sciences.

Scale bridging modelling of hydride formation

R. Spatschek, D. Korbmacher, C. Hüter, A. Chakrabarty, U. Aydin, J. Neugebauer

Max-Planck-Institute for Iron Research, Germany

Hydrogen embrittlement is a serious issue for many high strength steels, and still a thorough understanding of this phenomenon is lacking. Among the different suggested models the hydrogen enhanced decohesion picture is based on a change of fracture energy due to hydrogen accumulation. We discuss the role of hydride formation, especially near free surfaces and in the vicinity of crack tips, from a combined ab initio, atomistic, mesoscale and thermodynamic perspective. Here, in particular the presence of elastic deformations can largely influence the hydride phase formation, and we demonstrate how this aspect can be covered in a scale bridging approach.

Material and microstructure based design of anisotropic linear elastic properties of cubic crystal aggregates using zeroth-, first- and second-order bounds

Mauricio Lobos, Thomas Böhlke

Karlsruhe Institute of Technology (KIT), Karlsruhe 76131, Germany

A simple scheme based on analytical results is presented for the design of the anisotropic linear elastic properties of cubic crystal aggregates. The scheme is based on analytical results of zeroth-, first- and second-order bounds, delivering a total of 12 design variables which span the design space. The first-order bounds are known as the Voigt and Reuss bounds while the considered second-order bounds are the Hashin-Shtrikman bounds derived in Böhlke and Lobos (2014). These first- and second-order bounds are represented in terms of the one-point statistics of the polycrystal, the crystallographic texture, through the usage of a fourth-order texture coefficient. After having chosen which properties are to be designed, a physically suitable material, which fulfills prescribed criteria, is selected. This is achieved by using zeroth-order bounds and material data. Consequently, a homogenization scheme consistent with the considered bounds is chosen as an approximation for the real material behavior. Using the chosen homogenization scheme, the focused properties are analyzed in order to obtain their possibilities and limitations through microstructure adaptation. Finally, the optimal crystallographic texture with the best approximation of the prescribed properties is identified.

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Integrated experimental-numerical methodology to map microstructural strain and stress evolution in bulk nanostructured alloys

C.C. Tasan, D. Yan, M. Diehl, F. Roters P. Shanthraj, C. Zambaldi, D. Raabe

Max-Planck-Institut für Eisenforschung,
Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Microscopic strain and stress partitioning among the present phases govern the macroscopic mechanical response of multi-phase alloys. However, these phenomena are challenging to probe due to the multiple scales involved, dynamic nature of the deformation process, and lack of dedicated methodologies. The challenge is even more enhanced for multi-phase alloys with features smaller than micrometer scale.

A novel approach is introduced in this work that strengthens the connection between microstructure and mechanical properties in such alloys. To this end, numerical simulations and experiment analyses are carried out in an integrated manner to investigate the microstructural deformation mechanisms in multiphase microstructures.

For the experiments, a novel, *in-situ* SEM imaging and digital image correlation (DIC) based methodology is developed that allows concurrent microstructure and strain mapping at sub-micron resolution. Strain mapping is achieved by the application of a layer of nanoparticles on the sample surface (as the DIC pattern) that are selectively imaged during deformation. Concurrent microstructure mapping is achieved by optimization of imaging conditions to minimize the interference of the DIC pattern nanoparticles.

For the simulations, the electron backscatter diffraction (EBSD) map of the undeformed state of the same *in-situ* investigated microstructural patch is used to create the model. 2D full-field crystal plasticity simulations are run employing a recently developed spectral solver suitable for high-phase contrast materials [1, 2] implemented in the crystal plasticity simulation-kit DAMASK [3, 4]. The individual phase properties are obtained by additional inverse CP simulations of nanoindentation experiments carried out on the original microstructure [5].

The methodology will be demonstrated here on the example of martensite-ferrite dual phase (DP) steel, for which promising correlation between the simulations and experiments is achieved, despite the complex micro-mechanics of this material.

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Microstructure-sensitive modeling of the mechanical behavior of polycrystalline materials with direct input from emerging 3-D characterization methods

Ricardo Lebensohn, Reeju Pokharel

Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Emerging characterization methods in experimental mechanics pose a challenge to modelers to devise efficient formulations to permit exploitation of the massive amount of data generated by these novel techniques. In recent years, we have developed Fast Fourier Transform (FFT) based methods for polycrystals (e.g. [1]), which can efficiently use voxelized microstructural images of heterogeneous materials as input to predict their micromechanical and effective response.

Furthermore, models based on polycrystal plasticity are increasingly used in engineering applications. These models require a proper consideration of the single crystal plastic deformation mechanisms, a representative description of the microstructure, and an appropriate scheme to connect the microstates with the macro response. FFT-based methods are ideal candidates to fulfill these requirements, albeit at the expense of numerically very demanding computations.

In this talk, we will discuss the latest numerical implementations of the FFT-based formulation for complex constitutive behaviors [2,3] and amenable to input and validation from 3-D characterization methods [4], as well as our recent efforts to embed this kind of models in Finite Elements, to solve complex boundary-value problems with microstructure-sensitive material response.

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Computational Process-Structure-Properties Modeling of Thermal Sprayed Coatings

Tatu Pinomaa, Anssi Laukkanen, Kenneth Holmberg, Erja Turunen, Tarja Laitinen

VTT Technical Research Centre of Finland, Espoo, Finland

We present a predictive multiscale model for microstructure formation and evaluation of material properties in thermal spray coatings. The model is linked to a multiscale nano-microstructure based continuous material model to predict material properties and wear resistance of powder metallurgy based end products.

The studied coating technique is called high velocity oxygen-fuel spray (HVOF). In this process, oxygen and fuel is ignited inside a nozzle, leading to a high temperature exhaust gas flow that – due to the high combustion pressure – accelerates to supersonic velocities. Coating powder is injected into this gas stream, which is dragged into high velocity, and is partially or fully molten in flight. The powder particles hit the surface, and during several microseconds, simultaneously deform into disk-shaped "splats". Subsequent particle impacts lead to a lamellar coating microstructure. Based on specified process parameters, we use computational fluid dynamics (CFD) to describe a reacting and supersonic gas flow inside the nozzle, followed by a lagrangian particle model for the propagation and heating of injected coating particles. This model provides particle velocities and temperatures upon impact, which are used as input for a phase field simulation of coating particle impact and rapid solidification. Subsequent particle impact simulations can be used to model the coating formation.

This process-structure model, complemented with metallurgical and thermodynamical information yields the microstructure for a structure-property computational model. The process analysis results are coarse grained to yield a statistically representative model of the thermal spray coating, the structure being explicitly included in the imaging based property computation utilizing a finite element approach. The nano-microstructural model is subjected to simulated testing for its mechanical and wear responses, and a feedback loop to the coating processing model is presented for material tailoring. The microstructure can be linked to a multiscale representation of material response on larger spatial scales using methods such as the Arlequin method, which provide the basic material properties of the coating in a product and component environment, e.g. porosity, splat-substrate adhesion, and splat-splat cohesion and their effects can be evaluated and quantified. The methodology can also be used to link the coating response to specific external environments – for example degradation due to wear, high temperatures, or erosion-corrosion.

An inverse optimization strategy to determine single crystal mechanical behavior from polycrystal tests: application to Mg alloys

V. Herrera-Solaz¹, Javier Segurado^{1,2}, Javier LLorca^{1,2}

¹Department of Materials Science, Polytechnic University of Madrid, 28040 Madrid, Spain

²IMDEA Materials Institute, 28906 Getafe, Madrid, Spain

An inverse optimization strategy was developed to determine the single crystal properties from experimental results of the mechanical behaviour of polycrystals. The optimization method is based on computational homogenization of the polycrystal behavior by means of crystal plasticity finite element simulations of a representative volume element of the microstructure in which the dominant slip and twinning systems were included in the constitutive equation of each grain [1-2]. The inverse problem was solved by means of the Levenberg-Marquardt method, which provided an excellent fit to the experimental results. The iterative optimization process followed a hierarchical scheme in which simple representative volume elements were initially used and successively by more realistic ones to reach the final optimum solution, leading to important reductions in computer time.

The new strategy was applied to identify the initial and saturation critical resolved shear stresses and the hardening modulus of the active slip systems and extension twinning in Mg alloys. It was found that if only two stress-strain curves were used as input in the optimization procedure, the parameters obtained from optimization were not able to accurately predict the mechanical behaviour of the polycrystal under different loading conditions. Thus, a minimum of three independent stress -strain curves was necessary to determine the single crystal behaviour from polycrystal tests in the case of highly textured Mg alloys.

This methodology was applied to study the critical resolved shear stresses (CRSS) of two magnesium alloys, MN10 and MN11 containing 0.5wt.% and 1wt.% Nd, respectively. The initial CRSSs were observed to change drastically with increasing RE content. In particular, the CRSSs of basal and twinning modes increased while the CRSSs of pyramidal and prismatic systems decreased to an extent that all values become similar for alloying additions of 1wt.%. This is consistent with the isotropic yielding behaviour observed in the MN11 alloy. The changes in CRSS with RE addition lead to the promotion of twinning at the expense of basal slip and to enhance the activity of non-basal systems.

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Identification of constitutive parameters by inverse simulation of indentation in single crystals and close to grain boundaries

Claudio Zambaldi¹, David Mercier¹, Yang Su², Philip Eisenlohr², Thomas R. Bieler², Martin A. Crimp², Dierk Raabe¹, Franz Roters¹

¹Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

²Michigan State University, East Lansing, MI, USA

We present findings based on a recently introduced method [1,2] to extract critical resolved shear stresses and hardening parameters from quasi single crystal indentation. Individual grains of known orientation were probed by nano- or microindentation far away from the grain boundaries for their single crystal mechanical response. The resulting pile-up topographies were characterized by atomic force microscopy or confocal microscopy. In this way the orientation dependent activation of different deformation systems was analyzed by comparing the measured pile-up topographies against crystal plasticity finite element simulations of the indentation process.

Non-linear optimization of the constitutive parameters for the underlying crystal plasticity model, allowed us to extract a single set of parameters which represents the experimentally observed data for all indented orientations. In this way the relative activation of plastic deformation modes could be quantified based on simple indentation experiments.

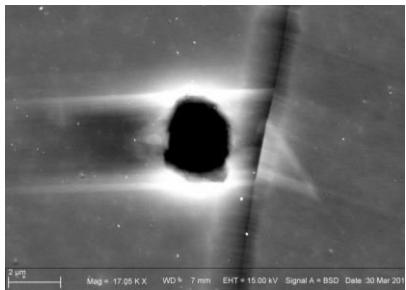


Figure 1: Nanoindentation close to a grain boundary in magnesium. Twinning is initiated in the adjacent grain.

After the initial development of this method on pure titanium [1] it has been applied to a number of metals and alloys with hexagonal (titanium alloy, magnesium [3]) and bcc (ferrite phase [4], tantalum, molybdenum) structure. The specific findings for the relative activation of different mechanisms in each phase will be presented and discuss.

Furthermore, the approach to quantify micromechanical effects by evaluating the anisotropic pile-up profile was extended to characterize the micromechanical effect of grain boundaries. In this case the possibility to efficiently probe many locations on a sample was important since it enabled the rapid acquisition of experimental data. Again the topographic data was compared to crystal plasticity finite element simulations of the deformation during indentation of a bicrystal. From the observed level of agreement between experimental data and simulation results, the slip transfer through the different types of grain boundaries was assessed.

element simulations of the deformation during indentation of a bicrystal. From the observed level of agreement between experimental data and simulation results, the slip transfer through the different types of grain boundaries was assessed.

This work was performed under the NSF/DFG Materials World Network initiative under Contracts NSF-DMR-1108211 and ZA523/3-1.

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Building realistic atomic models of kerogen using Hybrid Reverse Monte Carlo simulations

Colin Bousige^{1,2}, Benoît Coasne^{1,2}, Franz-Josef Ulm¹, Roland Pellenq^{1,2}

¹Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge MA 02139, USA

²<MSE>2, UMI 3466 CNRS-MIT, 77 Massachusetts Avenue, Cambridge MA 02139, USA

Gas and oil shale are unconventional deposits of hydrocarbons that represent important reserves worldwide. Organic-rich shales are natural composites as they consist of different inorganic minerals and a disordered porous carbonaceous material, called kerogen. Understanding and predicting the adsorption, transport, and mechanical properties of such disordered carbons requires having realistic atomistic models that can be used to establish reliable structure – property relationships. Such models can be obtained using Hybrid Reverse Monte Carlo (HRMC) simulations [1,2] in which a numerical atomic model having a structure factor identical to the experimental structure factor is built while using a force field to describe the chemistry of the material.

In this presentation, we will report realistic models of various kerogens obtained using HRMC. We will first show that this HRMC procedure can be computationally accelerated and, hence, applied to much larger systems by combining it with Molecular Dynamics simulations [3]. Thanks to the use of the REBO force field [4], these HRMC can be used to generate numerical models of kerogens with different chemical compositions and maturities. After standard characterization of the different structures in terms of pore size distributions and chemical analysis, the atomistic models of kerogen will be tested against a panel of measurements, accessible to both experiments and molecular simulations, such as nitrogen and water adsorption isotherms, vibrational density of states, and mechanical properties. These refined atomic models will also be used to test the importance of heteroatoms on the hydrophilicity of kerogen.

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Integrated Computational and Experimental Structure Determination for Nanoparticles

Min Yu, Andrew B. Yankovich, Amy Kaczmarowski, Dane Morgan, Paul M. Voyles

University of Wisconsin - Madison, Madison, Wisconsin 53706, USA

Advanced experimental techniques, such as scanning transmission electron microscopy (STEM) provide structural images of materials at atomic resolution. However, a single image provides only a two-dimensional projection of the structure, and three-dimensional tomographic imaging at atomic resolution and single-atom sensitivity remains extremely difficult. Experimentally driven structural refinement approaches typically rely on minimizing the error between forward simulation from atomic models and the experiment data. Such optimizations are challenging with limited data and rely on knowing good initial guesses for the ground state, which may be insufficient for predicting metastable, out of equilibrium states. Such optimizations also typically make no direct use of information about the energy of the potential structures. Genetic algorithms (GAs) have proven to be extremely effective in structure prediction for a wide range of complex structures, including clusters, crystals, and grain boundaries, and have also been used to accelerate matching STEM data to a nanoparticle of known structure. We will discuss development of an integrated GA optimization tool that can reverse engineer the 3D structure of a nanoparticle by matching forward modeling to experimental STEM data and simultaneously minimizing the energy. This tool integrates the power of GAs for complex optimization and utilizes both available experimental and energetics data simultaneously. We demonstrate this nanostructure determination tool on STEM data of Au nanoparticles.

Towards efficient fatigue simulation and parameter identification using models with multiple time scales

Guillaume Puel, Denis Aubry

Laboratoire MSSMat (Ecole Centrale Paris/CNRS UMR8579), Grande voie des vignes,
92290 Chatenay-Malabry, France

When dealing with the numerical prediction of material fatigue, classical life estimation methods, such as those described in [1], can give poor results as far as one is interested with complex loading histories (such as a loading with a slow-evolving average) or inertia effects (for high frequency loadings). It seems indeed more relevant for such cases to use time transient models describing how internal variables, such as plastic strain, or isotropic damage, change with respect to time. However, the computational cost associated with such simulations can become prohibitive if each individual cycle has to be computed.

Therefore a specific method is proposed here to drop the calculation cost by factors up to several thousands: it relies on periodic time homogenization, which is similar to what is usually developed in space homogenization. Moreover, the method is based on a sound mathematical framework, which can guarantee the accuracy of the derived equations and solutions. A first formulation of this method has been proposed in [2]: it is based on the assumption that two different time scales (a fast one, associated with the fast cycles, and a slow one) can be defined and decoupled. Using asymptotic expansions of the scale ratio, it then allows to solve the different equations at the slow time scale only, by taking into account the averaged effect of the fast cycles in the homogenized solution. Since this reference, several extensions have been studied, such as the dynamic framework [3] or how to describe an isotropic damage evolution [4,5].

Moreover, it is possible to address the parameter identification process for such time-homogenized problems. This latter is solved by minimizing a misfit function defined as a norm quantifying the discrepancy between the available measurements and the associated quantities derived from the model [6]. Work is in progress to address the main questions arising when one tries to use in the identification process the time-homogenized model rather than the reference problem.

Eventually, this should lead to a suitable strategy for addressing accurate fatigue predictions and associated parameter identification for arbitrary cases of study, whereas the computational cost remains affordable.

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A coupling method for stochastic polycrystalline models at different scales

Régis Cottereau

Laboratoire MSSMat, École Centrale Paris, CNRS, F-92295 Châtenay-Malabry, France

In this study, we present an approach that allows to couple two stochastic continuum models [1]. In particular it allows to couple a homogeneous (or slowly fluctuating) continuum mechanics model with random constitutive tensor and a polycrystalline model with stochastic anisotropic grains. The latter model represents the micro-scale model while the former would be its upscaled (or homogenized) version. The coupling strategy is performed in the Arlequin framework [2], which is based on a volume coupling and a partition of the energy between two models. The main interest of this framework is that it allows to couple models that are different in nature: discrete vs. continuous, deterministic vs. stochastic, linear vs. nonlinear, with vs. without defects or cracks.

A suitable functional space is chosen for the weak enforcement of the continuity between the two models. The choice of this space ensures that the ensemble average of the two stochastic solutions are equal point-wise in the coupling area, and that appropriate boundary conditions on the stochastic dimension are passed from one model to the other. However, it does not impose any strong continuity, that would induce undue strength localization from one model onto the other. The proposed coupling approach is an extension of a previous work dealing with the coupling of a stochastic model with a deterministic one [3]. It leads to a mixed problem. This choice of functional spaces and coupling operator ensures that the mixed problem has a unique solution that can be approximated by spectral finite elements or a Monte Carlo technique.

This presentation will be focused on showing the interest of such an approach for identification of polycrystalline models when the information comes from experiments performed at different scales. This is for instance the case when measuring concurrently elastic strains through X-ray diffraction during in situ mechanical tests coupled with image correlation. In general, different models are identified at different scales using different experimental information. However, using all the information concurrently and making sure that models at the different scales are compatible (in the sense of homogenization [4]) is a key to relieving some numerical difficulties encountered in the identification process.

Extension to the coupling of dynamics of dislocation models and polycrystalline models will be highlighted if time permits.

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Banding, grain fragmentation and texture formation in f.c.c. polycrystals: ‘stack of domains’ model

Arul Kumar Mariyappan¹, Sivasambu Mahesh²

¹Materials Science and Technology Division, Los Alamos National Laboratory,
Los Alamos, NM, 87545. USA.

²Department of Aerospace Engineering, Indian Institute of Technology, Madras,
Chennai, 600036. India.

Grains of a f.c.c. polycrystals undergoing heterogeneous deformation even under imposed homogeneous deformation. Heterogeneous deformation within the grains develop substructures like shear and deformation banding. Formation of banding produces significant lattice misorientation within the grains and it affects the texture formation followed by grain fragmentation. Recently developed computationally efficient rigid plastic rate-independent crystal plasticity based ‘stack of domains’ model of a grain is employed to study the banding followed by grain fragmentation and texture formation in f.c.c. polycrystalline material under rolling and Equal-Channel Angular Pressing (ECAP) deformation. Banding simulation under rolling and ECAP deformation is performed on f.c.c. polycrystalline copper comprised of 2048 initially randomly orientated grains. Predicted banding and grain fragmentation response is mapped over the entire orientation space. Model banding and texture predictions are validated with the experimental observations reported in the literature.

Multiscale modeling of hydrogen enhanced local plasticity and its application to homogenous nucleation of dislocation in Ni-H systems

Gerard Paul Leyson, Blazej Grabowski, Jörg Neugebauer

Max-Planck-Institut fur Eisenforschung

One of the major paradigms used to explain hydrogen embrittlement is *Hydrogen enhanced local plasticity (HELP)*. However, a quantitative connection between dislocation-hydrogen interaction and the actual embrittlement process is not well understood. To make this connection, it is necessary to model large length- and timescales while also taking into account atomistic effects, such as hydrogen-hydrogen interaction. In this work, a multi-scale approach is adopted, in which an analytic model that is informed by atomistic calculations is developed. In particular, the model takes, as input, hydrogen-hydrogen interactions and the dislocation core structure through the Peierls-Nabarro model. The local hydrogen concentration around the dislocation is calculated self-consistently with the hydrogen binding energy and the dislocation core is allowed to relax as a function of the local hydrogen content. The hydrogen concentration profiles given by the model are in excellent agreement with previous Embedded Atom Method-Monte Carlo simulations in Ni-H systems while being four orders of magnitude faster. The model is then applied to *Homogenous Dislocation Nucleation (HDN)* occurring in nano-indentation experiments. Unlike previous analyses, the complex nature of the dislocation field as well as the equilibrium hydrogen concentration around the loops is taken into account. The onset of HDN as a function of bulk hydrogen concentration and temperature is quantified and is in good agreement with experiments.

Multiscale modeling of a multi-component system: towards the understanding of Oxide Dispersion Strengthened steels

Caroline Barouh, Chu-Chun Fu, Thomas Jourdan

CEA, DEN, Service des Recherches de Métallurgie Physique, F-91191 Gif-sur-Yvette Cedex,
France

A multiscale-modeling approach is applied to investigate key properties of Oxide Dispersion Strengthened (ODS) steels, which are promising candidate materials for fusion and advanced fission reactors. They are suggested to exhibit improved radiation and swelling resistance, thanks to the presence of highly stable nano-precipitates containing Y, O, Ti and potentially vacancies. Accurate information on structural and compositional properties of these precipitates is however scarce, from both experiment and modeling. On one side, experimental data on the nascent clusters are difficult to obtain, due to limitations of spatial resolution. On the other side, addressing nano-scale features in multi-component systems by atomistic simulations is still highly challenging. For instance, first-principles methods are computationally too expensive for this purpose, while empirical potentials and effective interaction models may not be reliable enough for systems involving multiple chemical species.

We aim, in the present study, at understanding the mechanisms of the nucleation of the nano-precipitates. A combined Density Functional Theory (DFT) and Cluster Dynamics (CD) approach is employed. The DFT calculations are performed to gain insights into the nature and strength of interactions between various solutes (O, Y and Ti) and between solutes and vacancies in a bcc iron lattice, the solute diffusion properties, and the energetics of small solute clusters. The obtained DFT data are systematically used to parameterize a highly efficient CD model, based on the Rate Theory, where time evolution of the concentration of all the solutes, vacancy and solute clusters can be predicted.

In this presentation, we show the ability of our approach to perform real-time simulations as close as possible to typical experimental conditions of annealing time, temperature and dislocation density, in order to elucidate the role of vacancies on the nano-precipitate formation in a model ODS steel, which has been a subject of controversy raised by previous theoretical studies [1-2].

This work is supported by the joint program "CPR ODISSEE" funded by AREVA, CEA, CNRS, EDF and Mécachrome under contract n°070551.

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The use of discrete harmonics in direct multi-scale embedding of polycrystal plasticity

N. R. Barton¹, J. V. Bernier¹, R. A. Lebensohn²

¹Lawrence Livermore National Laboratory, Livermore, CA 94551, USA

²Los Alamos National Laboratory, Los Alamos, NM 87544

In efforts related to multiscale embedding of plasticity, there has been a recent emphasis on computationally tractable approaches that include polycrystal mechanics and texture evolution. The crystallographic texture, or orientation distribution function, is a key factor in determining material anisotropy. Here we will discuss an approach that allows for evolving texture by employing discrete harmonics, effectively decoupling considerations related to accurate integrals in the homogenization from those related to adequate representation of the evolving texture. We will discuss the basic behaviors of the model, including model fidelity as a function of the degree of the expansion used in representing the texture. Specific applications focus on the deformation of titanium, including the effects of twinning. Finally we will discuss the possibilities for use of the new modeling approach in the context of adaptive sampling to mitigate computational cost. The discrete harmonic based approach allows for a compact representation of the texture and its evolution, and appears to offer a viable path forward for use with adaptive sampling.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 (LLNL-ABS-650499).

Dislocation dynamics simulations of HCP beryllium single crystals at high strain rates

Moon Rhee, Sylvie Aubry, Gregg Hommes, Tom Arsenlis

Lawrence Livermore National Laboratory, PO BOX 808, 7000 East Ave., Livermore, CA
94550

LLNL has developed a three dimensional dislocation dynamics (DD) code ParaDiS (Parallel Dislocation Simulator) for the last decade to investigate the fundamental deformation behavior of cubic metals at extreme conditions. Recently, we have incorporated the infrastructure for HCP (hexagonal-closed-packed) single crystals into ParaDiS to study deformation modes of HCP beryllium under various loading conditions. Due to the low symmetry of HCP crystal structure, different loading directions may lead to unexpected mechanical properties and associated deformation mechanisms. Through DD simulations, we investigate the effect of loading directions on mechanical property at high strain rates. Dislocation mobilities of $\langle a \rangle$, $\langle c \rangle$ and $\langle c+a \rangle$ type dislocations are obtained from molecular dynamics simulations. Junctions can be formed based on the interaction energetics of dislocations. In beryllium, unlike other HCP metals, the interaction between $\langle c \rangle$ and $\langle a \rangle$ dislocations is very weak due to the exceptionally low Poisson's ratio. Experimental evidence reported in the literature suggests that the $\langle c+a \rangle$ dislocations in pyramidal planes can be easily dissociated into $\langle c \rangle$ and $\langle a \rangle$ dislocations. We enabled the mechanism of decomposition of pyramidal $\langle c+a \rangle$ dislocations into prismatic $\langle c \rangle$ and basal $\langle a \rangle$ dislocations. A mechanism to permit dislocation cross-slip is also enabled. Loading directions are varied to induce single and multi-slip deformation. Preliminary results indicate that there is no strain hardening during deformation under simple shear on the basal plane. We observe, however, high degrees of strain hardening for all uniaxial loading conditions including $[0001]$, $[\bar{1}\bar{2}0]$ and $[\bar{1}\bar{1}21]$ directions. This presentation will describe results obtained from DD simulations for HCP beryllium single crystals deformed at high strain rates as well as detailed description of dislocation flux and slip analysis during deformation.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory in part under Contract W-7405-Eng-48 and in part under Contract DE-AC52-07NA27344.

Impact of magneto-vibrational couplings on the thermodynamic properties of iron: A hierarchical *ab initio* approach

F. Körmann, B. Grabowski, B. Dutta, T. Hickel, J. Neugebauer

Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237,
Düsseldorf, Germany

Thermodynamic first-principles modeling of paramagnetic materials is a delicate task. One of the main issues is the interplay of magnetic and atomic degrees of freedom. Practical approaches allowing the computation of atomic forces at finite magnetic temperatures are up to now only rarely available, but are decisive for an accurate description of the thermodynamics in many material systems. For this reason, we have recently developed an *ab initio* approach to compute effective paramagnetic atomic forces [1]. They are obtained from SQS structures for the magnetic disorder combined with a spin- space averaging procedure. Employing this method we calculate the paramagnetic quasi-harmonic (vibrational) free energy for fcc iron. The derived thermodynamic properties such as phonon spectrum, expansion coefficient, and bulk modulus are in good agreement with experiment. In particular we demonstrate how the experimentally observed anti-invar effect in fcc Fe can be understood from first- principles. Coupling QMC and DFT simulations allows us to eventually compute the interatomic forces from the fully magnetically ordered (ferromagnetic) up to the completely magnetically disordered (paramagnetic) state in bcc Fe. The coupled QMC-DFT approach enables hitherto not achievable insights into the temperature-dependence of phonon frequencies in magnetic systems and may be used to further improve the experimental evaluation of vibrational entropy contributions in iron-based alloys.

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Uncertainty Analysis of Materials Phase Diagrams

Kristin P Lennox, Charles Tong, Vasily Bluatov

¹Lawrence Livermore National Laboratory, Livermore, California 94550, USA

Phase diagrams are used extensively in materials sciences to assess phase stability and to evaluate possible routes for processing of materials. A phase diagram can merge information from multiple experimental and computational sources for a chemical system and produce an image identifying the phase structure of the system at varying temperatures and compositions. This gives insight into, for example, ideal compositions for alloys and potential avenues for improving synthesis. Due to their reliance upon multiple data sources, phase diagrams are sensitive to the differences in uncertainty for various data sets. This is generally handled by using expert judgment to provide relative importance weights for competing data sets; however, the final phase diagram is essentially a point estimate, and gives no insight into the uncertainty of phase boundaries due to either limited data or expert uncertainty. We have developed a new phase diagram generation tool for binary systems that allows uncertainty to be incorporated into the final phase boundaries. This tool allows users to directly examine the sensitivity of phase diagrams to disparate data quality and varying assumptions about the functional form of thermodynamic potentials. This is demonstrated using a phase diagram of the binary iron-chromium (Fe-Cr) system.

This work is supported by the Critical Materials Institute, an Energy Innovation Hub funded by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, Advanced Manufacturing Office. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

First principles thermodynamics of magnetically disordered materials: defect formation in iron and steel

Vsevolod I. Razumovskiy¹, Andrei Reyes-Huamantinco¹, A. V. Ruban^{1,2}

¹Materials Center Leoben Forschung G.m.b.H. Roseggerstraße 12, Leoben 8700, Austria

²Department of Materials Science and Engineering, Royal Institute of Technology KTH, Brinellvägen 23, Stockholm 100 44, Sweden

Finite-temperature description of iron and steel is an important task within the framework of the Integrated Computational Materials Engineering approach. This task represents a complex and non-trivial problem at all scales starting from the fundamental level of density functional theory *ab initio* calculations. One of the challenges of *ab initio* calculations is the description of magnetic order/disorder transitions, in particular, the problem of an accurate description of the paramagnetic state. Here, we would like to present a method for *ab initio* calculations of the ideal paramagnetic state (IPM) and demonstrate its applicability to calculation of thermodynamic properties of paramagnetic iron and steel.

The spin-wave method [1] for *ab initio* description of the paramagnetic state provides one with an alternative to existing methods way to describe the disordered magnetic state using non-collinear calculations of planar spin spirals shown in Figure 1. One of the main advantages of the methodology is the possibility to calculate defects in the disordered magnetic state without need for additional averaging over a large set of magnetic configurations (including the effect of local lattice relaxations) as the formalism is based on averaging over the spin spiral spectrum. The latter problem can be reduced to a calculation of just a few high symmetry points in the Brillouin zone which simplifies *ab initio* calculations of the IPM a big deal. The method has been combined with standard supercell approach to obtain vacancy and stacking fault formation energies in paramagnetic pure iron as well as in paramagnetic Fe-Mn steel. Calculations have been performed using the Projector Augmented-Wave (PAW) method as implemented in Vienna Ab-initio Simulation Package (VASP) and the Exact Muffin Tin Orbitals method.

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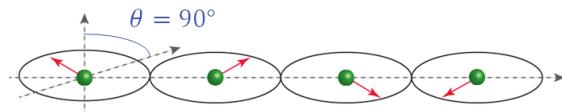


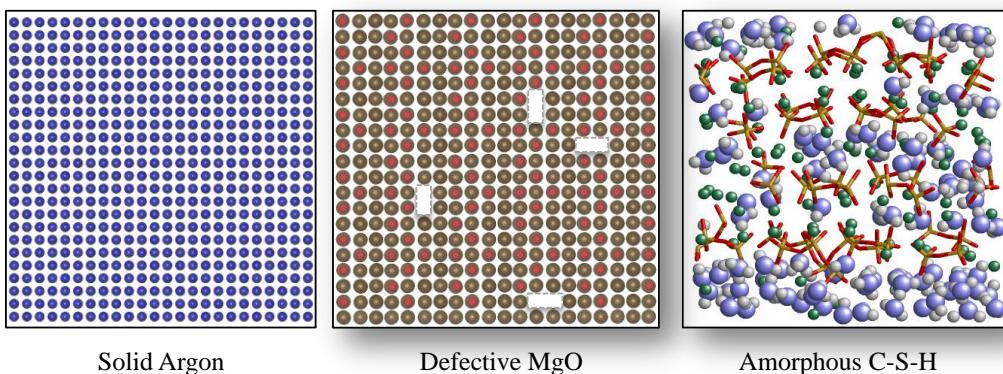
Figure 1: Planar spin spiral. Arrows represent schematic orientation of magnetic moments on atoms (green circles)

Multiscale Modeling of Heat Transport in Glassy and Amorphous Materials

Mohammad Javad Abdolhosseini Qomi, Mathieu Bauchy, Franz Ulm, Roland Pellenq

Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

This work presents a bottom-up approach to study heat diffusivity of amorphous and glassy materials from the nano-scale, to the engineering scale. The thermal conductivity of materials originates from the propagation of phonons at the nano-scale and depends strongly on the molecular structure and the energy landscape describing interatomic interactions. Such a non-equilibrium property is calculated for number of materials ranging from crystals (solid Argon and Magnesium Oxide), defective crystals (Effect of Vacancies), glass (silica glass) and Amorphous materials (calcium-silicate-hydrate (CSH) the main binding phase of cement paste) via the Green-Kubo approach in equilibrium molecular dynamics (see the figure below). We comment on the effect of textural properties on the heat transport and mean free path of phonons at the nanoscale in different materials. Calculating the phonon density of state (DOS) we show that how defects affect the local and collective motion of atoms at short and medium-range scale. Using the insight from crystals, defective and glassy materials, we are able to provide a clear picture of heat transport at the nanoscale. We show that the three principle thermal conductivities of Amorphous materials can be statistically different and we describe why the volumetric thermal conductivity of CSH is mostly unaffected by the defect population while on the contrary incorporating nano-scale defects in crystals directly effects their thermal conductivity. Since the mean free path of phonons is much less than cement nano-grains, 4-5nm, statistical micro-thermo-mechanics approaches are applicable and hence applied to calculate the homogenized thermal properties at micron and macro scales. Using a Monte Carlo sampling scheme, self-consistent micro-thermo-mechanical equations are randomly sampled to statistically upscale heat transport to micron scale. We show that the experimental values lie within the range of homogenized thermal conductivity at micron-scale of varying porosity and saturation level.



Modeling Multiple-site Brittle Fracture in Tungsten During Thermo-mechanical Transients with Discrete Volterra Dislocation Arrays

Andrew Sheng, David Rivera, Tamer Crosby, Nasr M. Ghoniem

Department of Mechanical & Aerospace Engineering, University of California at Los Angeles (UCLA), 420 Westwood Plaza, Los Angeles, CA 90095-1587, U.S.A.

Tungsten samples subjected to transient plasma heat flux conditions have been shown to exhibit plastic behavior during plasma exposure. Upon cooling, elastic strain recovery results in residual tensile stresses that can trigger the onset of fracture on the sample surface. These cracks, which also extend below the surface, are present both along grain boundaries and in the bulk [1]. Existing methods for modeling fracture have been limited in their ability to handle complex geometries, loading conditions, and high crack densities. Here we present a method for modeling the thermo-fracture process in 2D that utilizes a finite element thermo-elastoplasticity model in combination with a discrete dislocation representation of cracks. The finite element model is used to calculate the residual stresses present in a sample after plasma exposure. These stresses are used to determine the equilibrium configuration of distributed Volterra dislocations, which represent cracks in an infinite medium. The solution to a boundary value problem in a finite domain, which represents the sample, is then superimposed onto the elastic field in the infinite medium to obtain the solution for cracks in the finite domain. The stress intensity factor (SIF) for each crack is determined through the equivalence between the J-integral and the Peach-Koehler forces acting on the dislocations representing the crack tips [2]. By comparing the SIF to the fracture toughness of the material, crack propagation is represented by moving the crack tip dislocations.

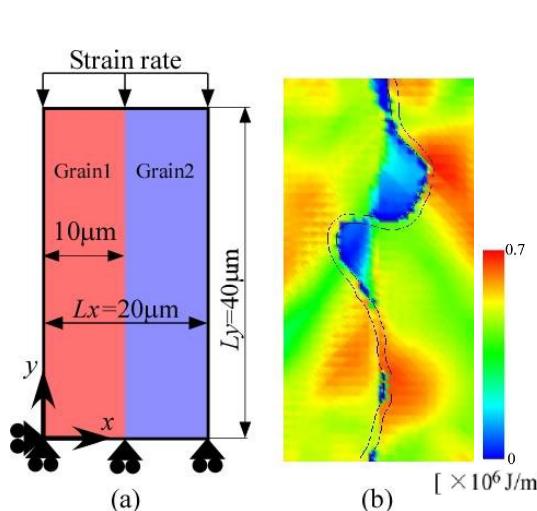
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Development of Multi-phase-field Crystal Plasticity Model for Grain Boundary Bulging during Dynamic Recrystallization

Takato Yamaguchi¹, Tomohiro Takaki¹

¹Mechanical and system engineering, Kyoto Institute of Technology, Matsugasaki, Sakyo, Kyoto, 606-8585, Japan

In hot working of metal material with low to medium stacking fault energy, microstructures are refined due to dynamic recrystallization (DRX). During the DRX, grain boundary bulging serves as a major nucleation origin of DRX grains [1]. Therefore, in order to accurately predict the nucleation site of DRX grains, it is important to understand the nucleation mechanism of DRX grain by grain boundary bulging. For that purpose, it is essential to develop a numerical model for DRX. However, because DRX is a highly complicated phenomenon where grain growth and plastic deformation occur simultaneously, to our knowledge, models that can express the grain boundary bulging have not been reported so far.



In this study, we develop a DRX model by coupling crystal plasticity (CP) model and multi-phase-field (MPF) model [2] to make clear the DRX nucleation mechanism due to grain boundary bulging numerically. In this model, non-uniform deformation, dislocation density and crystal orientation of poly crystalline structure are computed by CP finite element method. At the same time, MPF simulation is performed to express grain growth driven by stored energy of dislocations and redistribution of dislocation density due to the grain boundary migration. Dislocation densities and crystal orientations are exchanged between these two computations.

Figure 1: (a) Computational condition for compression simulation of bi-crystal material. (b) Grain boundary and stored energy distribution at 32% compression.

Fig.1 (a) shows the computational condition for compression simulation of bi-crystal material with different crystal orientations. Fig.1 (b) shows the calculation result of MPF simulation at 32% compression. Color and solid line indicate stored energy distribution and grain boundary, respectively. It is observed that the grain boundary migrate to the area with high stored energy and the stored energies behind the migrated grain boundary become small. From this result, it is confirmed that the developed model can express grain boundary bulging during DRX well.

This work was supported by JSPS KAKENHI Grant Number 25630011.

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Analytical method for estimating the thermal expansion coefficient at high temperature

So Takamoto¹, Shun Oinuma², Yujiro Nakatani², Satoshi Izumi¹, Shinsuke Sakai¹

¹ School of Engineering, The University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

² Power & Industrial System R&D Center, Toshiba Corporation, 1–9, Suehiro-cho, Turumi-ku, Yokohama 230–0045, Japan

Recent years, the development of materials for high temperature environments, in the field of the high-efficiency thermal power plant has become active. Since try-and-error scheme has reached the limitation, the estimation of physical properties by atomic-scale simulation is desired. In estimating of the thermal properties at high temperature, thermal expansion coefficient is one of key material property. It is said that the thermal expansion of the crystal is caused by the anharmonicity of the lattice vibrations. Conventional method based on the quasi-harmonic approximation [1] is known that the accuracy decreases at high temperature because the model does not sufficiently include the effect of the anharmonic vibrations [2].

In this study, we proposed an analytical method for calculating the thermal expansion coefficient at high temperature by estimating the distribution of interatomic distances based on the phonon-dispersion relation. The model incorporates the anharmonic effect caused by the increase in the amplitude of the phonons.

Classically, the pressure can be calculated by the interatomic potential and the radial distribution function using the Virial equation. Therefore, assuming the harmonic approximation, we estimated the radial distribution function from the relationship between the energy and the amplitude of the phonons. We take into account several anharmonic effects, such as the variation in the frequency of the phonons, the increase in

the distance between atoms due to the vibration, the asymmetry of the interatomic potential. By considering these effects quantitatively, our proposed model allows us to estimate the thermal expansion coefficient analytically over a wide temperature range.

Development of the interatomic potential which reproduces the thermal expansion coefficient at high temperature has become possible. We have developed the interatomic potentials for Ni and Fe to reproduce the thermal expansion coefficients over a wide temperature range.

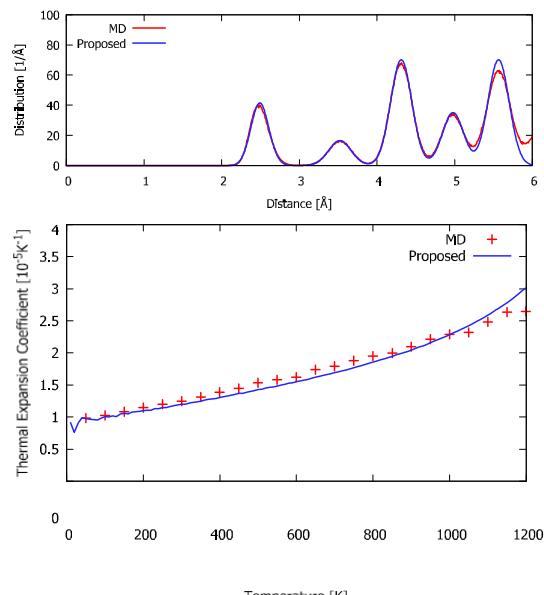


Figure 1: Estimation of radial distribution function (upper) and thermal expansion coefficients (lower) of Nickel.

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Dynamic Recrystallization Modeling by Multi-phase-field Method Considering Misorientation Dependent Interface Properties

Eisuke Miyoshi¹, Tomohiro Takaki¹

¹Mechanical and System Engineering, Kyoto Institute of Technology, Matsugasaki, Sakyo,
Kyoto 606-8585, Japan

Dynamic recrystallization (DRX) occurs during hot-working of metallic materials with low to medium stacking fault energy. Macroscopic mechanical behaviors during the hot- working with DRX are largely affected by the microstructure evolutions, or DRX grain growth. Therefore, in order to estimate and predict hot-working properties with high accuracy, it is key to develop a multi-scale model for DRX, which can compute the macroscopic mechanical behaviors depending on the microstructure evolutions.

We have developed a multi-phase-field dynamic recrystallization (MPF-DRX) model [1-3], where the evolution of dislocation density, or plastic deformation, is modeled by the Kocks-Mecking model and DRX grain growth is simulated by a multi-phase-field (MPF) method. Average stress of the computational domain is computed by Bailey-Hirsch equation using the average dislocation density of the domain. This MPF-DRX model enabled us to compute the mechanical behaviors of the domain based on the DRX grain growth, or multi-scale simulation of hot-working with DRX. On the other hand, the MPF- DRX model assumed that the dislocation density is constant in a grain and the grain boundary energy and mobility are constant independent on the grain boundary misorientation. In order to perform more accurate evaluations of hot-working, the model needs some improvements.

In this study, we develop the modified MPF-DRX model by introducing misorientation dependencies of grain boundary energy and mobility to the MPF model and a preferred nucleation site. The MPF model used in the present MPF-DRX model, which was developed by Steinbach et. al. [4], is difficult to introduce grain boundary energies and mobility with large difference. To improve the point, we introduce novel way to accurately express the grain boundary properties at triple points. In addition, the information of preferred nucleation site, such as triple point, grain boundary and inside of grain, is introduced to the MPF-DRX model. By performing a series of simulations using the modified MPF-DRX model, we confirm the accuracy of the model and the effects of the modified points on the results. In addition, the modified MPF-DRX model is incorporated to the MPFFE-DRX simulation [5] and we try to simulate more realistic hot-working multi-scale simulations.

This work was supported by JSPS KAKENHI Grant Number 25630011.

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Computational model verification using multiplexed photonic Doppler velocimetry for high velocity projectile impact on steel targets

Robert S. Hixson¹, Brendan O'Toole², Mohamed Trabia², Shawoon Roy², Michael Pena¹, Steven Becker¹, Edward Daykin¹, Eric Machorro¹, Richard Jennings², Melissa Matthes²

¹National Security Technologies, LLC, Las Vegas, Nevada 89193, USA

²University of Nevada, Las Vegas, Las Vegas, Nevada 89154, USA

Metal plates are subjected to high stress and strain rate deformation in penetration experiments and results are modeled using two complementary approaches. This work presents a unique approach to experimentally measuring the velocity of the back surface of the target at several points during the early deformation phase. Crater details are measured after the impact and all measurements are compared to computational simulations.

A two-stage light gas gun was used to launch cylindrical Lexan projectiles at velocities from 4 to 6 km/s at a 12.7 mm (0.5") thick ASTM A36 steel plate. The impact creates a small crater in the front of the plate and a bulge on the back surface, which typically leads to fracture and spallation of material near the back face. The free surface velocities from multiple points on the plate's back surface are measured using a Multiplexed Photonic Doppler Velocimetry (MPDV) diagnostic system. PDV is an interferometric fiber-optic technique that can determine velocity by measuring the Doppler shift of light reflected from the moving surface.

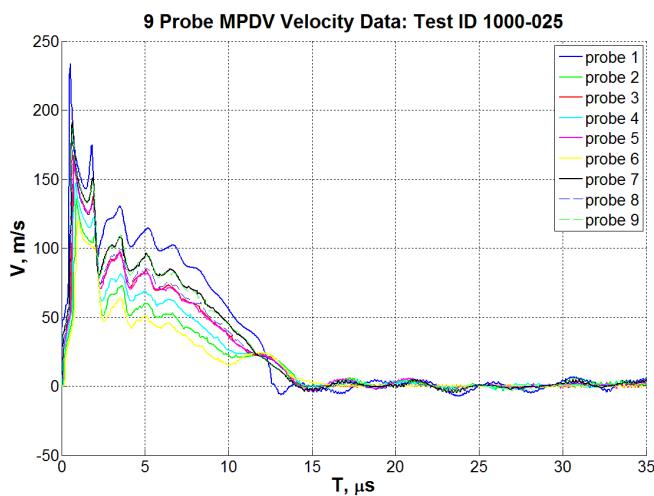


Figure 1: Sample data from a penetration experiment

Grüneisen equation of state. Experimental data and simulation results are compared to verify the accuracy of the computational models during ballistic impact events.

This work was supported by National Security Technologies, LLC, under Contract No. DE-AC52-06NA25946 with the U.S. Department of Energy and supported by the Site-Directed Research and Development Program.

A multiphase-field model with Onsager reciprocal relations

Reza Darvishi Kamachali, Ingo Steinbach

ICAMS, Ruhr-University Bochum, 44801 Bochum, Germany

A generalization of the multiphase-field model [Steinbach I. and Pezzolla F.; Physica D 1999;134;385] to include kinetic cross coupling to a conserved field [Brener E.A. and Boussinot G.; Phys Rev E 2012;86;060601] is presented. We show that this model is consistent with phenomenological relationships given by Onsager and his predecessors including symmetric reciprocal relations having a positive-definitive matrix of kinetic parameters (positive entropy production). At junctions, the interaction between each phase-field is attributed by a coupling term to all other existing phase-fields and the respective conserved order parameters. The model shall be applicable to phase transformations with kinetic constraints on the transformation rate at dual interfaces and junctions between an arbitrary numbers of fields.

Modelling nonlinear behavior of heterogeneous geomaterials by extended finite-element method

Naima Belayachi¹, Senjun Wu¹, Dashnor Hoxha¹, Duc-Phi Do¹

¹University of Orléans, INSA-CVL, PRISME, EA 4229, F45072, Orléans, France

Predicting the behavior of heterogeneous materials has attracted the attention of the research community mainly because they are used in various engineering applications coupled with more restrictive safety rules. However, both for natural and industrial materials, accurate behavior modeling is still a challenge despite of the fast progress of modeling techniques because of the need for a more precise knowledge of the mechanical properties for the structural behavior. Moreover, geomaterials like rocks or soils used for the nuclear waste disposal are known to have a non linear behavior and are particular class of heterogeneous material strongly influenced by their geological history and their natural composition and requires considerable efforts. To describe the mechanical behavior of such material, two approaches have been proposed. The macroscopic one suppose the material homogeneous, have the same behavior at any point , and use a well-established plastic viscoplastic and damage models identified by laboratory tests. The micromechanical approach complements the first by considering the microstructure of the material and the behavior of each constituent by highlighting the role of the microstructure and the interaction of their mechanisms on the macroscopic behavior. In spite progresses of numerical upscaling approach with complex behavior, the microstructure is simplified and described the well known unit cell. Alternatively to classic finite element method, XFEM offers to homogenization method the possibility to describe a more complex microstructure [1].

The M-H-M argillite rock studied in this work shows macroscopic nonlinear strains caused by slip of clay sheets of argillaceous matrix, and the damage of the matrix or grains [2]. In this paper, we are interested in modeling the behavior of the argillite rocks by numerical homogenization based on XFEM (extended finite element method). To describe the nonlinear behavior of the constituent the associated Drucker-Prager model is integrated in the XFEM computer code developed with Matlab [3]. The material is considered as biphasic composite with elstoplastoic matrix and elastic inclusions and pores with different shape and spatial distributions.

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Crack Propagation Simulations in Polycrystal by Multi-phase-field-crack Model

Shinya Mori¹, Tomohiro Takaki¹

¹Mechanical and System Engineering, Kyoto Institute of Technology, Matsugasaki,
Sakyo, Kyoto 606-8585, Japan

Crack propagation problem is the important and difficult point of study among the fracture mechanics. In particular, a prediction of crack propagation path in a complicated microstructure is very difficult. In numerical prediction and estimation, finite element methods are widely used to simulate the crack propagation. Meanwhile, finite element method needs to track the crack tip position and to select a direction of crack propagation. Therefore, it is thought to be difficult to simulate crack propagation in complicated microstructure only by finite element method.

Recently, studies where a phase-field method is applied to the prediction of crack propagation are done actively [1]. In phase-field method, crack and material is distinguished by an order parameter, or phase-field variable, and the crack interface is express as a variation region of the phase-field. The merits of the phase-field method are that we do not need to track the crack tip and that the crack propagation direction is determined automatically. Therefore, the phase-field method is promising method in the problem of crack propagation prediction.

In this study, we have develop multi-phase-field-crack (MPFC) model which can predict crack propagation in complicated microstructure of brittle material. In this model, we use the multi-phase-field model proposed by Steinbach et. al. [2] for grain growth and polycrystalline phase transformation. Elastic anisotropy, crystal orientation, difference of fracture toughness inside grain and at grain boundary, and misorientation dependent grain boundary energy are introduced into the MPFC model. By simulating crack propagationin polycrystal using the developed MPFC model, we confirm the validity of the developed model.

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Impact of extended defects on the mobility of grain boundaries: A molecular dynamics study

Sherri Hadian¹, Blazej Grabowski², Christopher Race³, Jörg Neugebauer²

¹Max-Planck Institute, ²Max-Planck Institute, ³University of Manchester

Classical molecular dynamics simulations are commonly used to explore the migration of grain boundaries. Our previous research has shown that conclusions drawn from such studies are highly dependent on systems size and driving force [1]. In particular the concept of an intrinsic mobility must be abandoned for perfectly flat, symmetric grain boundaries below the roughening temperature.

The present study extends our research towards grain boundaries deviated from their perfect and symmetric arrangement. Such boundaries constitute in fact the majority of experimentally observed moving boundaries. We introduce defects of different configurations into several low sigma high angle grain boundaries through systematically inclining the boundary plane from a symmetric equilibrium boundary. The results of the simulations show how the mobility of a boundary increases as the level of planar asymmetry increases. The results further show that the propagation of steps (which asymmetric boundaries relax into) is the rate determining mechanism of migration of the studied grain boundaries.

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On the strength properties of ductile porous solids with a Mohr-Coulomb matrix: theoretical formulation and numerical assessment

Kokou Anoukou¹, Franck Pastor², Philippe Dufrenoy³, Djimédo Kondo¹

¹Institut Jean Le Rond d'Alembert, UMR 7190 CNRS, Université Pierre et Marie Curie, 4 place Jussieu, F-75005 Paris, France

²Athénée royal Victor-Horta, rue de la Rhétorique, 16, Bruxelles, Belgium

³Laboratoire de Mécanique de Lille, UMR 8107 CNRS, Université Lille 1, Cité scientifique, F-59655, Villeneuve d'Ascq, France

We propose a new analytical macroscopic strength criterion for porous solids having a rigid-perfectly plastic matrix obeying Mohr-Coulomb yield criterion. In the context of a standard limit analysis, an associated flow rule is considered. We derive in a parametric form a closed-form expression of the macroscopic criterion. To this end, and similarly to the pioneering study by Gurson [1] (for von Mises matrix) and Guo et al. [2] (for a Drucker-Prager matrix), we perform a kinematic limit analysis homogenization of a hollow sphere under axisymmetric loadings. In the present study, a minimization problem, arising in the determination of the macroscopic plastic dissipation potential, has been solved analytically by means of Lagrangian methods of inequality constrained optimization. The predictive capabilities of the derived strength criterion are successfully assessed by comparison with numerical limit analysis results delivering lower and upper bounds of the macroscopic criterion of the porous solids with a Mohr-Coulomb matrix [3,4]. The influence of the third stress deviator invariant on the macroscopic strength surface is also highlighted through the asymmetry of the macroscopic yield surface with respect to pure hydrostatic axis. Moreover, it is shown that the tension-compression asymmetry of the Mohr-Coulomb yield surface at micro-scale, with respect to the pure deviatoric axis, is transposed at macro-scale by the homogenization procedure.

This work was performed under the financial support of the program “Transports durables et mobilité” via the French project ANR CoMatCo.

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Diffusion of oxygen in TiNiHf high temperature shape memory alloy: A first-principles approach

Hak-Sung Lee¹, Chang-Seok Oh¹, Jeoung Han Kim¹ and Jong Taek Yeom¹

¹Light Metal Division, Korea Institute of Materials Science
Changwon, Gyeongnam 642-831, Korea

The need of high temperature shape memory alloys (HTSMA) is increasing due to their potential applications for various mechanical devices such as actuator in automobile engine. In order to increase the operating temperature of SMA, various alloy systems including NiTi-X(X = Pd, Pt, Au, Rh, Zr and Hf) have been examined extensively. In a point of view of a materials cost the Ni-Ti-Hf system is a one of promising candidates which exhibit high transformation temperature and superior shape memory characteristics. However, the Ni-Ti-Hf HTSMAs have not been commercially available yet due to processing difficulties such as control of chemicals and mechanical processing partially coming from oxidation, as with other TiNi based HTSMA systems.

The oxidation behavior of $\text{Ni}_{0.5}\text{Ti}_{0.5-x}\text{Hf}_x$ alloy should be examined carefully because annealing and fabrication temperature of this alloys are enough high to be readily oxidized. Recently, one of authors reported that the oxygen diffusion in $\text{Ni}_{0.5}\text{Ti}_{0.5-x}\text{Hf}_x$ alloy is much faster than that in NiTi based on isothermal oxidation experiment with a TGA, however, the effect of dopants on the oxygen diffusion was not fully understood [1]. Therefore further systematic investigations via both of experimental and theoretical methods are necessary to understand the oxidation behavior.

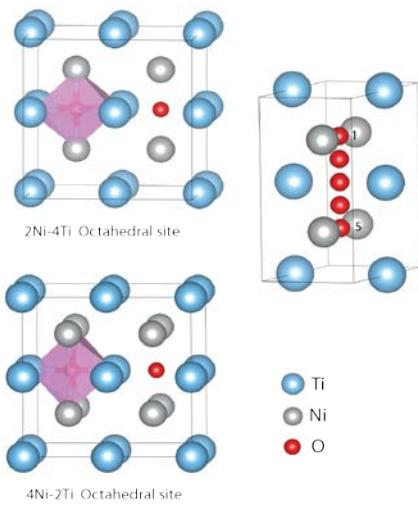


Figure 1: Two kinds of octahedral sites in NiTi and diffusion path

In this presentation, systematic nudged elastic band (NEB) calculations were performed with the VASP to obtain the activation energy of oxygen diffusions. In NiTi, there are two kinds of octahedral sites as shown in Fig. 1. It was found that the interstitial oxygen diffuses the neighbors with the lowest activation energy via two different octahedral sites and the activation energy is strongly related to the size of octahedral site. In order to understand the effect of dopant, a bigger calculation cell containing Hf atoms was carried out and the effect of structural relaxation around the defect was examined systematically. In addition, the effect of dopant concentration with special quasi random structures will be discussed.

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Phase transformations in Fe-C bulk and nanowire systems: molecular dynamics simulation and free-energy calculations

Emilia Sak-Saracino¹, Binjun Wang¹, Nina Gunkelmann²,
Luis Sandoval³ and Herbert M. Urbassek¹

¹ Physics Department and Research Center OPTIMAS, University Kaiserslautern, D-67663
Kaiserslautern, Germany

² Institute for Multiscale Simulations, University Erlangen , D-91052 Erlangen, Germany

³Theoretical Division T-1, Los Alamos National Laboratory, Los Alamos, NM
87545, USA

Using molecular dynamics simulation, we study the austenite-martensite phase transition in the Fe-C bulk system for C contents up to 1 at% [1]. The systems are subjected to a heating/cooling cycle. The transition temperature can be determined from the hysteresis of the system volume with temperature. We observe that the martensite temperature decreases with C content, as in experiment. In the austenite phase we find strong twinning.

We supplement the studies with free-energy calculations based on both thermodynamic integration and perturbation theory [2]. The results agree well with our atomistic simulations.

We employ the Meyer-Entel potential for describing Fe-Fe interactions [3], while the pairwise potential by Johnson et al. [4] was used to model Fe-C. C-C interact by the Tersoff potential.

In addition, we study nanowire systems in order to assess the influence of free surfaces on the mechanism of transformation [5].

The bulk system follows the Nishiyama-Wassermann path, while the Kurdjumov-Sachs orientation relationship is fulfilled in the nanowire. Under axial stress in nanowires, the martensite transformation is partially suppressed, creating strong plastic deformation.

This work is carried out in the Collaborative Research Center CRC 926 “Microscale Morphology of Component Surfaces”. Funding by Deutsche Forschungsgemeinschaft is gratefully acknowledged.

Figure 1: Dependence of the system volume on temperature during a heating / cooling cycle (bulk system). C concentrations are 0.3, 0.5, and 0.8 at %.

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Principal component analysis of necking in sintered nanoparticles

A. Dutta

S. N. Bose National Centre for Basic Sciences, Sector – III, Salt Lake, Kolkata -700098,
India

Sintering mechanism of nanoparticles have been a subject of wide interest owing to its role in the deciding their catalytic properties. Reduction of surface energy is believed to be the principal driving agent of nanosintering. Even though several attempts have been made to understand the underlying thermodynamics through modeling and atomistic simulations [1,2], expression of the kinetics remains a difficult problem. A major obstacle in this regard arises from the fact that the particles consist of thousands of atoms and the state of the system at any instant needs a very large number of variables to be expressed. Therefore, somewhat crude measurements like neck-width and radius of gyration are often used to specify the current state of the system.

In the present work, I propose the use of dimensionality reduction by means of principal component analysis [3] and employ the principal projection of atomic coordinates to express the instantaneous state of nanoparticles undergoing the process of sintering. Once the principal component of the atomic trajectories is obtained, other kinetic parameters, like the rate of sintering process, effective thermodynamic forces and the effective thermodynamic inertial are obtained easily. This technique has been applied for two cases: first, the sintering simulation is carried out under isothermal conditions and second, the sintering takes place under linearly rising temperature. The fundamental differences between these two modalities have been explained and they are analyzed from the perspective of their corresponding principal components.

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Reversible multiscale homogenization for obtaining effective strength-elastic properties of composite materials with incomplete set of initial data

Alexandr P. Sokolov¹, Vitaliy N. Schetinin¹, Vyatcheslav M. Makarenkov¹

¹Bauman Moscow State Technical University, Moscow, Russia

This work presents the continuation of series of research works about developing mathematical models of mechanical properties of composite materials [1,2] based on multiscale homogenization method or asymptotic averaging method (known under this name in Russian scientific journals). Like in previous works the effective strength-elastic properties of composites are the main objective, but the difference is that at it was made an attempt to handle the situation when the set of initial data is incomplete. New computational technique tries to estimate missing data first before making a decision of simplification the model of material of components of composite. New computational method and corresponding software implementation were built and some of its main features are presented here. This software was created to support the design process of new composite materials with predetermined properties. Expected that new computational method make it possible to increase the accuracy of final computed effective properties of modeled composite materials in comparison with experimental data in case when the set of initial data is incomplete (for example: strength-elastic properties of carbon fibers in transverse direction to the fiber axis are usually unknown). To find the solution of the problem in such case direct and inverse tasks of the mechanics of composites were solved together. All of these tasks were combined into the single network model of the whole task automatically by means of usage of developed software. New computational method was named Reversible multiscale homogenization (RMH). Some computational results are presented at Fig. 1.

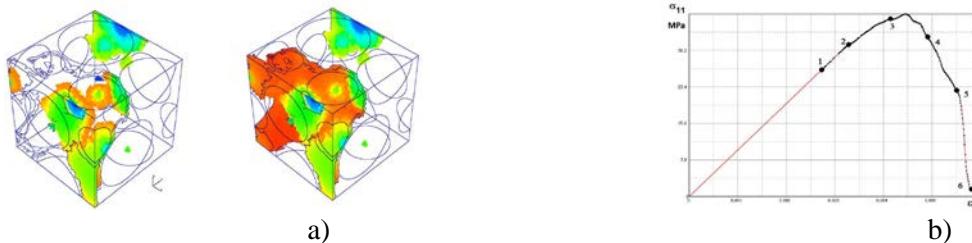


Figure 1: Computed Stress-strain diagram (a) of the model of unit cell of fiber-reinforced composite material (b). Destruction process simulation.

This work was performed with financial support from the Ministry of Education and Science of the Russian Federation (grant of President of Russian Federation MK-6573.2013.3 and State Order to Higher educational institutions □1.6260.2011).

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Bridging Crack Propagation at Atomistic and Mesoscopic Scale with Hybrid Multiscale Methods

Ross Stewart¹, Taolong Xu², Xiangguo Zeng², Jinghong Fan¹

¹Kazuo Inamori School of Engineering, Alfred University, New York, 14802, USA,

²College of Architecture and Environment, Sichuan University, Chengdu, 610065, China

Modern methodology to the modeling and simulation of crack propagation uses cohesive finite element methods (FEM) based on some type of cohesive constitutive laws. Physically, these laws should be developed based on the data obtained from atomistic crack simulation following the fact that crack propagation originates from the atomistic scale. However, reports show that directly use the data from atomistic-based simulation for FEM and meso- and macroscopic analysis is not practical. In most cases, one needs to revise the data such as reducing the obtained traction stress greatly or using empirical traction-displacement law to make the simulation convergence towards the realistic experimental results. This large discrepancy between the method based on physics and the empirical practice has motivated the present work to see whether this is caused by the simulation method itself. To reach this goal, we use a hybrid multiscale method which combines the concurrent generalized particle dynamics (GP) method proposed by Fan et al. since 2009^[1-4] and the bottom-up hierarchical method to transfer the GP-obtained physical parameters to the upper mesoscale FEM to investigate the meso- and microscopic crack propagation.

Here, the high-accuracy of atomistic crack simulation is essential and is warranted by the GP method. GP is one kind of coarse grain methods, but it has special features that the model consists of several particle domains of different scales with scale n=1 being atomistic scale and a large scale n=2,..m corresponds to continuum. The GP uniqueness include: First, the structure of all particle domains is the same as the atomistic domain and all calculations in the particle domain are conducted in its corresponding atomistic domain by the inverse mapping method. Second, the GP concept of scale duality can allow material being particles by a lumping process and being atoms when they are near, say, crack tips and interface by decomposition. This feature makes GP capable to extend MD models with sizes several orders larger than MD to raise its accuracy. To get detail physical data in terms of the crack propagation distance, Δa , from the tip O of pre-setting edge crack of length a, 20 rectangular rectangle atomistic subdomains I ($I=1, 2..20$) are divided for the area in front of the origin crack tip O. The center coordinate of each generic subdomain is $X_I = I * 20A$ where 20A is the width of the subdomain and its height is 80A. We take the subdomain I as the fundamental material object to observe the material behavior against the crack propagation when the current crack tip propagates to the subdomain, i.e., when $\Delta a = X_I$. In this way, for each subdomain I ($I=1, ..20$) three important physical variables are obtained: (1) The maximum resistance stress, $\sigma_{I-\max}$, of the material to against the crack passing through the subdomain I. (2) The rate of the resistance increase to reach $\sigma_{I-\max}$ measured by the initial slope of the stress-crack surface separation diagram (i.e., $\sigma_I \sim \delta$ curve). This parameter indicates the material hardening behavior to crack propagation. (3) The area under the $\sigma_I \sim \delta$ curve gives the energy release rate G_I which is an important energy variable for crack propagation. The GP results by drawing curves connected all the points of $\sigma_{I-\max}$ and G_I for all the 20 subdomain show interesting feature of the subdomain resistance. Inputting directly these GP-determined data sets for a cohesive finite element analysis of a compact fracture specimen, the critical force P as well as the critical stress intensity factor K_{IC} for the crack propagation is obtained. The result seems reasonable and encouraging. In the presentation, we will show more results in relation to using the hybrid method for the mixed mode loading, rate effects, and the FEM results from the data set at different subdomain as well as the discussion related to the common used cohesive constitutive law and methods.

Modeling of buckling under residual stresses by arlequin method and asymptotic numerical method: application to rolling of thin sheet metal

Kékéli Kpogan¹, Hamid Zahrouni¹, Michel Potier-Ferry¹, Hachmi B. Dhia²

¹Université de Lorraine, Laboratoire d'Etude des Microstructures et de Mécanique des Matériaux(LEM3), UMR CNRS 7239, Ile du Saulcy 57045 Metz, France ; DAMAS, Laboratory of Excellence on Design of Alloy Metals for low-mAss Structures, Université de Lorraine, France

²Ecole Centrale Paris, Laboratoire de Mécanique des Sols, Structures et Matériaux(MSSMat), Grande Voie des Vignes, 92295 Châtenay-Malabry Cedex, FRANCE

In this paper we present a new numerical technique to model the buckling phenomena under residual stresses induced by rolling process. This technique consists in coupling two finite element models: the first one consists in a three dimensional model based on 8-node tri-linear hexahedron which is used to model the three dimensional behaviour of the sheet in the roll bite; the second model is based on a shell formulation well adapted to large displacements and rotations, it will be used to compute buckling of the strip out of the roll bite [1]. We propose to couple these two models by using Arlequin method [2]. The originality of the proposed algorithm is that in the context of Arlequin method, the coupling area varies during the rolling process. Furthermore we use the asymptotic numerical method to perform the buckling computations taking into account geometrical nonlinearities in the shell model [3]. This technique allows one to solve nonlinear problems using high order algorithms well adapted to problems in the presence of instabilities.

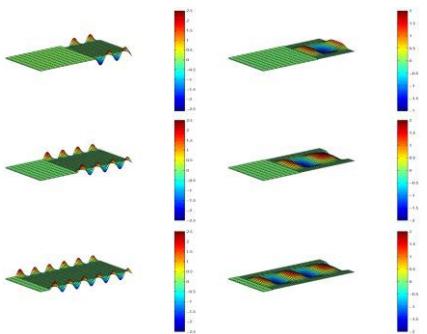


Figure 1: Propagation of the edge-waves flatness defects

The proposed algorithm is applied to some rolling cases where “edges-waves” and “center-waves” defects of the sheet are observed. The numerical results are compared with experimental data. To simulate the advance of the sheet in the process, the residual stress field is translated along the sheet. The position of the roll and the coupling area are located by a parameter which varies along the length of the sheet. The propagation of the edge-waves and the center-waves buckling are presented in the figure 1.

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Molecular Description of Mechanical Behavior for a Semicrystalline Polymer

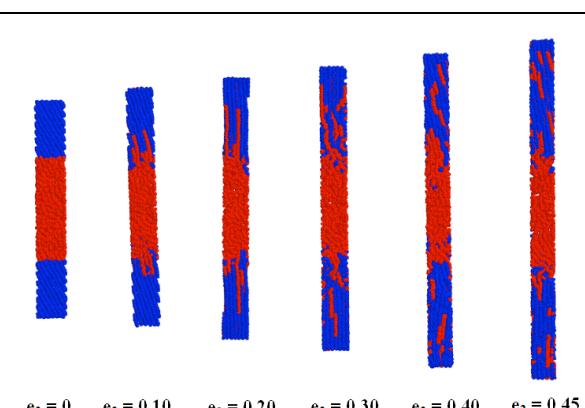
Gregory C. Rutledge¹, Jun Mo Kim¹, Sanghun Lee¹, C. Rebecca Locker²

¹Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

²ExxonMobil Research and Engineering Company, 1545 Route 22E, Annandale, NJ 08801, USA

Semicrystalline polymers, predominant among which are polyethylene (PE) and polypropylene as well as several other important engineering polymers, constitute the majority of plastics in production worldwide. These materials have achieved their commercial and technological success through a combination of low cost and remarkable mechanical properties. Nevertheless, despite decades of study and application, it remains a challenge to understand how these materials deform, and to model this deformation across the entire range of relevant length scales, from atomistic to macroscopic. We have recently proposed a fully atomistic Semicrystalline Model, based on our earlier Monte Carlo studies of the topology of the crystal/amorphous interphase,[1] and applied it to the study of large strain deformation of a semicrystalline PE using nonequilibrium molecular dynamics.[2] The model consists of a stack of alternating crystal and amorphous layers, as illustrated by the leftmost snapshot in the figure. Even a relatively simple deformation applied

macroscopically to the typical semicrystalline PE gives rise to a variety of locally distinct modes of deformation, due to the complex nature of the semicrystalline morphology, which may include spherulites and other, mesoscale structures. To unravel this behavior, we assess the mechanisms by which the Semicrystalline Model responds to large strain deformation for a variety of important modes of deformation, including extension, compression and shear, and different deformation rates. Consistent with the complex, seemingly contradictory conclusions drawn from experimental observations, a number of different mechanisms are observed, the importance of which varies with the mode of deformation, extent of strain, and strain



Snapshots of the Semicrystalline Model of PE, under uniaxial extension to different levels of strain, e_3 . Atoms initially located in the crystal domain are color-coded blue, while those initially in the noncrystalline domain are red. Periodic boundary conditions are employed in all directions.

rate. Both the crystalline and noncrystalline domains play important roles in the overall response. The concept of “bridging entanglements” is introduced to explain the hardening behavior observed at intermediate strains, just prior to yielding. In the realm of multiscale modeling, an effort by Ghazavizadeh and coworkers, using micromechanical homogenization methods, to dissociate the small strain noncrystalline response into amorphous and interphase hyper-elastic components suitable for use in finite element simulations may be described.[3]

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Tracking a glassy polymer on its energy landscape in the course of small time-dependent deformations

Maxime Delhorme¹, Nikolaos Lempesis², Georgios G. Vogiatzis³, Georgios C. Boulogouris⁴, Lambert C. A. van Breemen¹, Markus Hütter¹, Doros N. Theodorou³

¹Eindhoven University of Technology, Mechanical Engineering, Polymer Technology,
Eindhoven, The Netherlands

²Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, USA

³School of Chemical Engineering, National Technical University of Athens, Athens, Greece

⁴Department of Molecular Biology and Genetics, Democritus University of Thrace,
Alexandroupolis, Greece

Predicting the mechanical response of polymers in the glassy state upon deformation has been an ongoing project for 30 years. Many molecular, mesoscopic, and macroscopic simulation techniques have been employed to understand the different responses of glassy polymers: elastic regime, yielding, strain softening and hardening. In this contribution we present how the behavior of glassy atactic polystyrene can be investigated by considering the time evolution of molecular configurations on its potential energy landscape (PEL). In this approach, the polystyrene is represented in terms of an atomistic forcefield, while its PEL is described as basins (constructed around local energy minima) connected through saddle points.

In a first part, the linear elastic regime is studied using molecular dynamics simulations combined with the quasi-harmonic approximation (QHA)[1]. Stress-controlled uniaxial deformations are applied and the Young's modulus and Poisson ratio as well as their temperature dependencies, are extracted from the resulting changes in basin Gibbs energy. They are found in good agreement with experimental studies. The distortion of potential energy basins upon deformation is also quantified.

In a second part, the QHA is coupled with the Dynamic Integration of a Markovian Web (DIMW)[2] method. This approach tracks the temporal evolution of the distribution of the system's conformations among basins, via infrequent transitions (with rate constants down to $10^{-3}s^{-1}$) between them, starting off from a highly localized initial distribution. This simulation technique allows us to investigate the response of glassy atactic polystyrene to larger deformations, i.e beyond the elastic regime. Results for the stress-strain curve and underlying molecular mechanisms will be presented.

[1] N. Lempesis, G. G. Vogiatzis, G. C. Boulogouris, L. C. A. van Breemen, M. Hütter, and D. N. Theodorou, Mol. Phys. 111, 3641 (2013)

[2] G. C. Boulogouris and D. N. Theodorou, J. Chem Phys. 8, 084903 (2007)

Multiscale modelling of unfolded proteins

Ali Ghavami, Erik van der Giessen, P.R. Onck

Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

Fast and selective transportation of macromolecules between the cytoplasm and the nucleoplasm is essential for the proper functioning of eukaryotic cells. This is accomplished by the nuclear pore complex (NPC), a large molecular protein assembly with an estimated mass of 44-70 MDa that provides bidirectional pathways for passive transport of small molecules and facilitated transport of larger molecules. It is generally accepted that nuclear transport is mediated by natively unfolded proteins (FG-nups) that line the central channel of the NPC. These FG-nups have been shown to be essential for the viability of yeast and presumably all eukaryotes. However, how the biophysical properties of the FG-nups determine their function in passive and active transport is not well understood.

One of the reasons that have hampered the understanding of nuclear transport is the absence of experimental techniques that can probe the structure and dynamics of the disordered proteins inside the transport channel and during transport. This has led to the development of computational approaches to gain insight on the conformation of the FG-nups inside the NPC and their role in transport. Due to the large size of the system, high-resolution (all-atom) molecular dynamics simulations are restricted to study only a limited number of FG-nups. On the other hand, several low-resolution approaches have been used to study transport, but at the expense of losing detail at the scale of individual amino acids.

The goal of our work is to probe the full three-dimensional disordered domain of the yeast NPC by accounting for all FG-nups, each having a complete 20 amino acid resolution. To bridge the gap between the scale of individual amino acids and the scale of the full NPC, we have developed a one-bead-per-amino-acid molecular dynamics model [1,2]. The model captures the bonded interactions of the atomistic polypeptide chain as well as the non-bonded electrostatic and hydrophobic interactions between different aminoacids. The model is used to study the effect of the amino-acid sequence on the FG-nup conformation and to explore the relation between FG-nup distribution and cell viability (see Fig. 1). Finally, we will report recent results on the NPC energy barrier during passive and active transport.

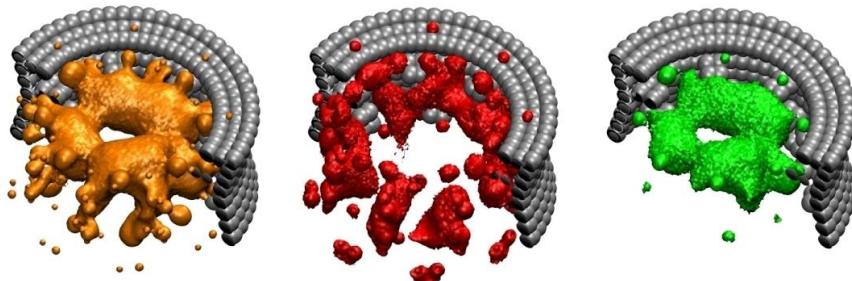


Fig. 1. The 3-dimensional distribution of amino-acids inside the NPC. All aminoacids (left), charged aminoacids (middle), FG-repeats (right).

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[2] A. Ghavami, E. van der Giessen and P.R. Onck, Probing the disordered domain of the nuclear pore complex through coarse-grained molecular dynamics simulations, submitted.

Prediction and Validation of Viscoelastic Properties of Polyurea with Systematically Coarse-Grained Molecular Dynamics

Jay Oswald¹, Vipin Agrawal¹, Kristin Holzworth², Wiroj Nantasetphong², Alireza V. Amirkhizi³, and Sia Nemat-Nasser²

¹ School for the Engineering of Matter, Transport and Energy, Arizona State University, Tempe, AZ 85287 USA

² Department of Mechanical and Aerospace Engineering, Center of Excellence for Advanced Materials, University of California, San Diego, La Jolla, CA 92093-0416, USA

³ University of Massachusetts Lowell, One University Avenue, Lowell, MA 01854

To improve understanding of the connection between microscopic structure and bulk properties of polyurea, a multiblock copolymer with excellent viscoelastic properties for the dissipation of shocks and ballistic impact loads, coarse-grained molecular dynamics simulations have been calibrated from atomistic simulations and validated against experiments conducted on a controlled, benchmark material formulated from pure methylene diphenyl diisocyanate (MDI).

A bead-spring model of polyurea, as shown in Figure 1, was systematically calibrated to match the structural distributions produced in molecular dynamics simulations of polyurea oligomers by the iterative Boltzmann inversion method. From canonical ensemble equilibrium simulations, the stress relaxation function was computed from the autocorrelation of virial stress fluctuations and rescaled in time by a time-dependent dynamic scaling function calibrated to match the self-diffusion of the atomistic and coarse-grained models.

Master curves computed from the stress relaxation function are then compared with dynamical mechanical analysis and ultrasonic wave propagation experiments mapped to a wide frequency range by time-temperature superposition principles with the Williams-Landel-Ferry equation. Computational simulations from monodisperse and polydisperse randomized unit cells representative of the benchmark polyurea both show excellent agreement with measurements over a multi-decade range of loading frequencies.

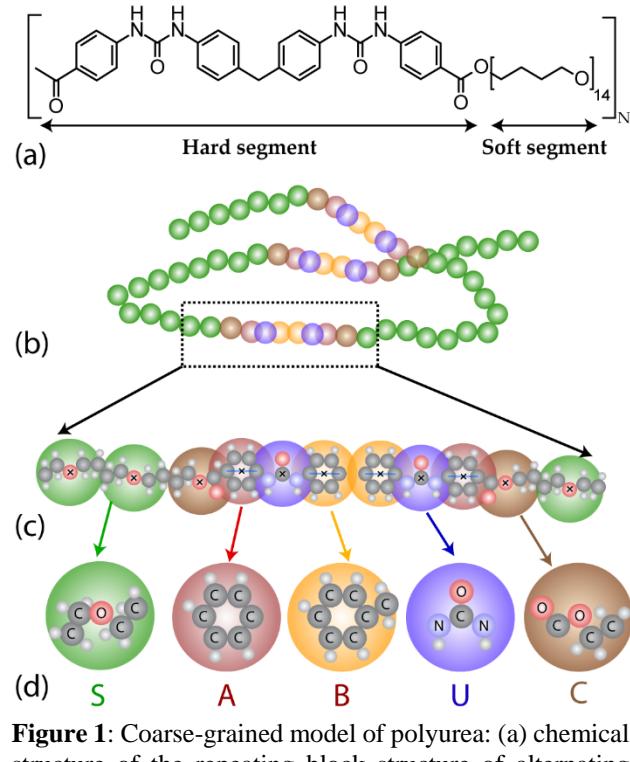


Figure 1: Coarse-grained model of polyurea: (a) chemical structure of the repeating block structure of alternating hard and soft segments, (b) figurative representation of a short polyurea chain composed of coarse-grained beads, (c) coarse-grained mapping of hard and soft segments of polyurea, (d) chemical structure of coarse-grained beads.

The authors gratefully acknowledge support from the Office of Naval Research under grant number N00014-09-1-1126 to University of California, San Diego.

Mechanical Properties of Biological Nanotubes with Multiscale Coarse-grained Models

Shyam Badu¹, Roderik Melnik¹, Maxim V Paliy², Sanjay Prabhakar¹, Bruce A Shapiro³

¹M2 Net lab, Wilfrid Laurier University, Waterloo, ON N2L 3C5,

²Department of Chemistry, University of Western Ontario, London, ON,

³Center for Cancer Research Nanobiology Program, Frederick, MD 21702, USA

The development of coarse-grained models leads to a possibility of explaining the properties of complex biological systems at large scales. Here we model the coarse-grained structures of RNA nanotubes built from the double strand RNA building blocks. An example of such a structure is shown in Figure 1. The self assembly of these biological nanostructures is straightforward due to high flexibility of RNA molecules. As far as the mechanical properties are concerned, in our earlier study the calculation of elastic properties, using the all atom Molecular Dynamics (MD) simulations, have been successfully performed for the RNA nanoring [1, 2]. The study of mechanical properties for large RNA nanoclusters is the subject of increasing interest to make these structures experimentally and biomedically compatible for their application. In view of this, we also study the elastic properties of these structures, including the energy-strain dependence of the RNA nanotube and its 2D surface modulus (i.e bulk modulus), using the MD simulations. In order to calculate these elastic properties of RNA nanotubes we carry out simulations of forced dynamics of nanocluster systems using NAMD and VMD and calculate the variation of energy as a function of strain. In particular, we apply the compressive and expansive forces via change in pressure of the system during Molecular Dynamics simulations. The elastic properties, calculated from our Molecular Dynamics simulations, are compared to the experiment.

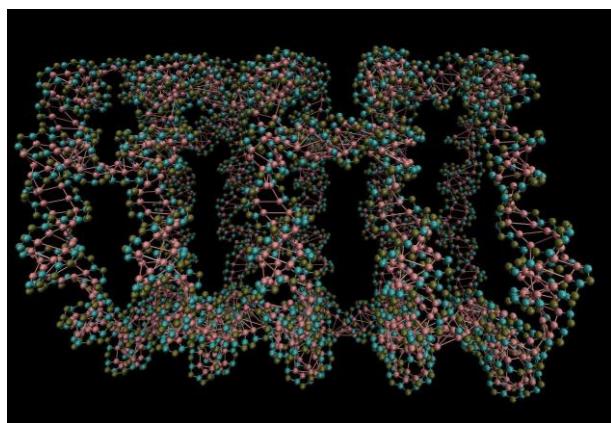


Figure 1: (a) Coarse-graining model for a five ring RNA nanotube

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Molecular Dynamics study on moisture-dependent properties of amorphous cellulose extended to poromechanical model

Karol Kulasinski¹, Sinan Keten², Sergey V. Churakov³, Dominique Derome⁴,
Jan Carmeliet^{1,4}

¹ ETH Zürich, Zürich 8093, Switzerland

² Northwestern University, Evanston, IL 60208-3109, USA

³ Paul Scherrer Institute, Villigen 5232, Switzerland

⁴ Empa, Dübendorf 8600, Switzerland

Amorphous cellulose is a soft polymeric material that can be found mostly in the outer regions of cellulose microfibrils, that give their strength to the cell wall of higher plants. Being strongly hydrophilic, amorphous cellulose adsorbs water in the nanopores and forms hydrogen bonds between available hydroxyl sites and water molecules. The adsorption of water influences many properties of this biopolymer and causes moisture swelling and stiffness decrease, two phenomena that are modelled.

The amorphous cellulose is constructed and simulated with Molecular Dynamics [1] in the full range of moisture content: from dry material to complete saturation. Explicit water molecules are put in the simulation box using simple Monte Carlo. The water is

found to break the hydrogen bonds within cellulose chains while increasing the porosity of the sample. Both swelling and weakening of the material are observed (Figure 1). The coupled mechanisms can be upscaled using a poromechanical approach, which is a rigorous way of taking into account the interaction of fluids with the solid matrix in porous materials, as per the following equations [2]:

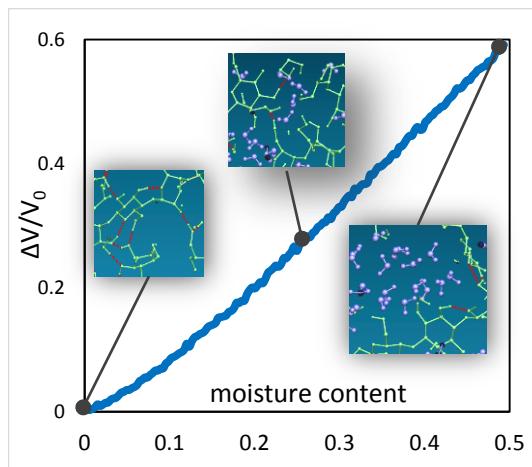


Figure 1: Volumetric swelling as a function of moisture content in amorphous cellulose.

compliance (C), Biot coefficient (B), and moisture capacity (M), as coupling constants. The coupling constants can be determined directly from the simulations.

The authors are grateful for the financial support of the Swiss National Science Foundation (SNF) under grants no. 125184 and 143601.

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$$d\epsilon = C d\sigma + B dp$$

$$du = B d\sigma + M dp$$

that relate strain (ϵ), stress (σ), moisture content (u) and pore pressure (p) using

Synchronized molecular dynamics simulation via macroscopic heat and momentum transfer for non-isothermal polymeric flows

Shugo Yasuda¹, Ryoichi Yamamoto²

¹Graduate School of Simulation Studies, University of Hyogo, Kobe 650-0047, Japan

²Department of Chemical Engineering, Kyoto University, Kyoto 615-8510, Japan

The synchronized molecular dynamics simulation via macroscopic heat and momentum transfer is applied to the non-isothermal polymeric flows. In this method, the molecular dynamics simulations are assigned to small fluid elements to calculate the local stresses and temperatures and are synchronized at certain time intervals to satisfy the macroscopic heat- and momentum- transport equations.

The rheological properties and conformation of polymer chains coupled with the local viscous heating are investigated with a non-dimensional parameter, i.e., the Nahme-Griffith number, which is defined by the ratio of the viscous heating to the thermal conduction at the characteristic temperature required to sufficiently change the viscosity.

The simulation results for polymer lubrication demonstrate that strong shear thinning and transitional behavior of the conformation of the polymer chains occur with a rapid temperature rise when the Nahme-Griffith number exceeds unity. The results also clarify that the reentrant transition of the linear stress-optical relation occurs for large shear stresses due to the coupling of the conformation of polymer chains and heat generation under shear flows.[1] The effects of the entanglement of polymer chains and thermal conductivity on the rheological property and conformation of the polymer chains are also discussed in the presentation.

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Mechanical and Thermal Properties of Cross-Linked Phenolic Resins: Towards a Multiscale Approach for Thermal Protection Materials for Space Vehicles

Joshua Monk¹, John Lawson¹, Justin Haskins¹, Charles Bauschlicher²

¹Thermal Protection Materials Branch, NASA Ames Research Center, Moffett Field, CA
94035

²Entry Systems and Technology Division, NASA Ames Research Center, Moffett Field,
CA 94035

Elastic and thermal properties of thermoset materials are critical in the design and performance of ablative composites which are used as heat shields to protect space vehicles during atmospheric reentry. To gain insight into the design of these materials for extreme environments, it is valuable to understand how the chemical make-up at the nano-scale can influence the thermal and mechanical bulk properties. In this study, molecular dynamics simulations of bulk phenolic systems were performed to produce key input parameters for constitutive models for microstructural simulations. An atomistic computational study allows us to manipulate the structural make-up of individual phenolic chains as well as generate various cross-linked (or cured) systems. An all-atom force field was chosen to investigate how the strength and thermal conductivity of the phenolic material varies as a function of the degree of cross-linking and chemical make-up of the phenolic chains. Small-scale mechanical tests were performed to compute various moduli for the phenolic systems above and below the glass transition at varied degrees of cross-linking. The thermal conductivity was obtained using the Green-Kubo approach for the virgin and cured phenolic systems. Atomistic parameters were used in continuum, microstructural computations to determine mechanical and thermal composite level properties.

Linking Composition and Topology to Mechanical Properties of Cross-linked Biopolymer Networks

G. Zagar, P.R. Onck, E. Van der Giessen

Zernike Institute for Advanced Materials, Groningen, the Netherlands

Biopolymer networks, such as those constituting the cytoskeleton of a cell, exhibit interesting mechanical properties, such as a remarkable nonlinear strain-stiffening when subjected to large deformations. The overall properties depend on the composition of the network in terms of concentrations of filaments and cross-linkers, their respective properties and the microstructure that they form.

We present a comprehensive treatment of an archetypical biopolymer network comprising filamentous actin, by using a combination of a simple theory to connect composition to topology and numerical simulations of discrete filament network models. Particular attention is given to the characteristics and physical origin of strain stiffening of these networks, in dependence on the ratio between cross-link versus filament

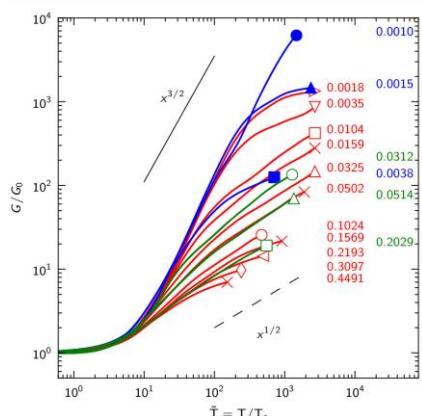


Figure 1: Normalized network stiffness as function of applied stress for different values of the material and topology dependent parameter.

properties. It will be shown that we can predict a broad range of behavior observed in in-vitro reconstituted networks. In addition, we provide simple models to understand the characteristic scaling laws for stiffening seen in simulations and in experiments.

It turns out that, eventually, the behavior of a network is determined by only a small number of parameters that combine information on constitution and topology. This insight culminates in master curves, shown on the left, from which the entire stress-strain response can be predicted just using known data on the stiffness of the constituents and on measurable concentrations.

Almost Ab Initio Nonlinear Rheology of Entangled Polymers

Marat Andreev, Rudi Steenbakkers, Jay D. Schieber

Center for Molecular Study of Condensed Soft Matter (μ CoSM) Illinois Institute of Technology 3440 S. Dearborn St., Chicago, Illinois, U.S.A.

We use a slip-link picture for entangled polymers to derive a set of integrated, well-defined mathematical models on varying levels of description. Each level is applicable to any chain architecture, molecular weight, or blend, and under any flow. For an atomistic basis we exploit primitive-path analysis [Everaers et al. *Science* (2004); Kröger *Comp.Phys.Comm.* (2005); Tzoumanekas and Theodorou *Macromolecules* (2006)], whereby one freezes the ends of the polymer chains in an atomistic simulation, and shrinks the length of all the chains while simultaneously preventing chain crossings. From the resulting statistics we are able to determine all but a single (monomeric friction) parameter in our most-detailed slip-link model. We then go through a series of coarse-graining steps to create a hierarchy of integrated slip-link models. This procedure produces a mathematical model whose calculations are 3 million times faster than the most-detailed level of description, and 20 billion times faster than atomistic-level calculations. Using any single member of the hierarchy, we can then fit our friction parameter to a dynamic equilibrium experiment of any chain molecular weight and chain architecture, and make predictions of the nonlinear rheology of any chain architecture, molecular weight, blends of these and in any flow field. Predictions of experiment are quantitative. More important than computational speed up is the dramatic reduction in the number of dynamic variables necessary to describe the system, which suggests a deep understanding of the physics of entangled polymers. Given that the time scales of the adjusted friction are order nanoseconds, truly ab initio rheology predictions of entangled homopolymers now seem possible.

Large scale Brownian dynamics simulations of complex viscoelastic Soft Matter

Wim Briels

University of Twente, Enschede, The Netherlands

In order to describe flow of soft matter in complex geometries detailed information is needed about how stresses depend on velocity gradients and concentration. Besides this, often compressible flow equations must be solved concomitantly with diffusion equations.

Since it is difficult to collect the appropriate information and to accurately represent it with a constitutive model, it is natural to develop particle based methods that can be applied to large portions of matter. In order to achieve this goal large, mesoscale objects must be represented by single particles, which move such that both the thermodynamic and the viscoelastic properties of the system are recovered. The latter usually result from a strong interplay between the dynamics at a large range of time and length scales of those degrees of freedom that have been eliminated in the coarse description. I will discuss a model in which the particles are dressed with additional variables which roughly reinstate the effects of the eliminated degrees of freedom.

I will describe the nature of the forces on the centers of mass of star polymers in a Kremer-Grest star polymer melt and present a model which is able to capture the global features.

In a second part I will present a model of deformable particles which is able to describe both the linear and the non-linear rheology of entangled polymer solutions.

Finally, I will present a Galilean invariant method to perform Brownian dynamics simulations of flowing soft matter in complex geometries.

Dynamic Phase diagram of soft colloids

Sudipta Gupta^{1,2}, Jörg Stellbrink¹, Manuel Camargo³, Jürgen Allgaier¹, Dieter Richter¹

¹JCNS-1 and ICS-1, Forschungszentrum Jülich, 52425 Jülich, Germany

²JCNS-SNS-Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

³Centro de Investigaciones en Ciencias Básicas y Aplicadas, Universidad Antonio Nariño, Kra 3 Este 47a-15 Bogotá, Colombia.

Soft colloids, e.g. polymer-coated silica particles, block copolymer micelles, star polymers etc., are hybrids between (linear) polymer chains and (hard sphere) colloids. Due to this hybrid nature, soft colloids macroscopically show interesting (phase) behaviour resulting from its unique microscopic structure. The combination of polymer-like properties, i.e. the formation of (transient) geometric constraints due to overlapping polymeric coronas and direct colloidal interactions due to the (hard) core in particular affects flow properties and non-equilibrium behaviour of soft colloids. Therefore soft colloids are frequently used in many technical applications (paints, shampoos, motor oils, polymer nano-composites etc.). The task of fundamental research on soft colloids is to investigate the basic principles of the so-called structure-property-relationship (SPR) that finally enables tailoring material properties for technical applications. Their macroscopic phase behavior and non-equilibrium flow properties are directly linked to the details of their unique microscopic structure.

We present a comprehensive study employing several experimental techniques covering micro-, meso- and macroscopic length and time scales (like SANS, DLS and rheology), which enables us to take the first step forward in establishing an generalized view in terms of structure property relationship (SPR) and structural dynamics of soft colloids. Using “frozen” block copolymer micelles as tunable model systems of the latter ones, we varied/tuned its aggregation number (N_{agg}), and consequently its softness, by changing the (solvophilic-solvophobic) block ratio $m:n$ (Fig. 1) from a symmetric to a highly asymmetric regime. Based on a simple and general coarse-grained model of the (micelle-micelle) interaction potential, we verify the significance of the interaction length σ_{int} as generic feature for this class of colloids, and elaborate a comprehensive comparison between theoretical [1,2] and experimental information [3-5] describing both structure and dynamics, without requiring adjustable parameters, and covering a broad range of volume fractions and regimes from soft star-like to hard sphere-like colloids.

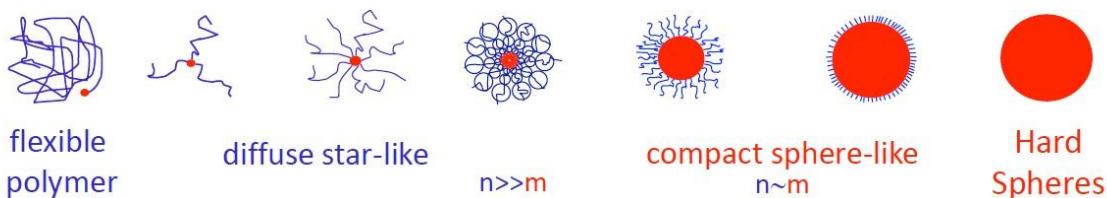


Fig. 1: Schematic representation of morphological evolution of star-like block copolymer micelles in selective solvent, from polymer-like Gaussian coil ($N_{agg} = 1,2$) to colloid like hard sphere ($N_{agg} \rightarrow \infty$). n and m denote the number of repetitive units for the solvophilic (blue) and the solvophobic (red) blocks, respectively.

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Thermodynamics of reductions in multiscale modeling

Miroslav Grmela

École Polytechnique de Montréal, C.P.6079 succ. Centre-ville Montréal, H3C 3A7,
Québec, Canada

Let $\mathcal{L}_1, \mathcal{L}_2, \mathcal{L}_3$ be three well established (i.e. well tested with experimental observations) levels of description ordered from the most microscopic to the least microscopic. By comparing solutions to the time evolution equations $\mathcal{E}_1, \mathcal{E}_2, \mathcal{E}_3$ on all three levels we can find relations $\mathcal{L}_1 \rightarrow \mathcal{L}_2 \rightarrow \mathcal{L}_3$ and $\mathcal{L}_1 \rightarrow \mathcal{L}_3$. Such relations give us: (i) relations $\mathcal{E}_1 \rightarrow \mathcal{E}_2 \rightarrow \mathcal{E}_3$ and $\mathcal{E}_1 \rightarrow \mathcal{E}_3$, (ii) relations $\mathcal{P}_1 \rightarrow \mathcal{P}_2 \rightarrow \mathcal{P}_3$ and $\mathcal{P}_1 \rightarrow \mathcal{P}_3$, where \mathcal{P} stands for material parameters, i.e. the parameters with which the individual nature of the system under consideration is expressed, and (iii) six entropies, namely $s^{(1 \rightarrow 2)}, s^{(1 \rightarrow 3)}, s^{(2 \rightarrow 3)}$ and $S^{(3 \leftarrow 1)}, S^{(3 \leftarrow 2)}, S^{(2 \leftarrow 1)}$. The entropies $s^{(i \rightarrow j)}, i < j$ are potentials generating the approach (as time goes to infinity) of the level \mathcal{L}_i to the level \mathcal{L}_j and $S^{(i \leftarrow j)}, i > j$ are the entropies $s^{(j \rightarrow i)}$ evaluated at the states on the level \mathcal{L}_i that are reached in the approach $\mathcal{L}_j \rightarrow \mathcal{L}_i$. These six entropies represent the multiscale thermodynamics corresponding to the sequence of levels $\mathcal{L}_1, \mathcal{L}_2, \mathcal{L}_3$.

In my talk I will illustrate this multiscale thermodynamics (and provide some of its applications) on the example of $\mathcal{L}_1 \equiv$ level of description of complex fluids on which inertia of the internal structure is taken into account, $\mathcal{L}_2 \equiv$ level of description of complex fluids without the inertia, and $\mathcal{L}_3 \equiv$ equilibrium thermodynamics of complex fluids.

A materials genome approach to engineering functional suprabiomolecular nanotubes

Luis Ruiz, Sinan Keten

Dept. of Civil & Environmental Engineering and Mechanical Engineering, Northwestern University, 2145 Sheridan Road TECH A133, Evanston, IL, 60208

Nanoscale biomolecular building blocks have unique chemical and structural features that may help overcome some of the persistent challenges in designing tough nanocomposites and separation membranes inspired from biology. However, it remains costly and time-consuming to uncover the hierarchical self-assembly principles and emergent properties of these novel systems through experimental trial-and-error. In pursuit of an accelerated pathway towards discovering novel biomolecular materials through computer simulations, this talk will summarize recent advances in predicting the assembly, mechanofunctionality, and transport capabilities of hybrid nanocomposites that blend the best aspects of biomolecules and engineering polymers. This talk will focus on polymer-conjugated cyclic peptide nanotubes (pc-CPNs) that self-assemble into biomimetic artificial nanochannels in polymer membranes. Predictive analytical relationships validated by both simulation and experiments will be presented to explain the breaking mechanisms and growth processes of pc-CPNs at the kinetic and thermodynamic limits. These discussions will culminate in a concept model that illustrates how the entropic forces arising from polymer conjugation could be utilized in directing the self-assembly of macrocycles towards nanochannels with spatially tunable interiors and thus engineered transport properties. More broadly, phase diagrams and kinetic growth models obtained provide general insight into the physics and mechanics of functional low-dimensional assemblies of soft nanoscale building blocks.

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Self-regulation in structure formation

Peter C. Rozemond, Martin van Drongelen, Gerrit W.M. Peters

Eindhoven University of Technology, Eindhoven, The Netherlands

Understanding and predicting structure development during flow is key in the processing of semi-crystalline polymers. It is well known that subjecting a polymer melt to a channel flow below the melting point, relevant for e.g. injection molding, yields a non-homogeneous microstructure in the sample after cooling. Most notably, a layer with high orientation appears in the high shear rate region near the walls [1]. The crystalline structure in this shear layer contains a high density of so-called shish-kebabs, consisting of a fibrous backbone (the shish, diameter of ~20 nm, length in access of 1 μm , inter-shish distance ~100 nm) with lamellar overgrowth (kebabs). It has been shown that this effect has a dramatic effect on the final properties of injection-molded products [2].

In this work we study the formation of shish-kebabs. To this end, experiments were performed at the European Synchrotron Radiation Facility to probe crystallization kinetics in a well-defined slit flow with high shear rates ($\sim 1000 \text{ s}^{-1}$) with in-situ Wide-Angle X-Ray Diffraction. Simultaneously the rheology is probed by means of a pressure drop measurement over the channel. It is shown that due to formation of shish, the viscosity of the polymer melt is strongly increased, freezing the crystalline structure in at a certain density, thus placing an upper limit on the shish density.

These findings are incorporated in a model to describe the flow-induced crystallization process. Formation of crystalline structures is governed by deformation on a continuum level. Rheological properties depend on crystalline structure. The model is extensively validated with experimental data. The coupling between continuum rheological properties and crystalline structure on the microscale proves to be a vital ingredient for modeling structure formation in polymer melts.

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Local stress calculations in biomembranes: importance of force decomposition

Alejandro Torres-Sánchez¹, Juan M. Vanegas², Marino Arroyo¹

¹LaCàN, Universitat Politècnica de Catalunya-BarcelonaTech, Barcelona 08034, Spain

²Sandia National Laboratories, Albuquerque, NM87123, USA

We present a molecular dynamics study of the microscopic stress in biomembranes. The microscopic stress in lipid bilayers has been a subject of profound studies due to its connections with protein function and different elastic properties, as predicted by thermodynamic approaches [1]. It also exemplifies the link between continuum and atomistic models through the so-called Irving-Kirkwood-Noll (IKN) procedure [2,3].

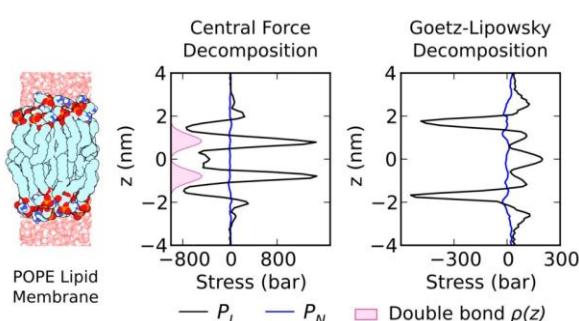


Figure 1: A comparison between lateral (P_L) and normal (P_N) stress profiles for a POPE bilayer with two different force decompositions.

Despite being an old field, the theory of the microscopic stress is not fully settled [4]. A key step in the IKN procedure is the decomposition of forces from multibody potentials. However, different decompositions lead to possibly different stresses differing by a divergence-free field [4,5]. Moreover, some force decompositions lead to non-symmetric stresses that are difficult to interpret from the continuum mechanics of simple bodies. Only recently have a force decomposition, the so-called central force decomposition (CFD), been

presented that produces symmetric stresses from first principles [5].

In a recent work [6], we compared stress profiles from the CFD and another common decomposition [7] in lipid bilayers. This common decomposition produces non-symmetric stresses for chiral lipids and very different stress profiles compared to those of CFD. This unsettling subjectivity of stress profiles calls for a reexamination of the physical grounds of the different force decompositions. An alternative approach to the IKN procedure based on equilibrium statistical mechanics may show that only the CFD leads to a valid stress from a thermodynamic viewpoint.

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Rheology and shear-induced diffusion in dense suspensions of red blood cells

F. Varnik¹, Markus Gross²

¹Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Germany

²Max Planck Institute for Intelligent Systems, Stuttgart, Germany

While the relaxation dynamics and rheological properties of hard sphere colloidal suspensions is rather well understood, a full theoretical understanding of these issues in the case of soft objects is still lacking. Deformability introduces additional time scales and degrees of freedom and thus makes a theoretical description more complicated [1].

This talk addresses this issue. A new effective medium theory is presented that takes accounts of effects arising from the deformability of a single object. The theory is then applied to a suspension of red blood cells (RBC). It is shown via computer simulations that the theory correctly describes the rheological response of the RBC suspension over a wide range of packing fractions and shear rates [2]. Moreover, shear-induced diffusion which becomes prominent at high concentrations is also investigated. A simple argument based on dissipation balance is used to predict the dependence of diffusion on imposed shear rate and packing fraction. These predictions are found to be in good agreement with results obtained from simulations [3].

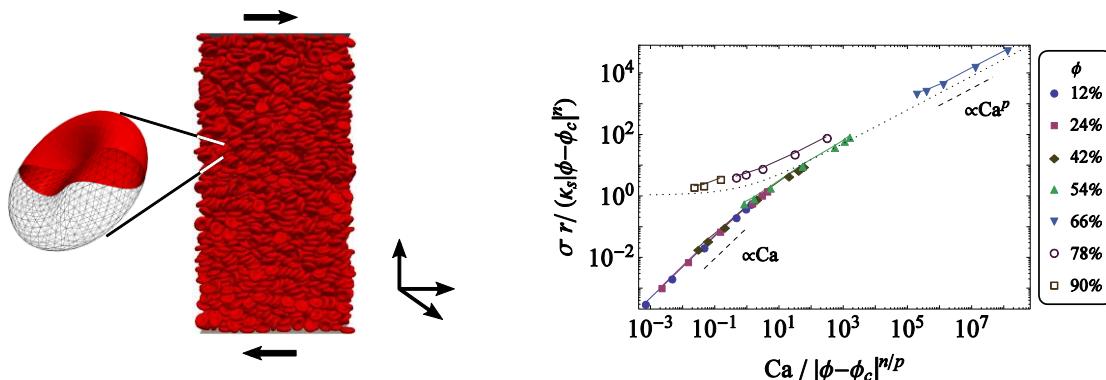


Figure 1: Left: A snapshot of the simulation box and a sketch of the surface mesh of a red blood cell. Right: Critical scaling plot of the suspension stress versus capillary number. Our data are in line with a critical jamming scenario with a critical packing fraction of $\phi_c=0.66$. Figures adopted from [2].

This work is supported by the German Research foundation (DFG) via the project Va205/5-2.

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Meso-scale Dynamic of Polymeric Glasses: Constitutive Models that Acknowledge Dynamic Heterogeneity

J.M. Caruthers

School of Chemical Engineering, Purdue University

The current physical picture of the glassy state involves dynamic heterogeneity, where nanoscopic regions of the glass have order-of-magnitude differences in local mobility even though the structure appears to be uniform. Moreover, these nanoscopic regions evolve with time where high mobility regions can become low mobility regions and vice-versa. Dynamic heterogeneity provides a critical challenge to the traditional nonlinear viscoelastic or viscoplastic continuum models where both temporal and spatial fluctuations are smoothed out as a result of the continuum postulate. In order to acknowledge dynamic heterogeneity, a Stochastic Constitutive Model (SCM) has been developed to describe the nonlinear viscoelastic behavior of polymeric glasses, where temporal fluctuations are explicitly included but spatially fluctuations are averaged in a mean field like approximation. In addition to the fluctuations, a key feature of the SCM is that the local mobility depends upon the local state of the material (e.g. local stress and local entropy) vs. the nonlinear viscoelastic/viscoelastic models where macroscopic mobility depends upon the macroscopic state. The SCM is able to describe a number of nonlinear relaxation phenomena that cannot be predicted by traditional nonlinear viscoelastic/vicoplastic models, including (i) post-yield stress softening and its dependence on annealing time, (ii) the inversion of the strain dependence of nonlinear stress relaxation with the loading rate and (iii) tertiary creep and creep-recovery. Because the SCM includes fluctuations, the SCM may provide an effective mesoscopic link between molecular dynamic simulations where fluctuations are significant and continuum models that can predict the response for engineering useful times.

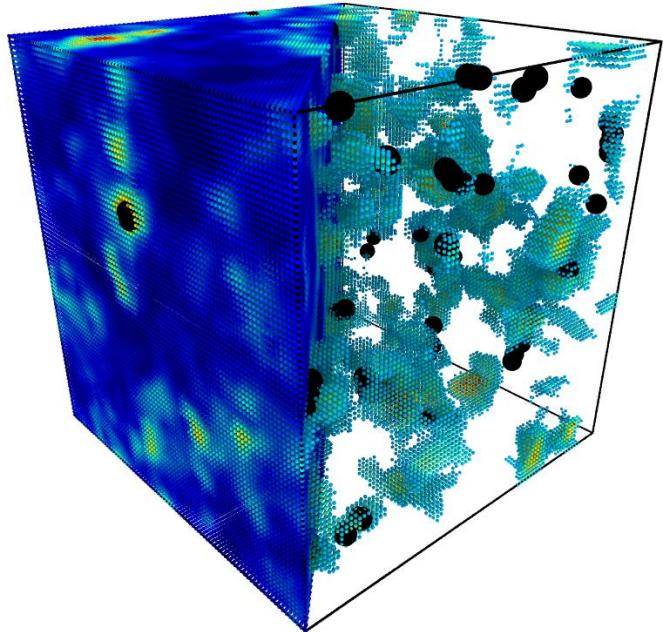
Predicting segmental relaxation in quiescent and deformed polymer glasses

Anton Smessaert and Joerg Rottler

Department of Physics and Astronomy, The University of British Columbia,
6224 Agricultural Road, Vancouver, British Columbia V6T 1Z4, Canada

Structural recovery and plastic flow in polymer glasses occurs in a highly heterogeneous fashion through cooperative segmental relaxation events. While simulations have elucidated many aspects of this dynamical heterogeneity, the connection to structural properties has remained elusive. In this contribution, we show that the low energy

vibrational spectrum of the amorphous polymer can be used to predict the location and direction of segmental motion. A “softness field” is constructed from a superposition of the amplitudes of the lowest energy normal modes, which reveals essentially the elastic heterogeneity of the solid. Segmental relaxation events are identified as discrete “hops” of particles out of their local cages with a numerical technique developed previously [1]. We find that these hops occur preferentially at the softest regions in the polymer. Moreover, the *direction* of the hops can be accurately predicted from the direction of the normal mode polarization field (a harmonic property). Thus, the soft modes predict not only where the



Softness map of a polymer glass with softness increasing from blue to red. Cutaway shows only the top 10% softest regions. Black dots indicate the location of structural relaxation events in a small time interval right after the map was constructed.

polymer will relax, but also how. We explore the evolution of the correlation between softness field and relaxation events for different temperatures, different ages, and for active deformation with molecular dynamics simulations of a coarse-grained bead-spring polymer model. The softness field decays very slowly (logarithmically) on time scales much longer than the vibrational timescale, which indicates that it is a robust structural feature suitable to detect local regions vulnerable to irreversible relaxation events. Parallel work on models for amorphous metals suggests that these “soft spots” are indeed the counterpart of dislocations in disordered materials.

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Filled polymer glasses; the sum of its parts?

Sam Krop, Han. E.H. Meijer, Lambert C.A. van Breemen

Eindhoven University of Technology, Mechanical Engineering, Polymer Technology,
5600MB Eindhoven, The Netherlands

Since polymers play an increasingly important role in both structural and tribological applications, understanding their intrinsic mechanical response is key [1]. Therefore, much effort has gone into the development of models, such as the Eindhoven Glassy Polymer (EGP) model [2], which captures the polymers' response quantitatively. In practice, however, these polymers are filled, e.g. with colorants and impact modifiers.

To characterize the effect of filler particles on the intrinsic mechanical response, model systems of polycarbonate and epoxy are filled with either hard (TiO_2) or soft (MBS) particles are tested in uniaxial compression. Since experimentally only macroscopic effects are probed, simulations are needed to reveal the effects at the inter-particle level. Therefore, representative volume elements (RVEs) are constructed, where the matrix material is modeled with the EGP model and the fillers with their individual mechanical properties.

Comparing the simulated response of the RVEs with the experiments shows that the macroscopic response is captured well. Only at large deformations the simulations fail to capture the response of the hard-filled system. Moreover, the simulations clearly show that all the rate-dependence originates from the polymer matrix; fillers only change the magnitude of stress.

In the simulations it is assumed that the particles perfectly adhere to the matrix. In reality, for the hard-filled system, this interface or the polymer itself will fail at some point; the local strains significantly exceed the macroscopic applied deformation. But since the local deformations are now available quantifying the onset of failure is within reach. Subsequently, this method proves to be beneficial as a design tool too: different scenarios, e.g. altering or even combining filler properties, are easily tested without the need of tedious experiments.

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Hierarchical composites reinforced with microscopic fibers and nanotubes: the modelling challenge.

Valentin S. Romanov, Stepan V. Lomov, Ignaas Verpoest, Larissa Gorbatikh

Department of Materials Engineering (MTM), University of Leuven (KU Leuven),
Kasteelpark Arenberg 44 - bus 2450 B-3001 Leuven, Belgium

The toughness improvement of fiber reinforced polymer composites is an important area of research in the field of composites. Despite superior strength and stiffness, these materials are susceptible to early onset of matrix cracking. The cracks start as debonding at the fiber/matrix interface where high stress concentrations are generated and then develop through the matrix into larger cracks. This type of damage can be suppressed by adding carbon nanotubes (CNTs) into the polymer matrix of the composite or by growing CNTs directly on the fiber surface [1]. There are several possible explanations for the toughening effect. One of them is a re-distribution of stresses on the micro-scale caused by the presence of CNTs.

In order to investigate a hypothesis that CNTs can have a significant effect on stress concentrations, we developed an advanced two-scale model. The unique feature of this model is that microscopic fibers and nanotubes are modelled simultaneously. The challenge lies in modeling of reinforcements with a significant difference in relative dimensions—diameters carbon fibers and CNTs differ more than 700 times. Recent literature survey showed that there are no models of nano-engineered composites that are able to meet such a requirement.

In the present work we introduce the 3D FE model, in which CNTs are represented as 3D solid bodies implemented into a polymer already reinforced with microscopic carbon fibers. It was achieved with the embedded regions (ER) technique that allows for co-existence of two independent FE meshes. The model does not require intermediate homogenization steps or transferring of parameters from the nanotube scale to the fiber scale. The effect of different CNT configurations on stress fields in the matrix is investigated.

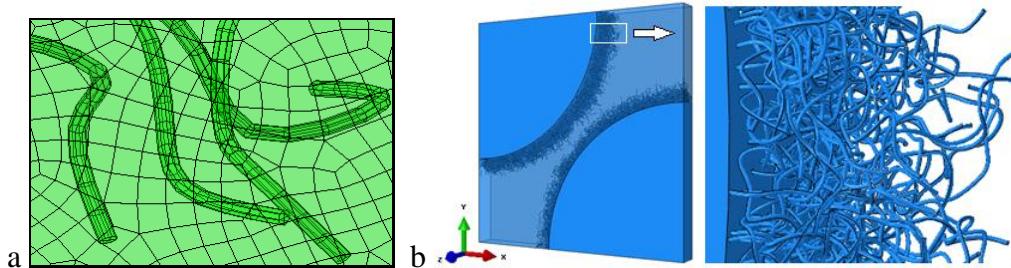


Figure 1: (a) ER technique - the combination of two independently created FE meshes: CNT mesh and matrix mesh; (b) a 3D model of a unidirectional fiber reinforced composite with introduced CNTs showing the unit cell and the zoom-in on the geometry of the grown CNT forests on the fiber surfaces.

This model was developed in the IMS&CPS project (Innovative Material Synergies & Composite Processing Strategies) funded by the EU FP7 program. The analysis of CNT configurations was performed in the framework of the GOA/10/004 project (New model-based concepts for nano-engineered polymer composites) funded by the Research Council of KU Leuven.

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Concurrent two-scale model for the elasto-viscoplastic behavior of silica-filled rubber

Markus Hütter, Mykhailo Semkiv

Eindhoven University of Technology, Department of Mechanical Engineering,
Eindhoven, The Netherlands

A dynamic two-scale model for describing the mechanical behavior of silica-filled elastomers is developed. The closed system of evolution equations is derived, consisting of evolution equations for the macroscopic momentum density, the temperature, the macroscopic deformation gradient and a mesoscale structure variable. The latter is given by the product of the number density of filler particles and the distribution function of particle-particle separation vectors. The system under consideration is strongly non-linear. The origins of non-linearity are the following: (i) the rubbery matrix, in which the particles are imbedded, expresses non-linear elastic effects; (ii) around the nanofillers, the matrix material forms glassy layers that overlap for sufficiently close particles, and consequently create temporary glassy bridges with a characteristic time scale that depends on the applied load (e.g. [1]). Extending earlier efforts to model nonisothermal and finite-deformation elasto-viscoplasticity [2, 3] with the GENERIC framework of nonequilibrium thermodynamics [4, 5, 6], we obtain the constitutive relation for the macroscopic stress tensor in terms of the filler-particle arrangement. Moreover, the filler-particle dynamics and the thermodynamic driving force for the breaking and recombination of the glassy bridges are derived. Finally, it is shown that the mesoscale dynamics can be cast into a stochastic differential equation in 6-dimensional space, amendable to Brownian dynamics-type simulations on the filler-particle level.

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Micromechanics modeling of the linear viscoelasticity of nano-reinforced polymers with an interphase

Julie Diani, Pierre Gilormini

PIMM, UMR 8006 CNRS, Arts et Métiers ParisTech, 151 bd de l'hôpital, 75013 Paris,
FRANCE

A first study [1] showed experimental evidences and micromechanics analysis supporting the existence in carbon-black filled styrene butadiene rubbers, of a filler-rubber interphase with viscoelastic properties and reduced mobility due to the possible confinement at the particle-matrix interface.

Using a simple spherical rigid representation for the carbon-black and a viscoelastic behavior for the rubber within the 4-phase model [2], it has been possible to determine the viscoelastic behavior of the interphase and its thickness was estimated to 5 nm.

In order to discuss this arguably reasonable value of 5 nm, the self-consistent model based on morphological representative pattern [3] was applied. Such a model introduces microstructure parameters such as the particle dispersion, particle size distribution or interparticle distance distribution allowing the study of the impact of such parameters on the material viscoelasticity. Results show that the 4-phase model give an upper bound of the interphase thickness and that the particle dispersion and the interparticle distance distribution have a significant impact on the nanoparticle reinforced polymer while the particle distribution has little effect [4].

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Coupled Digital Image Correlation and Fracture Mechanics analysis for the identification of cohesive models in polymers at the micron scale

Rafael Estevez¹, Julien Réthoré²

¹University of Grenoble, SIMAP, UMR CNRS 5266, Grenoble-INP, UJF

²University of Lyon, INSA Lyon, LaMCoS, UMR CNRS

We present a new methodology [1] for the identification of a cohesive model which describes the material's failure. The goal is twofold: (i) to provide insight in the mechanism underlying failure and (ii) derive information for a realistic description within a cohesive model approach. The material under consideration is a thermoplastic (PMMA) which is known to fail by crazing. PMMA has been elected as the size of its process zone is of few microns in opening with a process zone tens of microns long. A sample of PMMA with a natural crack is tested under four points bending. The study is conducted at the micron scale with the observation of the displacement fields at the notch tip. These are measured optically by Digital Image Correlation. In a first analysis, the displacement is searched for as a decomposition over Williams' series [2]. As shown in [3], it allows for extracting not only stress intensity factors but also the position of the crack tip. The equivalent elastic crack is thus determined as the crack within a perfectly elastic material which produces the same far-fields. The evolution of the equivalent elastic crack position is obtained from this analysis. The advance of this tip during the test corresponds to the development of crazing within a cohesive zone. In a second step, X-FEM simulations with a cohesive model are performed using the displacement obtained by DIC as boundary conditions. The obtained displacement field is projected onto the Williams' series so that the equivalent elastic crack from the X-FEM simulation is determined. The parameters of the cohesive law are then adjusted so that the gap between the crack tip position obtained the experimental analysis and the numerical simulation is minimized. For the PMMA under consideration, the methodology allows to capture the onset of crazing, the traction- separation profile and the maximum opening corresponding to the nucleation of a crack locally. The identified cohesive parameters are consistent with results available in the literature. In addition, the model enables the characterization of the normal and tangential mode of the cohesive model. Further, the proposed methodology allows to access to the mechanical state inside the cohesive law whereas its length is far smaller than the usual resolution of DIC. The methodology is exemplified in a fracture test on PMMA but the framework allows for investigation of the cohesive zone between in other polymers in which no cohesive zone are available at the moment and cohesive zone representing the interface between assembled bulk part.

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A Thermodynamically Consistent Finite Deformation Enhanced Strain Formulation for the Coupled Diffusion in Gels

Christian Linder, Andreas Krischok

Department of Civil and Environmental Engineering, Stanford University Stanford, CA
94305, USA

This presentation is concerned with the development of a large-deformation, continuum-level theory to describe the coupling of the interaction of mechanics and chemistry for polymeric networks, capable of absorbing fluid-like chemical species. The mixture of solid and solvent is treated as a homogenized continuum. To avoid numerical difficulties, a new approach for the approximation of the different field variables is presented in the context of the finite element method. In particular, an enhanced strain formulation within the finite deformation context is proposed to avoid otherwise resulting diffusion driven locking phenomena. A thermodynamically-consistent theory that is in full agreement with the supposedly incompressible behavior of both the solid and the solvent phase of the mixture is presented. The change in entropy due to mixing the fluid and the polymer network is based on the Flory-Huggins model and the change in the configurational entropy due to stretching the network is based on a model for Gaussian chains. A statistical mechanics approach for a pre-swollen reference configuration is presented. Several numerical simulation outline the performance of the new approach.

Micromechanical modeling of elastoplastic damage behavior of the human femur under compression loading

Jamila Rahmoun¹, Hakim Naceur¹, Julien Halgrin²

¹LAMIH, Université de valenciennes, France

²Institut des Sciences du Mouvement, Université de la Méditerranée, France

Osteoporotic hip fractures represent a burden of mortality on the growing population of old patients. To estimate hip fracture and plan the preventive intervention, the strength of the proximal femur must be precisely quantified. To this end, computed tomography based Finite Element analysis which incorporates information on both 3D architecture and bone density, can be used. Furthermore, micromechanical approaches coupled with CT-based FE models were revealed to be more appropriate when the robustness of computation and accuracy of results are of interest.

In this study we propose a micromechanical elastoplastic model of the human femur bone behavior in view of an integration of bone damage for the simulation of necking and rupture initiation. The damage is carried out by the framework of the limit analysis based on the MCK criterion [1]. We first present the methodology allowing the estimation of elastic anisotropic properties of porous media by means of the Mori-Tanaka homogenization scheme [2]. Then, we develop the formulation of the integrated yield criterion derived by considering trial velocity field inspired from the Eshelby inhomogeneous inclusion solution [3]. The obtained micromechanical model is implemented via a User Material routine within the explicit dynamic code LS-DYNA. To illustrate the potential of the current approach, a right adult human femur was simulated until complete fracture under sideways loading.

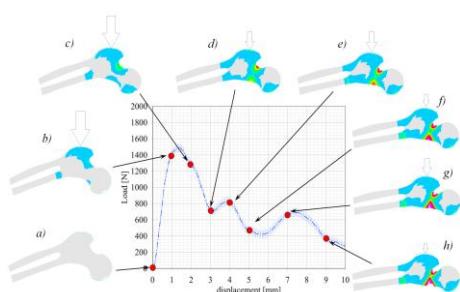


Figure 1: Damage evolution in the cancellous femoral bone during compression loading.

The obtained numerical load-displacement response matches globally the experimental results. Our results showed progressive fracture profiles depending on the vertical trochanter stroke (see Figure 1). The predicted fracture path follows a diagonal line from the inner surface of the neck (basal) to the outer surface towards the greater trochanter. A comparison between predicted fracture path and radiographs of basicervical fractures from the literature shows a quite good agreement, even if loading conditions may be different. Thus, the proposed micromechanical model improved the strength prediction of metastatic femurs by representing the failure risk in a more realistic approach.

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Modeling and simulation of the mechanical behavior of hierarchical bovine enamel

Swantje Bargmann^{1,2}, Ingo Scheider¹, Tao Xiao¹, Ezgi Yilmaz³, Gerold Schneider³, Norbert Huber¹

¹ Institute of Materials Research, Materials Mechanics / ACE-Centre, Helmholtz-Zentrum Geesthacht, Germany

²Institute of Continuum Mechanics and Materials Mechanics, Hamburg University of Technology, Germany

³Institute of Advanced Ceramics, Hamburg University of Technology, Germany

Dental enamel is the outermost layer of a tooth crown consisting of a hierarchical and graded structure. Approx. 85 vol. % of enamel consists of the mineral hydroxyapatite mineral, the rest being protein and water. The hierarchical organization of bovine enamel can be characterized in 3 different levels. Mechanical properties such as stress-strain behavior or the elastic modulus differ greatly on different hierarchical levels.

This contribution is concerned with the modeling and computation of the mechanical behavior, in particular with the failure, of the enamel of a bovine tooth. The model [1] accounts for non-linear, large-deformation kinematics, linear viscosity and softening at each level, i.e. at each scale. The numerical implementation is carried out with the help of the finite element method. A complex microstructure representing bovine enamel is studied in the multiscale numerical examples. The results capture major features of the physical experiments, such as nonlinear stress-strain behavior, stiffness and failure strength.

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Correlating the Free-Volume Evolution to Plastic Deformation of Highly Cross-Linked Polymers from Large Scale Coarse-Grained MD Simulations

Amin Aramoon¹, Stephen A. Barr², Timothy D. Brietzman², Jaafar A. El-Awady¹

¹ Department of Mechanical Engineering, Johns Hopkins University, Baltimore, MD
² Air Force Research Laboratory, Wright-Patterson AFB, OH

Highly cross-linked polymer networks (e.g. epoxies) are widely used in many automotive, marine, and aerospace applications. Predicting the damage and failure of such systems is of crucial interest for the reliable performance of these class of materials. The evolving free volume (voids) in these networks under loading plays a critical role in both their elastic and plastic response. Macroscopic properties such as elasticity, glass transition temperature, and failure can be experimentally determined. In addition, the distribution and size of free volumes can be measured using positron annihilation techniques. However, in such studies it is not always easy to identify the micro-structural features controlling plasticity and failure. On the other hand, numerical methods such as quantum mechanics (QM) and molecular dynamics (MD) simulations can shed light on the atomic processes involved, but are computationally expensive and limited to modelling extremely small volumes, and further linking the outcome of these methods with continuum models still requires further developments.

In this work, a MD coarse-grain model has been developed to study the plastic behavior of epoxy materials. The polymerization of a highly cross linked polymer network in different curing conditions such as temperature, cross-linker functionalities and degree of cross linking are studied using a dynamic cross-linking algorithm. The effect of chain size, length of monomers, and degree of cross-linking on the evolution of the free volume density and subsequently plastic deformation (e.g. hardening and failure). Free volumes are measured by fitting unit volume cells in the network. From these simulations we also develop a direct correlation between the evolution of plastic deformation and the free volume density of the epoxy.

Universal Structure-Material-Property Map for Natural and Biomimetic Platelet-Matrix Composites and Stacked Heterostructures

Navid Sakhavand¹ and Rouzbeh Shahsavari^{1,2}

¹ Department of Civil and Environmental Engineering, Rice University, Houston, TX 77005

² Department of Material Science and NanoEngineering, Rice University, Houston, TX 77005

Many natural and biomimetic platelet-matrix composites -such as nacre, silk and clay-polymer -exhibit a remarkable balance of strength, toughness, and/or stiffness, which call for a universal measure to quantify this outstanding feature given the structure and material characteristics of the constituents. Analogously, there is an urgent need to quantify the mechanics of emerging electronic and photonic systems such as stacked heterostructures, which are composed of strong in-plane bonding networks but weak interplanar bonding matrices. Herein, we present the development of a unified framework to construct a universal structure-material-property diagram that decodes the interplay between various geometries and inherent material features in both platelet-matrix composites and stacked heterostructures in the shear mode. Validated by several 3D-printed specimens and a wide range of natural and synthetic materials across scales, this universally valid diagram (Figure 1) has important implications for science-based engineering of numerous platelet-matrix microstructures and stacked heterostructures while significantly broadening the spectrum of strategies for fabricating new composites through incorporating contrasting platelets. Given the conference theme of “Microstructural Frontiers”, this work opens up several new opportunities to further extend the proposed diagram to include inelasticity, locking mechanisms, stacked multiheterostructures, extrinsic hierarchical toughening processes, etc. to identify and delineate new boundaries and overlaps in mechanistic processes of platelet-matrix microstructures with the goal of unveiling other mysteries in multi-phase multi-functional materials.

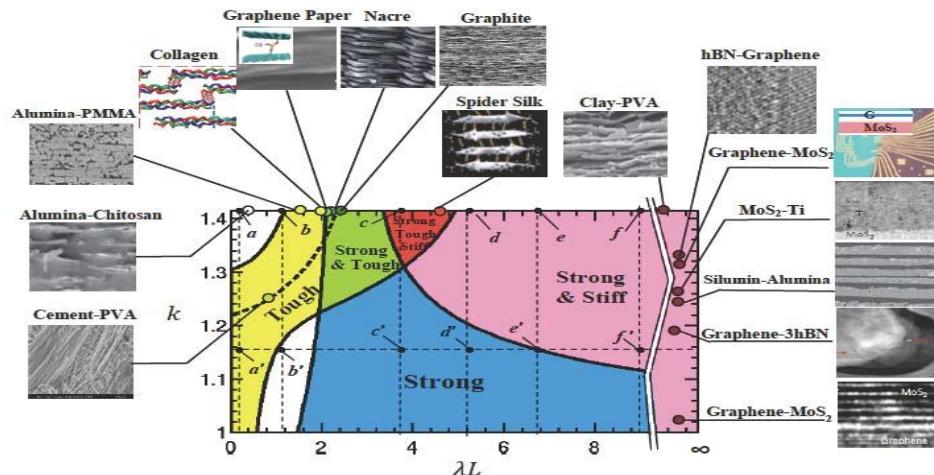


Figure 1. Universal Structure-Material-Property Map for Platelet-Matrix Composites and Stacked Heterostructures

Figure 1. Universal Structure-Material-Property Map for Platelet-Matrix Composites and Stacked Heterostructures

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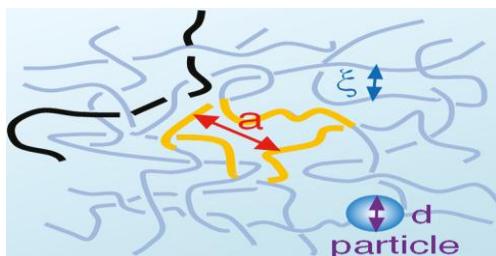
Scaled dynamics of nanoparticles in semi-dilute polymer solution

Sudipta Gupta¹, Michael Ohl¹, Ralf Biehl², Margarita Krutyeva², Dieter Richter²

¹JCNS-SNS-Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA ²JCNS-1 and ICS-1, Forschungszentrum Jülich, 52425 Jülich, Germany

In recent times the diffusion of nanoparticle in complex polymeric fluids has proven to be of considerable importance in understanding the underlying dynamics of the solvent itself [1] and is of immense technological interests, like chromatography, electrophoresis, and drug delivery. In this regard, one can understand biological phenomena involving transport of proteins through a media consisting of concentrated biopolymer like DNA or through polysaccharide solutions. The novelty of such process also lies in detail understanding of colloidal diffusion [2] and sedimentation through a solution of non-adsorbing polymer chains, such as polymer solutions [3], melts [4], bio-macromolecular solutions [5], cells and colloid suspensions [6]. In these connection passive microrheological measurements [7] provides important information about the local/internal viscoelastic properties.

We used two independent systems consisting of human globular protein in an aqueous solution of Poly(ethyleneoxide)(PEO) and POSS hybrid plastic nanoparticles in a Polyethylene (PE) Xylene solution implementing state of the art neutron spin echo (NSE) and pulsed field gradient-NMR (PFG-NMR) technique to study the dynamics of the nanoparticles in semi-dilute polymer solution. Following the recent scaling predictions by Cai et al. [1] We found power law dependency of the normalized terminal diffusion coefficient (D_t/D_s) to the polymer volume fraction (ϕ) where D_s is the particle diffusion coefficient in pure solvent. Using both PFG-NMR and NSE we found $D_t/D_s \sim \phi^{-1.52}$ dependency in the intermediate scaling regime $\xi(\phi) \leq d \leq a(\phi)$ and $\phi_d^\xi \leq \phi \leq \phi_d^a$, where ξ is the correlation length or the polymeric mesh size, d diameter of the probed nanoparticle and $a(\phi)$ is the concentration dependent tube diameter of the corresponding polymer solution (Fig. 1), ϕ_d^ξ and ϕ_d^a are the crossover concentrations at which the concentration dependent correlation length $\xi(\phi)$ and tube diameter $a(\phi)$ becomes equal to the particle size (d). Both NSE and PFG-NMR reveals the presence of a fast and slow diffusion mode, which has been identified as diffusion inside and outside of the mesh.



- Fig. 1: From reference [1]. Schematic representation of a particle of size "d" in polymer solution.
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Welding and healing of polymer interfaces: Connecting structure, dynamics and strength

Mark Robbins¹, Ting Ge², Gary Grest³

¹Johns Hopkins University, USA

²University of North Carolina, USA

³Sandia National Laboratory, USA

Applying heat to polymer interfaces is a common means of welding polymer components or healing cracks in polymers. Once chains have diffused by their radius of gyration, the properties of the interface should be indistinguishable from those of the bulk. In practice, welds can achieve bulk strength at much shorter times. The mechanism of strength growth is difficult to determine with experiments, because they cannot directly access the evolution of molecular configurations and entanglements. Large-scale simulations were used to follow the dynamics of interdiffusion at welds and cracks and the associated changes in density and molecular conformations[1]. The evolution of entanglements was tracked using Primitive Path Analysis and shown to be directly related to the mechanical strength under shear and tensile loading. As in experiment, the maximum shear strength σ_{\max} of a homopolymer interface rises as a power of welding time t and then saturates at the bulk value. Simulations show that σ_{\max} is proportional to the areal density of interfacial entanglements at short times and saturates when chains have formed 2-3 entanglements across the interface. Enthalpy limits interdiffusion across heteropolymer interfaces, and there is a corresponding reduction in interfacial entanglements and mechanical strength. A minimum loop length of order the entanglement length must diffuse across the interface to form entanglements. Cracks are more complicated because of the presence of short segments produced during fracture. Segments that are too short to confer bulk strength, but longer than the entanglement length, remain near the interface for long time intervals. This leads to a plateau in strength that is below the bulk value. Crazes form under tensile loading. A low interfacial entanglement density can stabilize craze formation and significantly enhance the fracture energy, but the bulk fracture energy is recovered at about the same time as bulk shear strength.

Supported by NSF Grant DMR-1006805, CMMI-0923018 and OCI-0963185.

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Multiscale Analysis of Multilayer Composite Pipes

Pham Dinh Chi, Sridhar Narayanaswamy

Engineering Mechanics Department, Institute of High Performance Computing
1 Fusionopolis Way, #16-16 Connexis, Singapore 138632

The use of composite materials in offshore applications has constantly increased towards the development of deepwater technology and ultra-deepwater feasibility. Cylindrical composite pipes are the most principal components in floating and offshore platforms. Composite pipes could be grouped into bonded and unbonded structures. Typical bonded composite structures comprise a core angle ply laminate cylinder sandwiched between an inner liner and an outer liner made of elastomer or metal alloys. On the other hand, unbonded composite pipes such as flexible pipes in floating platforms consist of multiple metallic and polymeric layers, among which tensile wires play essential roles in providing axial and bending stiffnesses. The flexibility in motion of each layers of the unbonded composite pipe and the complexity in their geometries and materials make the analysis of unbonded composite structures very challenging. In this work, multiscale non-linear analyses of unbonded flexible risers are carried out and the non-linear behaviors of individual riser layers as well as stick-slip mechanisms between them are studied. In addition, the work also discusses the potential of flexible fiber-reinforced pipe where metal armour strips may be replaced by fiber-reinforced composite materials to significantly enhance the structural performance of conventional pipe.

Nucleation barrier to registration of lipid bilayer domains

J. J. Williamson, P. D. Olmsted

Department of Physics, Georgetown University, Washington DC 20057, USA

In cellular processes involving lipid bilayer phase separation, equally as important is registration (alignment) of domains between the two leaflets. Most work has focused on measuring or calculating a free energy per area for “direct” inter-leaflet coupling taking place across the midplane [1, 2]. This coupling would favour registration of like domains, as typically seen for macroscopic domains in experiment [3].

However, we show that hydrophobic mismatch between lipid species leads to an additional “indirect” coupling acting to minimise overall thickness variations, favouring *antiregistration*. Thus, domain registration is subject to a competition of two distinct coupling mechanisms.

We use a coarse-grained lattice simulation to show that this renders domain registration a *nucleation-like process*; bilayers may fail to reach their equilibrium, registered state. Given that antiregistration is often unresolvable in experiment, this has important implications for interpreting observed phase behaviour. Crucially, this applies even for a 50:50 mixture of phases, which would naively imply spinodal decomposition. The physics will also bear directly on cellular functions in which inter-leaflet coupling plays a role, e.g. protein signaling [4].

A continuum theory is developed to explain the dependence of nucleation energetics on material parameters. The results show the complex role of lipid length mismatch, and motivate a variety of future work in which the transition between antiregistration and registration is considered.

This work was initiated under the CAPITALS programme grant funded by EPSRC UK.

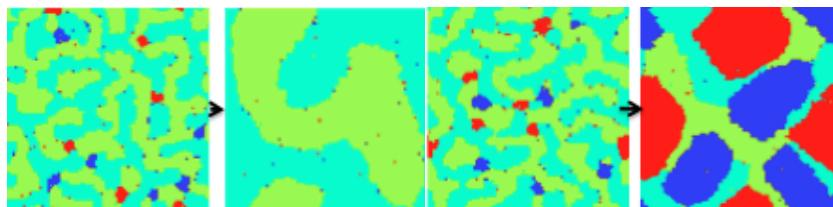


Figure 1: Two trajectories with identical parameters. Registered domains (red/blue) form stochastically via *nucleation*. On the left, this is unsuccessful and the bilayer is metastably trapped out of registration.

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Molecular Mechanism of viscoelasticity in aligned polyethylene

A. Hammad¹, H. Hasan¹, T. D. Swinburne¹, S. Del Rosso², L. Iannucci², A. P. Sutton¹.

¹Department of Physics, Imperial College London, London SW7 2AZ.

²Department of Aeronautics, Imperial College London SW7 2AZ.

Ultra-High Molecular Weight Polyethylene (UHMWPE) is widely used in industrial applications due to its low density and high tensile strength. Extensive experimental work has been done to determine its mechanical properties, notably its viscoelasticity. However, an understanding of the link between these macroscopic mechanical properties and molecular processes has so far not been achieved. We begin to address this by considering a simple united atom model of polyethylene chains. We demonstrate the nucleation of solitons from chain ends, as one molecular chain is stretched with respect to another, and how load is transferred between chains in disregistry by intermolecular interactions. An analogy is drawn between solitons in UHMWPE and dislocation loops in a 3D crystal, giving a basis for the mechanical behaviour of UHMWPE in terms of the motion of solitons. Although solitons have been invoked to account for dielectric relaxation in crystalline regions of polyethylene, we believe this may be the first time they are discussed in the context of mechanical properties of aligned polyethylene.

Mesoscale Modeling of the Interfacial Mechanics of Nanocellulose with Glassy Transparent Polymers

Sinan Keten, Luis Ruiz

North Western University, Dept. of Civil & Environmental Engineering and Dept. of Mechanical Engineering 2145 Sheridan Road Tech A133 Evanston IL 60208

This talk will overview a simulation-based approach to enhancing the mechanical properties of novel transparent thin films and nanocomposites by utilizing cellulose – the most abundant and renewable structural biopolymer found on our planet. Cellulose nanocrystals (CNCs) exhibit outstanding mechanical properties exceeding that of Kevlar, serving as reinforcing domains in nature's toughest hierarchical nanocomposites such as wood. Yet, weak interfaces at the surfaces of CNCs have so far made it impossible to scale these inherent properties to macroscopic systems. A simple analysis on CNC interfaces that accounts for size and geometry effects will be proposed. Our theory and simulations converge on the prediction that the ideal cross-sectional dimensions maximizing the interfacial fracture energy of CNCs must be approximately 5 by 6 nm in dimensions, which intriguingly are very close to the universal dimensions of CNCs found in wood. This study sheds light on a new design principle pertaining to atomically layered nanomaterials that may guide the synthesis of novel nanocomposites. I will conclude with an outlook on how the nascent properties of nanocellulose building blocks could be further utilized in polymers through validated systematic coarse-graining approaches that marry chemical features with mechanical properties.

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The Microscopic Effect of Filler on Rubber Reinforcement: A Coarse-Grained Molecular Dynamics Study II

Kentaro Nagaya¹, Masatoshi Sato¹, Yosuke Kimura¹, Katsumi Hagita²

¹ Toyota Technical Development Corporation, NORE Sakuradori bldg, 2-28-23, Izumi,
Higashi-ku, Nagoya, Aichi, Japan

²National Defense Academy of Japan, 1-10-20, Yokosuka, Kanagawa, Japan

It is well known that adding filler particles such as carbon black to cross-linked rubber raises the stiffness, increases the hysteresis loss due to internal friction and causes stress softening in cyclic deformation (referred to as Mullins effect). Mechanisms by which these macroscopic changes occur are areas in active research. One of the key factors in understanding the occurrence of these phenomena is considered to be microscopic filler-rubber interaction.

In this research, we developed a microscopic approach to understand rubber reinforcement using coarse-grained molecular dynamics simulations^[1]. In our models, we considered two types of filler-rubber interactions exist: one is physical adsorption and the other is chemical bond. In addition, we also considered variation of filler distribution. Fillers are well dispersed or partially aggregate in our models.

We investigated static uniaxial tensile behavior of filled and unfilled rubber models, and found three reinforcement mechanisms. First is the same mechanism predicted by Guth^[2], which depends only on the volume content of fillers. We have confirmed this mechanism at small strain region. Second is caused by filler-filler network created by the advantage of chemical bond at large strain. In this region, some polymers linked fillers and were stretched, that is, these polymers generated tension. Last is caused by contact pressure of aggregated fillers at very small strain region. Aggregated fillers push each other in vertical directions against tensile direction (Poisson ration is 0.5). The third mechanism will be discussed in detail.

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Multiscale strain field measurement in fibrous membrane of connective tissue with photobleaching

M. Coret¹, C. Jayyosi², K. Bruyère-Garnier²

¹ LUNAM Université, GEM, UMR CNRS 6183, École Centrale de Nantes, Université de Nantes, France

² Université de Lyon, F-69622 Lyon ; IFSTTAR, LBMC, UMR-T9406 ; Université Lyon1, France

Multiphoton microscopy, combining two photon excitation fluorescence (TPEF) and second harmonics generation (SHG), has proved itself to be one of the most efficient ways to image collagen and elastin based structures. Indeed, considering elastin autofluorescence and collagen second harmonics generation, fibers' network can easily be seen and distinguished thanks to that microscopy technique. Therefore, it turns to be a valuable tool to study soft biological tissue microstructure, and, if coupled with a loading device, it allows seeing how the fibers' network reacts to mechanical loading. Photobleaching is usually seen as a drawback of multiphoton microscopy, as it corresponds to a loss of fluorescence that undergoes the sample when excited with too much laser intensity or too long exposure time.

In this study, using that loss of fluorescence, intrinsic markers were placed on the structure, designing a pattern of photobleached squares as seen on figure 1.

This grid was then used to compute local strain in human liver's capsule submitted to uniaxial tensile test, following the same approach adopted by Screen and Evans[1]. Local strain was derived from calculated displacements at various steps during loading up to failure, using the finite element method on a 4 nodes element mesh built from the photobleached grid. Observations about the geometry and kinematics of the fibers locally, revealed that this technique is non-destructive, and thus can be used to assess local strain in fibrous structures that contain elastin and collagen fibers [2]. These markers can be used in various ways, in order to help understanding the contribution of microstructure to the macroscopic mechanical behavior of the tissue and to study local phenomenon such as damage and failure mechanisms.

The authors thank the IVTV (ANR-10-EQPX-06-01) team for its help and support.

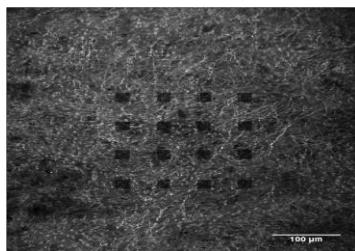


Figure 1: Image of the human liver's capsule with a photobleaching grid before loading

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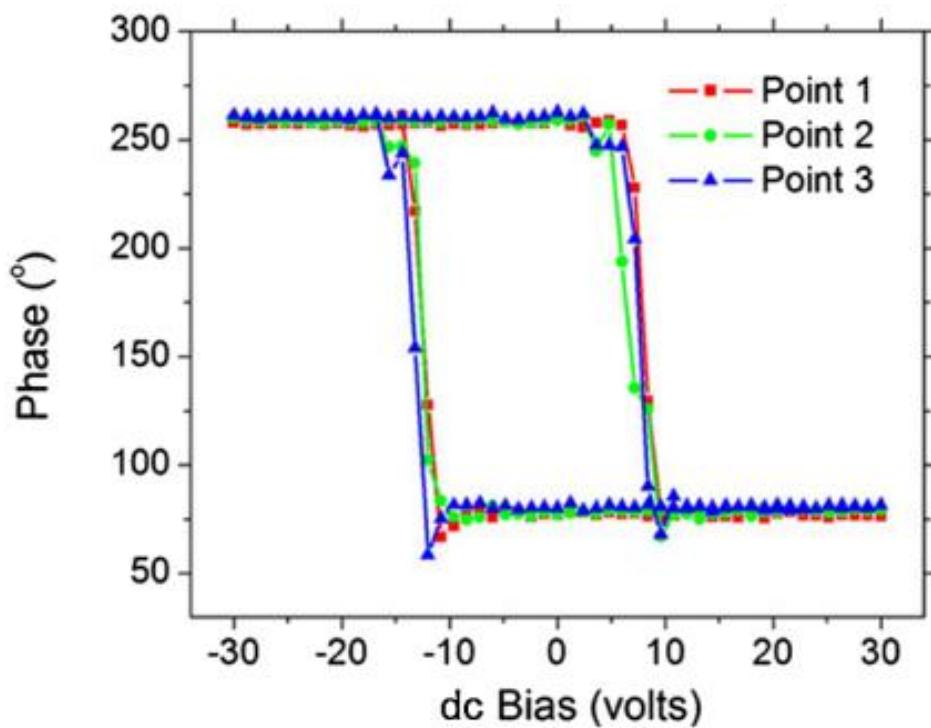
The Mechanism Underpinning Biological Ferroelectricity

Matthew Zelisko¹, Jiangyu Li², Pradeep Sharma¹

¹Department of Mechanical Engineering, University of Houston, Houston, TX 77204, US

²Department of Mechanical Engineering, University of Washington, Seattle, WA 98195, US

Ferroelectricity in biological materials, while speculated, has been a matter of much debate. Recent experimental discovery of this phenomenon in elastin---a key ingredient of aorta, lung, ligament, and skin has given rise to tantalizing questions regarding its origins as well as ramifications. In this presentation, motivated by the experiments performed by one of us, we present a two-scale modeling approach consisting of a coarse-grained statistical mechanics model and molecular dynamics to elucidate the microscopic mechanisms underpinning ferroelectricity in Elastin.



Ferroelectric hysteresis loops of porcine aortic walls observed through PFM¹

More recent experimental work done by Li *et al.*² has shown that the ferroelectric behavior of an elastin network may play an important role in the aging process among other things. As the concentration of glucose in the intercellular elastin matrix increases, similar to what happens as we age, elastin exhibits less of a ferroelectric response, and at high enough glucose concentrations the ferroelectricity of elastin is completely suppressed. Therefore it is hopeful that the statistical mechanics and molecular dynamics

model presented will later be useful in better understanding the aging process in living organisms.

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Mechanics Controls Catalysis (Sometimes)

M. F. Francis^{1,2}, W. A. Curtin¹

¹École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

²Brown University, Providence, Rhode Island, United States

The control and optimization of catalytic processes is a key goal in many technologies. Here, we demonstrate via computation that the application of mechanical stress can modify chemisorption energies at stepped surfaces, and thus catalytic activity, in ways not previously envisioned. Specifically, compressive stresses can induce stronger binding of chemical species at steps, which is the opposite of the well-established trend found on close-packed surfaces. The mechanism driving this new stress effect is shown to be the mechanical relaxation of the deformed material during chemisorption, which can be larger, and of the opposite sign, than the electronic effects due to changes in the d-band structure. Application of stress can thus simultaneously shift binding energies on steps up (or down) and on terraces down (or up), and potentially increase overall catalytic activity in wide classes of systems. These trends can be rationalized using the theory of elasticity, and suggest multiscale approaches for efficiently predicting stress effects on binding energies without full quantum calculations.

Strain Effects on Defects and Diffusion in Perovskites

Dane Morgan¹, Tam Mayeshiba¹, Yueh-Lin Lee¹, Milind Gadre¹, Anh Ngo¹, Yang-Shao Horn², Stuart Adler³

¹University of Wisconsin, Madison, WI 53706, USA

²Massachusetts Institute of Technology, Cambridge, MA 02139, USA

³University of Washington, Seattle, WA 98195, USA

Oxygen active materials are capable of actively incorporating and transporting oxygen through their bulk. Such materials are of interest for a wide range of applications, from solid oxide fuel cells to gas separation membranes to chemical looping. Recent work has shown that strain can play a significant role in altering the transport of oxygen through oxygen active materials, particularly in fluorite structured compounds. However, transition metal perovskites are an important class of oxygen active materials that have received only limited attention. In this work we use ab initio methods to model the coupling of strain and defect formation and migration energetics in a range of transition metal perovskites. We explore the formation volumes of oxygen vacancies and demonstrate how their sizes arise from a combination of local bond breaking and electron donation. We further find that the oxygen transport can be enhanced by orders of magnitude through tensile strain effects. Comparison is made to recent experimental results from Kubicek, et al. on $(\text{La},\text{Sr})\text{CoO}_3$ [1] and excellent agreement is found. We demonstrate that a simple strain model can qualitatively explain the ab initio results but with significant quantitative discrepancies.

We gratefully acknowledge financial support from the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under award number DE-SC0001284, NSF Graduate Fellowship Program under Grant No. DGE-0718123, and computing support from NSF National Center for Supercomputing Applications (NCSA - DMR060007).

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An *ab initio* investigation of the stability of ZnO in an electrochemical environment

Mira Todorova, Jörg Neugebauer

Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf,
Germany

Theoretical and modeling concepts in semiconductor defect chemistry and electrochemistry have hugely evolved over the last years and are crucial for their respective fields such as optoelectronics and semiconductor devices or corrosion and battery materials. Despite being based on the same fundamental building blocks - charged defects/ions - the underlying theoretical concepts and communities have little overlap. To bridge the gap we have recently developed a unified approach that is based on a fully grand-canonical description of both ions and electrons and that connects and “translates” the respective concepts [1].

Our method links ab initio calculations quite naturally to experimental observables, such as the pH-scale and the electrode potential, which determine and characterise the state of an electrochemical system. Employing this approach provides surprising new insight into apparently ”old” problems such as water stability, opens new routes to construct electrochemical phase (Pourbaix) diagrams, and gives a handle to an absolute alignment of electrochemical potentials. Applying the approach to ZnO, we will discuss the impact of an electrochemical environment on the stability of native bulk point defects as well as on the stability of the polar Zn terminated ZnO(0001) surfaces.

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A Multi-Scale Study of the Chemo-Mechanical Behavior of Battery Materials

Feifei Fan, Ting Zhu

Georgia Institute of Technology, USA

High-capacity lithium-ion batteries are critically important for a wide range of applications, from portable electronics to electric vehicles. However, they cannot meet requirements for more demanding applications due to limitations in capacity, charging rate, and cyclability. One leading cause of such limitations is the mechanical degradation and associated capacity fading in electrodes during charging/discharging processes. In this work, we use multi-scale simulations to study the chemo-mechanical responses of electrode materials including morphological evolution and stress generation. We will show how the chemical reactions lead to mechanical failures in electrode materials from atomistic scale to continuum scale. The results provide insights into chemical-reaction-induced microstructural evolution in nanomaterial electrodes, and have implications for an optimization of electrode design in next generation lithium-ion batteries.

Effect of Dislocations on the oxygen ion conductivity in reduced and doped Ceria

Lixin Sun, Dario Marrocchelli, Mostafa Youssef and Bilge Yildiz

Department of Nuclear Science and Engineering, Laboratory for Electrochemical Interfaces,
Massachusetts Institute of Technology, 24-210, 77 Massachusetts Avenue, Cambridge 02139,
USA

Enhancement of ionic conductivity in thin films or multilayers of oxide materials, i.e. doped zirconia and ceria, has sparked great interest in the search for fast ion conducting structures for fuel cells. The enhancement in ionic conductivity in such structures could be attributed to elastic strain arising from the lattice mismatch at the interface. However, this assumes that the interface between two materials is perfectly coherent, while in most cases dislocations are observed, which relax the interfacial elastic strain. The strain field and the electrostatic field that arises from the dislocations can also impact the defect stability, distribution and mobility in these materials; and yet, the role of dislocation on the ionic conductivity is not consistently reported in the literature nor is it clearly understood [1-3]. The aim of our work is to quantitatively assess the dislocation's influence on the ionic conductivity, especially in fluorite oxides by computer simulations.

A $1/2<110>\{100\}$ edge dislocation in reduced or doped ceria is studied by atomistic simulations with Born's model of potential. The atomistic structure is equilibrated by a hybrid algorithm combined the Monte Carlo and Molecular Dynamics simulations [5]. Starting from a uniform distribution of dopant cations and oxygen vacancies, the system is relaxed by rearranging the dopant cations and vacancies to find the most stable distribution of cations. Molecular Dynamics calculations are employed to study the transport properties of the dislocation system.

Asymmetric distribution profiles of dopant cations and oxygen vacancies were found upon after relaxation as a result of the strain field of the dislocation and also the association between dopant cations and oxygen vacancies due to elastic and electrostatic interactions. Dopant cations and oxygen vacancies enrich at the tensile strain field around the dislocation, while a depletion zone of dopants and oxygen vacancies is equilibrated on the compressive region around the dislocation. This is because the dopant cation (usually bigger than the host cation) is easier to be accommodated at the tensile region than the compressive region, and this is followed by the electrostatic attraction of vacancies to the zone enriched by aliovalently charged cations. As opposed to the speculations that regard dislocations as fast diffusion paths, the $1/2<110>\{100\}$ type edge dislocation was actually found to impede oxygen transport in these doped and reducible oxides. The ionic conductivity in ceria has a non-linear dependence on the dopant concentration, with a maximum at 8-10 % concentration of dopants. Therefore, both the high concentration ($>20\%$) of dopants in the enrichment zone and the low concentration ($< 5\%$) in the depletion zone around the dislocation impede oxygen transport and reduce the local ionic conductivity.

Our work demonstrates that dislocations can significantly change the distribution and mobility of dopant cations and oxygen vacancies, and their effects must be considered in quantitatively interpreting the experimental results aiming to assess the effects of strain in oxide ion conductivity.

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First-Principles Study of Oxygen Reduction Reaction on Bulk Metallic Glasses

Zhengzheng Chen and Gang Lu

Department of Physics & Astronomy
California State University, Northridge, California 91330, USA

Pt or Pd-based bulk metallic glasses (BMGs) are promising candidates for electrocatalysts in fuel cells due to their outstanding durability and structural controllability [1]. In particular, unlike conventional metallic catalysts, BMGs can sustain high strains - without nucleation of dislocations to relax the strains - that can be used to tune their catalytic activities. However, it is very challenging to characterize the catalytic activities of BMGs and to optimize their chemical compositions experimentally. Here we report the first computational effort to study stress-dependent oxygen reduction reaction (ORR) on Pd-based BMGs from first-principles.

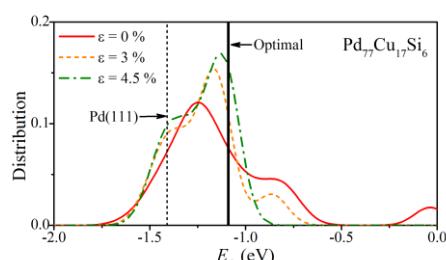


Figure 1: Distribution of binding energy (E_O) of $\text{Pd}_{77}\text{Cu}_{17}\text{Si}_6$ BMG under different biaxial strains

E_O distributions reveals that there is an optimal Si content for superior ORR activity. The effect of stress on ORR activity is examined as well and compression stresses are found to enhance ORR activity.

This work was sponsored by the Army Research Office – Multidisciplinary University Research Initiative under Contract W911NF-11-1-0353. We acknowledge Sharvan Kumar and Yiyi Yang for fruitful discussions.

Two chemical compositions of BMGs - $\text{Pd}_{77}\text{Cu}_{17}\text{Si}_6$ and $\text{Pd}_{77}\text{Cu}_6\text{Si}_{17}$ are examined in this work. The oxygen binding energy (E_O) on the surface is used as the descriptor for the ORR activity [2]. Owing to the amorphous nature of BMGs, a statistical analysis is necessary to characterize the ORR performance of BMGs. For example, the distribution of E_O exhibits a finite broadening, and is sensitive to the local chemical environments on the surface. It is found that local Si-rich environment is detrimental to ORR activity whereas local Cu-rich environment is beneficial to ORR performance. Detailed analysis on

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Role of solvation dynamics in influencing nanoscale corrosion and passive oxide breakdown

Subramanian K.R.S. Sankaranarayanan¹, Sanket A. Deshmukh¹ and Shriram Ramanathan²

¹Center for Nanoscale Materials, Argonne National Laboratory, Argonne IL-60439

²School of Engineering and Applied Sciences, Harvard University, Cambridge MA-02138

Pitting corrosion, a common form of electrochemical corrosion, occurs due to halide ion interaction with metal surfaces and is typically initiated at a lattice defect site. Although continuum theories have looked at possible pathways for pitting initiation in the metal/oxide environment, atomistic understanding of the role of solvent condition and solvation dynamics on electrochemical corrosion phenomena could advance our understanding further of this important problem. We perform an all atom reactive molecular dynamics simulation to probe the influence of chloride ion concentration on the local structure and dynamics of interfacial water near a passive oxide surface. Using representative example of MgO-Cl-water and FeO-Cl-water system, these simulations are being utilized to study electrolyte adsorption, solvation behavior and surface speciation on the passive oxide surfaces in the presence of aqueous media. Na⁺ and Cl⁻ ions with varying concentration are incorporated into the simulation cell to examine the ionic distribution in the near surface region of the oxide film and evaluate the role of solvation dynamics on Cl⁻ adsorption. Proximity effects on water molecules (H₂O) near a passive oxide surface at room temperature are evaluated based on various structural and dynamical correlation functions. In an aqueous environment without any chloride ions, we find significant ordering of water molecules in the two layers close to the oxide interface. The extent of ordering decreases with increasing distance from the oxide-water interface. Our simulations suggest that interfacial ordering is strongly correlated to the Cl⁻ concentration; a non-monotonic variation is observed with the extent of ordering decreasing strongly above a threshold Cl⁻ concentration. Subsequent studies will aim at correlating solvation dynamics with near-surface oxide layer stoichiometry, point defect concentration, passive oxide density and composition. The findings could provide insights into the role of solvation dynamics in influencing aqueous corrosion phenomena.

Acknowledgement: Use of the Center for Nanoscale Materials was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357

Diagnosis of the Mechanism of Anodic Oxide Film Growth on Platinum in H₂SO₄

Feixiong Mao^{1, 2}, Samin Sharifi-Asl², Digby D. Macdonald²

¹ School of Materials and Metallurgy, Northeastern University, Shenyang 110819, China

² Department of Materials Science and Engineering, The University of California at Berkeley, Berkeley, CA 94720

Diagnostic criteria for the growth of the anodic oxide film on platinum in H₂SO₄ are reported. The criteria apply to the generalized High Field Model, which postulates that the electric field within the film is dependent upon the applied voltage and film thickness, and the Point Defect Model, which describes the electric field as being constant during film growth. The constancy of the electric field in the passive film on platinum, as demonstrated in this work, is attributed to band-to-band Esaki tunneling, which buffers the electric field against changes in the applied voltage and film thickness. In this paper, we apply an analytical analysis of the oxide film growth transient on platinum in H₂SO₄ and demonstrate, unequivocally, that the PDM provides a superior theoretical framework than does the HFM for interpreting oxide film growth on platinum. Importantly, the criteria have been shown theoretically to apply to metal interstitial conduction, which is the mechanism of conduction in the HFM and in the PtO oxide film on platinum, rather than being restricted to oxygen vacancy conductors, as originally derived.

Nano-Mechanics of Pit Initiation on Metals and Alloys

Digby D. Macdonald

Department of Materials Science and Engineering, University of California at Berkeley,
Berkeley, CA 94720

For more than forty years, the conditions for the existence of the passive state, and hence for the existence of our metals-based civilization, which is based upon the use of the reactive metals (Al, Cr, Fe, Ni, etc) to build machines, have been described in terms of equilibrium thermodynamics in the form of Pourbaix diagrams. These diagrams plot equilibrium potential versus pH relationships for various reactions (e.g., $\text{Fe}/\text{Fe}_3\text{O}_4$, Fe/Fe^{2+} , $\text{Fe}_3\text{O}_4/\text{Fe}^{2+}$) to define regions of stability or predominance. However, Pourbaix diagrams provide an equilibrium view of passivity, whereas passive films are non-equilibrium structures, whose existence depends upon an appropriate relationship between the rate of formation and the rate of destruction. Accordingly, a more accurate and realistic description of the phenomena of passivity and passivity breakdown must be found in the field of electrochemical kinetics. It is this kinetic theory for depassivation (loss of passivity) that is presented in this paper. It is shown that the kinetic theory for depassivation not only accounts for transpassive dissolution, acid depassivation, flow-assisted corrosion, and fretting corrosion, but it also led to the discovery of a new form of depassivation, which is termed “resistive depassivation”. When applied to microscopic regions on a metal surface, at which cation vacancies that are generated at the film/solution interface by the absorption of chloride ion into surface oxygen vacancies condense at the metal/film interface, and hence cause cessation of the growth of the barrier layer into the metal, “depassivation” theory provides a natural account of passivity breakdown. This paper will present the theory of passivity breakdown according to the point defect model and will show that the theory accounts essentially for all that is known about this important phenomenon.

Emergent Piezoelectricity in Mono- and Bilayers of Inorganic Two-Dimensional Crystals

Karel-Alexander N. Duerloo¹, Dr. Mitchell T. Ong², Prof. Evan J. Reed¹

¹Stanford University, USA

²Lawrence Livermore National Laboratory, USA

Nobel Prize-winning work on graphene has placed atomically thin two-dimensional (2D) crystals at the focus of considerable research attention. The discovery of 2D crystals was groundbreaking because these materials possess several *emergent* properties that are not present in their bulk 3D parent crystal. 2D emergent properties include: exceptional mechanical strength, graphene's exotic electronic properties, and direct band gaps in transition metal dichalcogenides.

Our modeling work has discovered that piezoelectricity is an emergent property of many 2D crystals: BN, MoS₂, MoSe₂, MoTe₂, WS₂ and WSe₂. These atomically thin 2D crystals are piezoelectric, whereas their bulk parent crystals are not. This radically new notion of piezoelectric monolayers being isolated from an entirely non-piezoelectric 3D crystal suggests potential for intriguing electromechanical effects in the single- and few-layer regime.

In the single-layer case, our density functional theory calculations reveal that the piezoelectric coefficients of the studied 2D crystals are on par with commonly used 3D wurtzite piezoelectrics. Piezoelectric coupling in 2D crystals could have exciting implications for nanoscale piezotronics.

Piezoelectric effects also exist in the 2-layer case: we have studied a bilayer consisting of two BN monolayers and have found that flexural electromechanical coupling is yet another emergent property that is unique to the bilayer case. A BN bilayer can be seen as a cantilever-type heterostructure where one layer's strain is opposite from that of the other. This hints at the possibility of electrically controlling or sensing the curvature of a membrane that is only ~3 Å thick. More detailed analysis reveals that such a bilayer of BN amplifies piezoelectric displacements by a factor on the order of 10³-10⁴.

Our work was supported in part by the U.S. Army Research Laboratory, through the Army High Performance Computing Research Center, and was also partially supported by a DARPA YFA grant.

Chemistry in the double layer: Implications for developing better microkinetic models in electrochemistry, corrosion research, and alloy design

Santanu Chaudhuri, Aslihan Summer, Jie Xiao, Martin Losada

University of Illinois at Urbana-Champaign, Illinois Applied Research Institute, College of Engineering, Champaign, IL 61820

Intermetallic phases which are cathodic with respect to the alloy matrix are known to induce localized corrosion. Our research in search for a microkinetic model based first-principles guided multiscale modeling will be presented. Current computational approach at different length scales is somewhat segmented and remain unclear about connections to experimental work performed using rotating disk electrodes (RDEs) for unmodified electrodes and inhibited reaction kinetics. Need for a corrosion model that couples transport of ions through the electrochemical double layer (EDL) is an important input to the localized corrosion reaction on the cathodic precipitates. As a multiscale framework, progress in first-principles density functional theory (DFT) based calculations of the cathodic reactions on Cu surface and transport calculations using molecular dynamics simulations of the electrolyte adjacent to electrode surface will be discussed. A coupling between reaction kinetics on solvated electrodes and transport of reactive species such oxygen, hydroxyl and peroxy ions forms the basis for our microkinetic model. Moreover, alloy surfaces undergo segregation and morphological changes which alters electrode surface area and active site densities. Our ongoing effort in understanding energetic preference for segregation in binary and ternary cathodic precipitates will be briefly presented for underscoring the challenges for obtaining microstructures based kinetic insights on corrosion in metal alloys using a multiscale model. Finally, for understanding RDE experiments, analyzing the electrochemical reactions under solvent flow (basis for Levich Equation) is important. Our microscale model can incorporate solvent flow and the effects on the ionic equilibria. However, polarization of the double layer and changes in the ordering in the electrolyte layers which changes transport is poorly understood. Especially, classical force fields need polarizable framework to obtain reasonable agreements with experimental data for transport coefficients. A comparison with Cu RDE experiments will be presented to explain the current state-of-the-art in force field development and challenges in modeling reactions in the double layer under potentiodynamic conditions.

Ionic motion during field-assisted oxidation of aluminium studied by molecular dynamics simulations

Astrid Gubbels-Elzas, Barend J. Thijssse

Department of Materials Science and Engineering, Delft University of Technology,
The Netherlands

Molecular dynamics simulations with the REAX force field were performed to model the growth of an oxide layer on (100)-oriented aluminium in three different oxidation environments: atomic oxygen gas, liquid water, and an aqueous ammonium tartrate solution. The anodizing behaviour was studied at two different temperatures (300 K and 600 K), in the absence of an external electric field and with field strengths of 0.5 to 2.0 V/Å applied over the growing oxide. Figs. 1 and 2 show representative snapshots. The aim of this study is to determine how the ion motion in the oxide layer is affected by such an applied anodizing potential and by the oxidizing medium.

The principal findings are: (1) O and Al ions move through the oxide via interrupted sequences of short replacement steps rather than as a continuous motion across the oxide, (2) dissociation of H₂O molecules at the surface is crucial, and (3) the dependence of the ion motion on the electric field strength exhibits steps in the growth behaviour.

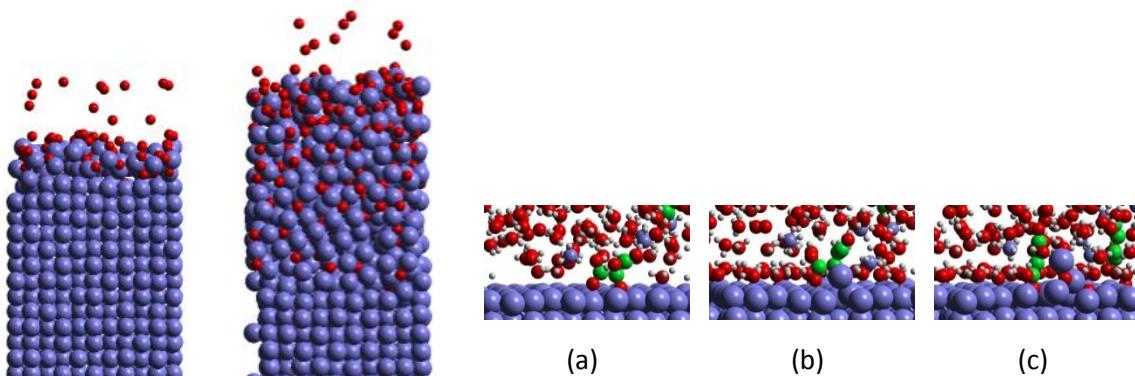


Figure 1: Configuration at 1000 ps for oxidation of Al in atomic oxygen gas at 300 K without an electric field (left) and at 600 K with a field of 2V/Å (right).

Figure 2: Tartrate ion (green) pulling Al atoms out of the surface and thereby assisting the growth of oxide.

Colours: blue=Al, red=O, grey=H, green=C, small blue=N.

The Volcano of Hydrogen Pickup in Zirconium Alloys Explained by p-type Doping of the Passive Oxide Layer

Mostafa Youssef, Bilge Yildiz

Massachusetts Institute of Technology, Massachusetts 02139, USA

Hydrogen pickup in zirconium alloys is a prominent challenge in front of the design of these alloys for fuel cladding in nuclear reactors. In 1960 a volcano-like relationship was identified between the fraction of hydrogen picked up in zirconium alloys and the 3d transition metals that are typically used to alloy zirconium. The peak of the volcano was found to be coincident with Nickel [1]. This empirical observation was used subsequently in the design of zirconium alloys without a physical understanding of its origin. Here we establish using a combination of density functional theory (DFT) calculations and thermodynamic analysis that the origin of this volcano is the variation in the ability of the 3d transition metals to p-type dope ZrO_2 . The latter is the passive layer that grows natively on zirconium alloys.

By modelling the defect equilibria in ZrO_2 co-doped with hydrogen and a transition metal, one at a time, we computed two metrics related to hydrogen pickup. The first is the solubility of hydrogen in ZrO_2 as a function of the transition metals. This metric exhibits a volcano-like relationship with the 3d metals similar to the one identified experimentally but the peak is coincident with Co. The second metric is the equilibrium chemical potential of electrons (Fermi level) in the co-doped ZrO_2 as a function of the transition metals. We found out that this metric exhibits a mirror image of the volcano with the minimum at Co as well. That is, Co is the element that achieves the most p-type doping of ZrO_2 among the 3d metals. It turns out that p-type doping lowers the formation energy of interstitial proton which, in turn, increases the solubility of hydrogen in ZrO_2 giving rise to the volcano of hydrogen solubility.

Beyond the above thermodynamic picture, there is a kinetic incarnation for these results. Lowering the chemical potential of electrons (p-type doping), increases the activation barrier for the electron transfer from ZrO_2 to the protons adsorbed on its surface. These protons are byproduct of water splitting. This electron transfer is needed to reduce the protons, form H_2 molecules, and avoid picking up hydrogen. Thus, p-type doping both increases the solubility of hydrogen in the bulk of ZrO_2 and obstructs the reduction of protons on the surface of ZrO_2 . The two effects synergistically lead to picking up hydrogen into ZrO_2 and the underlying zirconium alloy.

This physical understanding opens the route for physics-based design of hydrogen pickup-resistant zirconium alloys.

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Multiscale Corrosion Modeling and Computational Design of Aerospace Coatings Systems

E. Sapper¹, I.S.Cole², M. Breedon², C. Chu², F. Chen², M. Chen², J. Osborne¹

¹BOEING RESEARCH & TECHNOLOGY

¹PO Box 3707, Seattle, WA, USA, 98124

²CSIRO

²Private Bag 33, Clayton South, Victoria 3169

A multiscale model is being developed which connects aspects of aerospace material corrosion and performance at all relevant length scales, from atomistic corrosion mechanisms and metallic microstructures to in-flight exposure conditions determined by flight path, global wind patterns, and ocean currents releasing aerosolized electrolyte into the environment.

The complete multiscale model links a wide range of individual modules together, each residing in different length and time scale regimes. The model provides a means of assessing the impact of atomistic and molecular mechanisms such as species transport and adsorption, as well as component surface morphology, on the predicted service lifetime of an aerospace material, and will have significant impact in the design of protection systems for future aircraft. This presentation will focus on the design and decision-making aspects of the work, including exercising the model for existing and novel system for corrosion prevention.

Prediction of Crack Growth Rate in Type 304 Stainless Steel Using Artificial Neural Networks and the Coupled Environment Fracture Model

Jiangbo Shi^{1,2}, Jihui Wang¹, Digby D. Macdonald²

¹School of Materials Science and Engineering, Tianjin University, Tianjin 300072, P. R. China;

²Department of Nuclear Engineering, University of California at Berkeley, Berkeley, CA 94720, USA

It has long been recognized that intergranular stress corrosion cracking (IGSCC) in sensitized stainless steels reflects complex interactions between stress, material properties, and environmental parameters. This complexity can lead to significant scatter in the crack growth rate (CGR) that, in turn, leads to difficulties in predicting CGR with the desired engineering accuracy under any given set of conditions. In the present work, a crack growth rate database has been established from data reported in the literature and an artificial neural network (ANN) was developed having linear and sigmoid transfer functions. The ANN aims at predicting the CGR in sensitized Type 304 stainless steel and to delineate the dependencies of the CGR on each of the principal independent variables of the system (i.e. temperature, conductivity, stress intensity, degree of sensitization, electrochemical potential, and pH) using back propagation error minimization. The ANN revealed the underlying relationships that map the dependencies of the dependent variable (CGR) on the various input independent variables. A sensitivity analysis using the trained ANN establishes that IGSCC in sensitized Type 304SS in high temperature (288°C) aqueous environments is primarily electrochemical in character. The coupled-environment fracture model (CEFM), which is a deterministic, physico-electrochemical model for predicting crack growth rate, was customized to take into consideration the impact of the degree of sensitization on crack propagation rate and was then used to predict IGSCC CGR in Type 304 stainless in simulated Boiling Water Reactor (BWR) primary coolant circuits. Comparison of the ANN-predicted CGR and the CGR predicted by the CEFM as a function of the independent variables reveals good agreement between these two approaches.

Growth and breakdown of iron sulfide passivating corrosion films: Towards a mechanistic, multiscale model

Aravind Krishnamoorthy¹, F. William Herbert¹, Bilge Yildiz²

¹Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge MA 02139

²Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, Cambridge MA 02139

In sour (H_2S -containing) environments relevant to the oil & gas industry, the corrosion of steel components is partially inhibited by the formation of passivating, iron sulfide-containing films. Acting as a barrier layer, these films control metal loss but are susceptible to localized breakdown which can lead to catastrophic failure through pitting corrosion. Due to challenges in the characterization of these sulfide films, even fundamental mechanistic information such as the nature of the rate controlling unit process is not conclusively known [1]. Therefore, susceptibility of materials to failure in these critical systems is quantified largely using empirical formulae that have little basis in the mechanism of sulfide corrosion [2].

In this study, we present a multiscale model for the growth and breakdown of iron sulfide passive films based on the elementary unit processes of electron- and ion transfer reactions. The relative kinetic rates of these processes depends on a host of factors including system temperature, activity of sulfur and film thickness, necessitating the use of a multiscale model that can span all the requisite time scales. Our model couples activation barriers for surface reactivity calculated *ab initio* using Density Functional Theory (DFT) simulations and mesoscale diffusivity of Fe^{2+} ions in the iron sulfide film calculated using kinetic Monte Carlo (kMC). The calculated activation barriers are validated with experimental results from the authors' work and literature. We also provide a mechanistic pit initiation model adapted from the well-known Point Defect Model [3]. Taken together, these two results lead to a more deterministic description of the growth and degradation kinetics of sulfidic passive films on iron.

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Multiscale Nature of Stress Corrosion Cracking

G. S. Was

University of Michigan

Stress corrosion cracking (SCC) is an inherently multiscale process that requires a combination of experiment and simulation to understand. This talk will focus on the nature of stress corrosion cracking from atomistic to macroscopic length scales. Emphasis will be placed on the phenomenon of irradiation assisted stress corrosion cracking (IASCC) in austenitic stainless steels as an example of a process that can be understood only through combinations of techniques over a range of length scales. IASCC is believed to be driven by the combined action of localized deformation, grain boundaries and an aggressive environment. Using novel experimental techniques employing an in-situ capability, pre-determined and pre-characterized geometries for dislocation channel- grain boundary interaction, and molecular statics and molecular dynamics modeling of channel-boundary interaction, we are determining the basic processes and mechanisms by which IG cracking initiates in irradiated austenitic Fe-Cr-Ni alloys conducted in aggressive media at high temperature. A key aspect of this effort is that it embraces the essence of mesoscale science, providing the linkage from atomistic simulations of dislocation responses to the accommodation and emission of dislocations from grain boundaries, and direct observation of dislocations with irradiation defects and grain boundaries to macroscale experiments. A consequence of this combined effort has been the identification of the factors most likely responsible for establishing not only the local stress state at grain boundaries prone to failure but their location with respect to the macroscopic applied stress.

Multiscale simulations of stress corrosion effects and surface response to charging

J.-M. Albina^{1,2,3} Y. Umeno³, G. Moras¹, C. Elsässer^{1,2}, P. Gumbsch^{1,2}

¹ Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstr. 11, 79108 Freiburg, Germany

² Karlsruhe Institute of Technology KIT, Institute for Applied Materials, Kaiserstr. 12, 76131 Karlsruhe, Germany

³ Institute of Industrial Science, The University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan

Stress corrosion, tribochemical wear or the mechanical response of surfaces to charging are phenomena which require quantum mechanical treatment of the elementary physical phenomena but at the same time reveal their macroscopic consequences only by integration or interpretation on macroscopic scales.

As examples, I will address the dissociative chemisorption of H₂ molecules at the edges of hydrogen-induced platelet defects in silicon crystals which stabilizes the breaking up of highly strained silicon bonds. The resulting stress-corrosion fracture process yields atomically smooth cleavage of Si crystals along otherwise unstable (100) planes. Similar chemical reactions have a big influence on the tribological behaviour of diamond. Linear carbon chains that form during sliding of diamond surfaces undergo a fast degradation process upon exposure to air. This oxidative wear process is triggered by the chemisorption of O₂ molecules that lead to the splitting and to the shortening of such sp-hybridized structures.

Direct electrical charging of metal surfaces alters the surface properties significantly. Electronic structure calculations allow assessing the effect of tangential strain on the work function and the change in surface stress as a function of charging. This is demonstrated on the 4d series of transition metals. They mostly follow a parabolic behavior, which is dependent on the d-band occupancy until we reach the noble metals, which show an s-band occupation dependency. The variation of the stress-charge coefficients is interpreted in terms of a bonding-antibonding orbital occupation.

Multiscale modelling of materials chemomechanics: from catastrophic brittle fracture to stress corrosion cracking

James Kermode, Giovanni Peralta, Zhenwei Li,
Marco Caccin, Federico Bianchini, Alessandro De Vita

King's College London, Department of Physics, Strand, London, WC2R 2LS, United Kingdom

Fracture of oxides and semiconductors is the dominant failure process underlying many materials reliability issues, and is also relevant to mining, where huge amounts of energy are required to fragment thousands of tons of rock into fine powder raising ever more serious sustainability issues. At the same time, fracture remains one of the most challenging ‘multi-scale’ modelling problems: since crack propagation is driven by the concentration of a long-range stress field at an atomically sharp crack tip, an accurate description of the chemical processes occurring in the near tip region is essential, as is the inclusion of a much larger region in the model systems. Both these requirements can be met by combining a quantum mechanical description of the crack tip with a classical atomistic model that captures the long-range elastic behaviour of the surrounding crystal matrix, using a QM/MM (quantum mechanics/molecular mechanics) approach such as the ‘Learn on the Fly’ (LOTF) scheme [1], or more recently a novel information-efficient Machine Learning extension of LOTF, where the results of all QM calculations are stored in a database and used this to predict forces on new configurations whenever possible, thus calling upon QM only when it is strictly necessary [2].

Examples of the application of these techniques to ‘chemomechanical’ processes, where complex and interrelated chemical and mechanical processes that originate at the atomic scale go on to determine the mechanical behaviour of a material, include low-speed dynamical fracture instabilities in silicon [3], interactions between moving cracks and material defects such as dislocations or impurities [4], very slow crack propagation via kink formation and migration, and chemically activated fracture, where cracks advance under the concerted action of stress and corrosion by chemical species such as oxygen or water [5]. The mechanism underlying stress-corrosion cracking in silica forms the topic of ongoing work, enabled by an INCITE award from the US DoE and hosted at the Argonne Leadership Computing Facility [6]. An expansion of the modeling approach to metals is also underway, focusing on the mechanical properties of nickel-based superalloys, a class of materials that exhibit excellent strength and creep-resistance at high temperatures making them suitable for the construction of efficient turbines for energy generation and aerospace applications [7].

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Self-Healing Materials and Damage from Shock Induced Nanobubble Collapse: Reactive Molecular Dynamics Simulations

Priya Vashishta, Adarsh Shekhar, Ken-ichi Nomura, Rajiv K. Kalia, Aiichiro Nakano,
Kohei Shimamura, Fuyuki Shimojo

Collaboratory for Advanced Computing and Simulations

Departments of Chemical Engineering & Materials Science, Physics & Astronomy, and
Computer Science, University of Southern California, Los Angeles, CA 90089-0242, USA

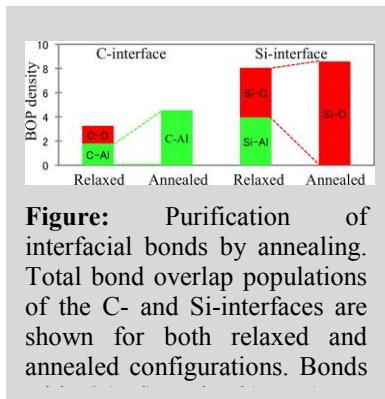


Figure: Purification of interfacial bonds by annealing. Total bond overlap populations of the C- and Si-interfaces are shown for both relaxed and annealed configurations. Bonds

Bonding and Structure of Ceramic-Ceramic Interfaces - Interfaces in multicomponent systems are critical in determining their material behavior. High-resolution TEM identified rich interfacial phases of thickness $\sim 10 \text{ \AA}$, which have distinct atomistic structures that do not exist in bulk phases. An archetypal ceramic/ceramic interface is formed between Al_2O_3 and SiC , which is important for broad applications such as matrix-nanoparticle composites, high-power electronic devices, and self-healing nanocomposites that autonomously heal cracks and recover strengths. For better understanding and design of $\text{Al}_2\text{O}_3/\text{SiC}$ interfaces, the central question is: What are the nature of interfacial bonding at the atomistic level and its consequence on interphase structures?

Our quantum molecular dynamics (QMD) simulations of $\alpha\text{-Al}_2\text{O}_3$ (0001)/3C-SiC (111) interfaces revealed profound effects of thermal annealing for producing strong interfaces consisting solely of cation-anion bonds. A Si-terminated SiC surface and Al_2O_3 form a stronger interface (Si-interface) with a Si-O bond density of 12.2 nm^{-2} , whereas the C-interface has an Al-C bond density of 9.46 nm^{-2} . The interfacial bond strengthening is accompanied by the formation of an Al_2O_3 interphase with a thickness of $2\text{-}8 \text{ \AA}$.

Damage on Silica Surface from Shock Induced Nanobubble Collapse - Despite a great deal of research on cavitation bubbles, several important questions about the mechano-chemistry of bubble collapse near a solid surface remain unanswered. In particular, an atomistic understanding is lacking. We have addressed these questions using billion-atom reactive molecular dynamics (RMD) simulations. These are the largest RMD simulations done on 163,840 processors IBM BlueGene/P at Argonne Leadership Computing Facility. The simulations revealed more chemical activity in water nanojets and vortex rings formed by collapsing nanobubbles, in cavitation pits on silica surface and around secondary shock waves. We found that the structural damage is intimately related to the chemical processes initiated by water nanojets, and can be mitigated by incorporating suitable gas in the nanobubble.

We examine chemical and mechanical damages due to shock-induced collapse of a nanobubble near a silica slab. We also performed two sets of simulations in which the nanobubble contained an inert gas at a density of 0.24 g/cc . The role of gas density in the stability of a single bubble is usually examined for gas densities around 0.5 g/cc . The simulated systems contained 10^9 and 10^8 atoms and the initial bubble radii in these systems were again 97.6 nm and 40 nm , respectively.

Acknowledgement: Research supported by DOE-BES Grant Number DE-FG02-04ER46130.

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Mapping Strain Rate Dependence of Dislocation-Defect Interactions in Zirconium

Yue Fan¹, Sidney Yip^{1,2}, Bilge Yildiz¹

¹Department of Nuclear Science and Engineering, MIT,
Cambridge, Massachusetts 02139

²Department of Materials Science and Engineering, MIT,
Cambridge, Massachusetts 02139

Probing the mechanisms of defect-defect interactions at strain rates lower than 10^6 s^{-1} is an unresolved challenge to date to molecular dynamics (MD) techniques. Here we propose a novel atomistic approach based on transition state theory and the concept of a strain-dependent effective activation barrier that is capable of simulating the kinetics of dislocation-defect interactions at virtually any strain rate, exemplified within 10^{-7} to 10^7 s^{-1} . In particular, we investigate the interaction between an edge type dislocation and an irradiation induced self interstitial atom (SIA) cluster in Zr as a model system.

The resulting interaction paths, energy barriers and critical stresses are found to depend significantly on the strain rates and temperatures considered. We found that, at low strain rate and high temperature conditions, the SIA cluster is eventually absorbed by the dislocation forming a jog structure, and thus, assists the climb. However, at high strain rate and low temperature conditions, the dislocation passes through the cluster. Both the dislocation and the SIA cluster fully recover their original structures, and this process has no contribution to climb. Our predictions of a crossover from a defect recovery at the low strain rate regime to defect absorption behavior in the high strain-rate regime are validated against independent, direct MD simulations at 10^5 to 10^7 s^{-1} . Implications of the present approach for probing molecular-level mechanisms in strain-rate regimes previously considered inaccessible to atomistic simulations are discussed.

Measurements and Observations on Adhesion to Brittle Materials

Rajan Tandon, Michael E. Chandross

Materials Science and Engineering Center, Sandia National Laboratories, Albuquerque,
NM 87185

Bonded systems between different material families (metals, ceramics, and polymers), and within each family are widely used. A few examples include: polymer coated dielectrics, encapsulated electronic packages, brazed and soldered assemblies, glass to metal seals, plated and coated electrical contacts, coatings on tribological materials, and arc-sprayed components. The performance of such multi-materials systems is often limited by the adhesion between the layers. Experimental observations and measurements of interfacial properties in ceramic-polymer/metal systems are described. Spherical shaped indenters have been used to induce delaminations at the interface. The load for initial delamination is used to measure the interfacial strength, while the load-crack length relationships are used to estimate interfacial toughness. In the ceramic-polymer system used for dielectric protection, surface chemical modifications led to enhanced interfacial toughness, and various modelling approaches needed to properly characterize the system are discussed. In the ceramic-metal cases described, the interfacial microstructure changes during processing or use (high temperature sealing, and solid-oxide fuel cell applications). Here we will highlight the reasons why multi-scale models are necessary for accurate descriptions of performance, and how experimental techniques can help in building these models.

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Decoding the chemomechanics of friction and scratch in complex granular hydrated oxides

Soroosh jalilvand¹, Rouzbeh Shahsavari^{1,2}

¹Department of Civil and Environmental Engineering, Rice University, Houston, TX 77005

²Department of Material Science and NanoEngineering, Rice University, Houston, TX 77005

Calcium-Silicate-Hydrate (C-S-H) is a structurally complex material that is the primary binding phase of all Portland cement concrete materials. C-S-H is typically considered as an assemblage of discrete nanoscale particles whose interactions are governed by nano-scale friction and interfacial cohesion. Despite the critical role of interparticle forces on mechanics of granular materials such as C-S-H, there is currently no unified understanding on the atomistic mechanisms governing the nanoscale friction, scratch and cohesion in C-S-H; a lack of knowledge, which presents a major barrier to decode the interplay between chemistry, structure and mechanics of various C-S-H systems. Here, we develop a molecular dynamics framework, coupled to a set of re-defined classical continuum relations, aimed at filling this gap.

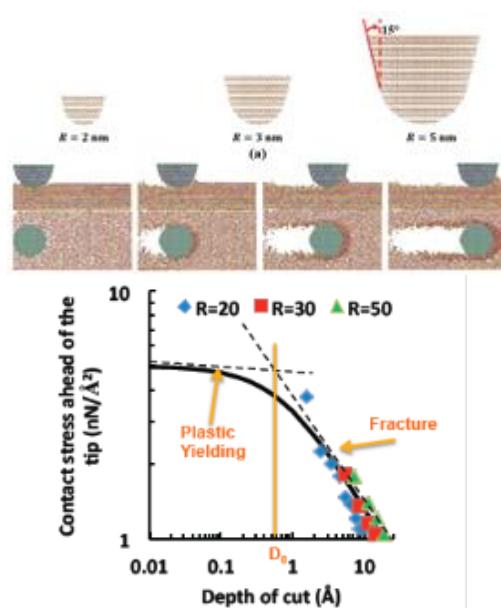


Figure 1. Typical scratch test in C-S-H (top). Classical fracture size-effect of quasi-brittle materials does not hold for nanoscale scratch test in C-S-H.

contribute most to the friction and normal forces. Finally, we probe the effect of pile-up and show that the nanoscale scratch test does not follow the classical laws of size-effect in fracture of quasi-brittle materials (**Figure 1**). Our findings, for the first time, provide an “atomistic lens” on nanoscale friction and contact phenomena in particulate C-S-H systems. This has a significant impact on fundamental understanding of C-S-H and modulation of its behavior, thus impacting the mechanics of granular cementitious materials.

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The normal force is calculated by relaxation of two C-S-H particles at various distances and crystallographic orientations. The effect of watery environment is studied by immersing the particles in water molecules, and the friction and scratch forces are calculated by sliding the tip over the substrate in various directions. Our study identifies the distinct contribution of van der Waals and electrostatic forces to the interfacial behavior of C-S-H particles. While the electrostatic forces govern the interaction of particles at short and large distances, the van der Waals forces are responsible for variations in the normal force at intermediate distances. We find that normal force varies sub-linearly with nanoscale contact area between the tip and substrate, while the friction force shows a linear trend. Our results demonstrate to what extent atoms of particular type contribute to the total interfacial forces. Due to large electronegativity, Si atoms (vs Ca, O and H)

Hybrid quantum-classical simulation of the reaction of breaking bond by water molecules in silica glass

Takahisa Kouno^{1,2}, Shuji Ogata², Tomoyuki Tamura², Ryo Kobayashi²

¹Institute for Solid State Physics, The University of Tokyo, Japan

²Graduate School of Engineering, Nagoya Institute of Technology, Japan

The silica glass is a fundamental of various kinds of glasses and is widely used, e.g., in the optical fibers. Due to the brittleness of the silica glass, the micro-cracks and impurities contained in it influence sensitively its strength and lifetime. It is experimentally well known that the water molecules, which migrate into the silica glass from the moisture environment, react with the silica atoms to break the stretched Si-O bond, resulting in accelerated breakage of the glass. The reaction mechanism of the bond breakage has been believed to follow the Michalske-Freiman reaction model ($\text{H}_2\text{O} + \text{-Si-O-Si-} \Rightarrow \text{-Si-OH} + \text{HO-Si-}$)[1].

We propose a novel reaction model between the water molecules and silica glass by performing reaction-dynamics simulation using the hybrid quantum-classical method. In the hybrid method, the quantum region treated with the electronic density-functional theory (DFT) is embedded in a large classical system: the quantum and classical regions couple mechanically with each other. We perform the hybrid simulation of a silica glass system (about four thousand atoms) with water molecules inserted in it (Figure 1 (a)). We set the quantum region as that composed of the water molecules and their surrounding atoms (Figure 1 (b)). For fast computation we use the real-space grid based implemented of the Kohn-Sham DFT (RGDFT) code.

In the cases where a single water molecule in highly stretched or expanded systems contrary to the Michalske-Freiman reaction model mentioned above. In the cases where two molecules are placed initially at neighboring sites, they attract each other to form a water-dimer in a relatively large site of the silica glass. Those self-dimerized water molecules react quite sensitively with the silica atoms to break the Si-O bond. Detailed analyses about the reaction mechanisms are presented.

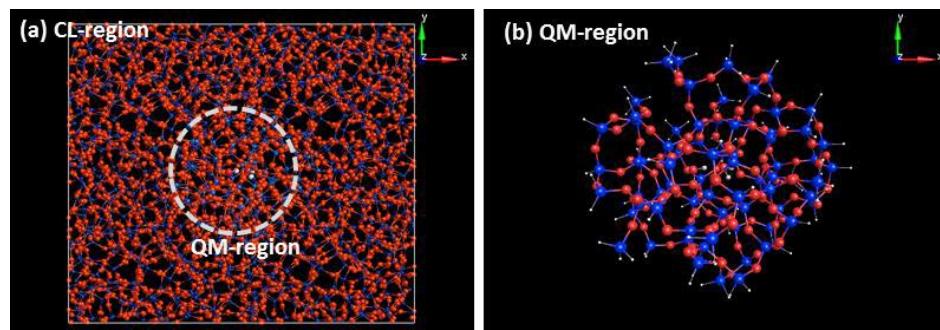


Figure 1: Hybrid Quantum-Classical simulation of SiO_2 . (a) Classical (CL)-region. (b) Quantum (QM)-region. Si is shown in blue, O in red, and H in gray.

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Simulation of impurity atom segregation formation kinetic in the vicinity of dislocations and crack tips

Andrei V. Nazarov^{1,2}, Alexander A. Mikheev³

¹ National Research Nuclear University (MEPhI), Moscow, Russia

² SSC RF Institute for Theoretical and Experimental Physics (ITEP), Moscow, Russia

³ Moscow State University of Design and Technology, Moscow, Russia

Elastic fields, generated by defects of the structure, influence the diffusion processes. To describe the stress influence on diffusion flows in interstitial alloys, we use an approach, developed earlier for the case of vacancy mechanism. This approach is in contrast to most other known takes into account atomic structure in the vicinity of the impurity atom and the structure changes under strains not only on rest position but also at the position of the saddle point. Stress fields alter the surrounding atom configuration and, as a consequence, the height of the activation barrier is changed. In contrast to our works [1,2], we consider, that in inhomogeneous systems, the barrier height depends on the two coordinates: rest position and saddle-point position and hence jump rate also depends on these two coordinates. Knowing the changes of the activation barriers it is possible to calculate the jump rates. The rates of atom jumps in different directions define the flux density of the defects, the explicit form of which can be derived by calculating the balance of different jumps and their contribution to the flux. We obtain the expressions for the interstitial diffusion fluxes in FCC and BCC structures for different kinds of atom jumps. In these nonlinear equations, influence of deformation tensor component on diffusion flux is determined by coefficients depending on atom interaction and atomic structures in the vicinity of the saddle point and rest position. New equations are differed sufficiently from the equations obtained in [2]. Our approach gives the possibility to use the equations at low temperatures, in conditions where the strain influence on the diffusion fluxes is manifested in maximal degree.

We use new equations for studying of interstitial impurity atom redistribution kinetics in the vicinity of crack tips or dislocations taking into account the strain generated by mentioned defects. Two levels of simulation are applied. First one is evaluation of mentioned coefficients that determine the influence of strain tensor component on diffusion flux. For this purpose we have developed a model into the framework of molecular static method taking into account an atom environment as near the interstitial site as for the saddle-point configuration. The second level is modeling of interstitial segregation formation based on nonlinear diffusion equations taking stress fields generated by defects. The results of simulation show, that the distribution of the interstitials near the crack tip has a quite complicated character and the hydrogen distribution has qualitatively different character as compared with carbon distribution.

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Understating pitting in the passive layer of carbon steel starting from first principles study of its point defects

Mostafa Youssef, Bilge Yildiz

Massachusetts Institute of Technology, Massachusetts 02139, USA

In a CO₂-rich anoxic aqueous environment as in some oil fields, a layer of siderite (FeCO₃) grows on carbon steel as a byproduct of steel corrosion. This layer acts as a resistive barrier that kinetically slows down further corrosion of steel. A safe and economic employment of carbon steel in such oil fields strongly relies on the coherence of this siderite layer. However, under certain conditions, yet to be discovered, siderite suffers pitting corrosion. The pitting is believed to initiate at weak spots in the siderite layer and proceed by the dissolution of the layer into the surrounding aqueous environment [1]. The weak spots, at which pits are initiated, are suggested to be weak due to the accumulation of point defects [2]. The purpose of this study is to understand the defect equilibria in siderite under various thermodynamic conditions as a first step to understand pit initiation.

We use density functional theory (DFT) with an on-site Coulomb interaction (U) for d electrons, to study iron, carbonate and electronic defects in FeCO₃. By applying charge neutrality condition, we compute the concentration of these defects as a function of the thickness of the siderite layer starting from the iron rich region (steel/siderite interface) to the carbonate rich region (siderite/water interface).

A multi-scale approach that links our atomic scale modeling with a rate-equations model such as the point defect model [2] provides a potentially predictive paradigm for pitting in carbon steel. A discussion of the capabilities and challenges of this paradigm will be discussed.

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Long term solute evolution in RPV steels: experimental and modeling convergence?

Pareige Philippe¹, B. Radiguet¹ and Malerba Lorenzo²

¹Groupe de Physique des Matériaux, Normandie Université,
76801 Saint Etienne du Rouvray, France

²Structural Materials Group, Institute of Nuclear Materials Science, SCK•CEN,
The Belgian Nuclear Energy Research Centre, Boeretang 200, 2400 Mol, Belgium

Radiation-induced embrittlement of steels used to build the irreplaceable reactor pressure vessels (RPV) is the lifetime limiting factor of existing nuclear light water reactors (LWR). The primary mechanism of embrittlement is the obstruction of dislocation motion produced by nanometric defect structures that develop in the bulk of the material due to irradiation. So far, two classes of nano-structural features are considered as the main contributors to the embrittlement of RPV steels: (a) clusters of solute atoms such as Cu, Ni, and Mn, generally catalogued as precipitates; and (b) the so-called 'matrix damage', generally interpreted in terms of clusters of point-defects

In the first class, one can distinguish between Cu-rich precipitates (CRP) and Mn-Ni-rich precipitates (MNP). The formation of the latter, which might also not contain Cu, is favoured by low(er) temperature and high Ni (and Mn and Si) content. MNP without Cu are detected only at sufficiently high neutron fluence, not only in (low-Cu) RPV steels, but also in FeMnNi model alloys. Today, the large amount of experimental works in this field of irradiated materials (vessel steels, model alloys, ferritic-martensitic steels,...) brings a lot of information on the behavior of solutes or impurities in bcc iron under irradiation. Common trends are observed and often explained or validated with numerical modeling.

Back to RPV steels, there is a belief that precipitates rich in Mn and Ni, once nucleated, will rapidly grow to large volume fractions. For these reasons, they are more commonly denoted as late blooming phases (LBP). Their appearance has been associated with the possibility of a sudden and unexpected increase of embrittlement above a certain dose, that cannot be predicted by current commonly used empirical correlations.

In this paper, insight gained lately from atomistic simulation and experimental results on the possible mechanism of formation of "dislocation obstacles" are described. Strong of this, a discussion of up to what extent the lateness and the blooming of these phases should be really considered a concern for nuclear power plants will be engaged. The modeling/experimental parallel suggests that these features start forming at early dose by heterogeneous nucleation on point-defect clusters and are therefore intimately connected with matrix damage, thereby following the same trend as the latter in terms of kinetics of formation versus dose.

Self-interstitial clusters with C15 Laves phase structure in bcc iron

M.C. Marinica, R. Alexander, L. Dezerald, L. Ventelon, F. Willaime

CEA, DEN, Service de Recherches de Métallurgie Physique, 91191 Gif-sur-Yvette, France

The morphology adopted by small self-interstitial atom (SIA) clusters in metals under irradiation cannot be resolved by experimental techniques. Molecular Dynamics simulations of cascades have shown that while most SIA clusters adopt the standard loop geometry and are highly mobile, a large remaining fraction is immobile [1]. Using a combination of Density Functional Theory (DFT) and empirical potential calculations we show that in iron a particular family of these immobile clusters has an unusual three dimensional periodic structure corresponding to the C15 Laves phase. These C15 aggregates are highly stable compared to the conventional 2D loops and they exhibit large antiferromagnetic moments with respect to the bcc matrix [2].

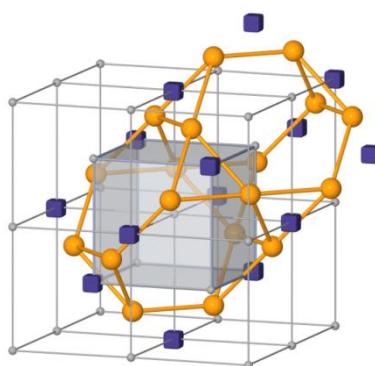


Figure 1: Tetra-interstitial cluster with C15 structure in a bcc lattice. Blue cubes: vacancies, orange atoms: self-interstitials, grey atoms: bcc lattice.

DFT calculations show that in iron the formation energies of C15 SIA clusters are lower by 1.5 eV than that of $<110>$ loops for tetra-interstitials and by 4 eV than that of $<111>$ loops for octa-interstitials [2, 3]. This characteristic is very well reproduced by the M07 EAM potential for iron but not by the Ackland-Mendelev potential. The systematic exploration of the energy landscape performed using the Activation Relaxation Technique (ART) and the M07 potential confirms the exceptional stability of these clusters and shows how they can grow by capturing self-interstitials. These clusters are predicted to be the lowest energy structures up to sizes of about 40 SIAs. According to DFT calculations this behavior does not occur in other bcc metals, except for Ta

but in a smaller range of sizes. This new morphology of self-interstitial clusters thus constitutes an important element to account for when predicting the microstructural evolution of iron base materials under irradiation.

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The thermal stability and structure of neutron irradiation induced vacancy-solute clusters in iron alloys

M. Konstantinović, G. Bonny, Monica Chiapetta

SCK•CEN, Nuclear Materials Science Institute, Boeretang 200, B-2400 Mol, Belgium

The structural properties of nanoclusters formed under neutron irradiation in iron-based alloys are essential for understanding embrittlement and hardening of reactor pressure vessel (RPV) steels. Even at nanometric sizes, the variety of solute, vacancy, interstitial clusters, and their mutual complexes strongly affects the dislocation motion, causing macroscopic changes in the mechanical properties. These changes, occurring in the RPV during service of a nuclear power plant (NPP), are of considerable importance for the safe operation and play a major role in the NPP life extension analyzes.

In this work the thermal stability and structure of clusters formed by neutron irradiation are studied by means of positron annihilation spectroscopy of postirradiation annealed FeCu, FeCuMnNi and FeMnNi alloys and rigid lattice calculations. While most of the vacancy-solute clusters dissolve in the temperature range between 650 K and 700 K, the presence of Ni and Mn solutes in vacancy-MnNi clusters provides an additional thermal stability and shifts the annealing stage corresponding to the dissociation of these clusters to higher temperature. Very good agreement between the measurements and calculations is obtained for vacancy-MnNi clusters of nanometric size, containing of about 25-50 % of vacancies.

Flux coupling between vacancies and interstitial solutes (C, N and O) in α -Fe solid solution

Thomas Schuler, Maylise Nastar

CEA, DEN, Service de Recherches de Métallurgie Physique, F-91191 Gif-sur-Yvette,
France

We show that even at very low concentrations of carbon, nitrogen and oxygen in α -iron (Fe), non-negligible concentrations of vacancy-solute clusters form under equilibrium or irradiated conditions. The net flux of vacancies towards point defect sinks is thus likely to induce an interstitial solute net flux, which can result in radiation induced segregation phenomena.

For each solute, a generalized Hamiltonian is derived on the perfect body-centered cubic lattice including substitutional and octahedral interstitial sites. Interactions are fitted to a whole set of DFT calculations of small vacancy-solute clusters binding energies. Other interactions are then added to the Hamiltonian, corresponding to interactions of Fe or solute atom at the saddle point with the surrounding atoms. The latter are fitted so as to reproduce DFT calculations of migration energies of solutes and vacancies in various environments.

We extend the Self-Consistent Mean Field (SCMF) formalism to systems containing two migrating species (interstitial solutes and vacancies) located on two different sublattices. This extension is validated against Atomic Monte Carlo simulations which are performed at high vacancy and solute concentrations. The atomic diffusion model is inserted into the SCMF formalism and Low Temperature Expansions are used to calculate the ensemble averages and the resulting full Onsager matrix of the system. For the first time, the contribution of multiple vacancies is considered. The amplitude and the sign of flux coupling is observed to strongly depend on the clustering tendency of vacancies and interstitial solutes. Mobilities of vacancy-solute clusters are calculated as well.

This work was supported by the joint program "CPR ODISSEE" funded by AREVA, CEA, CNRS, EDF and Mécachrome under contract n°070551.

Atomic Scale Strengthening Mechanisms due to Hard Obstacles in Fe

Yury Osetskiy, Roger Stoller

Materials Science and Technology Division, ORNL, Oak Ridge, TN 37831- 6138, USA

In this research we have studied dislocation – obstacle interactions over a wide range of environmental and microstructural parameters with the main objectives focused on the direct comparison with available and future experiments. Conventional range of parameters such as obstacle size, temperature range and dislocation speed effects was considered together with the specific output from “computer modeling experiment”. This includes stress-strain behavior, critical resolved shear stress (CRSS) temperature dependence and a complete analysis of the interaction mechanisms and their temperature behavior. For the mechanism analysis we used a recently developed new dislocation characterization and visualization technique that allowed us to define the dislocation line direction and the local Burgers vector with an unachievable so far accuracy. This new technique allows us to have a direct comparison with *in situ* deformation TEM experiments and especially with the recently developed 3D TEM tomography.

This work was supported by the US Department of Energy Office of Fusion Energy Sciences.

Effect of impurities on the mobility of self-interstitial clusters in α -Fe

Anna Serra¹, Napoleon Anento¹, Dmitry Terentyev², Yuri Osetsky³

¹Dept. Matemàtica Aplicada III, Universitat Politècnica de Catalunya, Barcelona, Spain

²SCK•CEN, Boeretang 200, Mol, Belgium

³Materials Science and Technology Division, ORNL, Oak Ridge, TN 37831, USA

Self-interstitial atom (SIA) clusters formed by <111> crowdions are highly mobile in pure iron. MD simulations have shown that cluster trajectories are one dimensional (1D) with an almost continuous motion and activation energy of the order of 0.05eV [1, 2]. However, there is an essential discrepancy between simulations and experiment in terms of the type of movement. Experimentally, 1D migration has been observed as discrete 1D jumps interrupted from time to time due to some invisible obstacles or traps at room temperature [3,4]. In this work, we address the problem of the SIA cluster's trapping mechanism that may lead to the slowing down or complete blockage of highly mobile small (tens of defects) <1 1 1> SIA clusters in bcc Fe due to impurity atoms in solid solution. Thus, we present the interaction of clusters with solute atoms such as C, Ni, Cu, and Cr as well as with the stable solute-vacancy complexes.

Whereas the activation energy for the diffusion of clusters in pure iron is independent on the cluster size, for clusters with diameters under 3nm, the presence of impurities introduces a dependence of the activation energy on the impurity type and concentration, cluster size and temperature.

This work was performed under the auspices of The Spanish ‘Ministerio de Economía y Competitividad’ (FIS2012-39443-C02-02) and the Catalan Government (AGAUR 2009SGR 1003). The computing was partly carried out in CSUC (www.CESUC.CAT). This work was partly supported by the CDP, an Energy Frontier Research Center at ORNL funded by US DOE. The authors acknowledge useful discussions with Dr. Lorenzo Malerba

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Combined Molecular Dynamics and Object Kinetic Monte Carlo simulations of ion implantation in Fe thin films

M. Aliaga¹, I. Martin-Bragado² and M. J. Caturla¹

¹ Dept. Física Aplicada, Facultad de Ciencias, Fase II, Universidad de Alicante, Alicante,
E-03690, Spain

² IMDEA Materials Institute, C/ Eric Kandel, 2, Tecnogetafe, 28906 Getafe, Madrid,
Spain

Ion implantation experiments are being used extensively to validate multiscale models of damage production in metals for fusion applications. In particular, in-situ TEM measurements can be taken during implantation providing detailed information about the process of defect production and evolution.

In this work we present a combined study using Molecular Dynamics (MD) and Object Kinetic Monte Carlo (OKMC) to reproduce the ion implantation experiments in Fe of Yao et al. [1]. Our objectives are, on the one hand, to study the effects of the surface on the distribution of damage and, on the other hand, to follow the evolution of the microstructure of the irradiated material.

These in-situ TEM irradiation experiments require of special conditions of the sample, in particular the use of thin films, with thicknesses that can be as small as 50nm. We prove, using Molecular Dynamics calculations with recent interatomic potentials developed for Fe, that the primary damage in thin films is very different from the primary damage in the bulk material. For example, large vacancy clusters are produced under ion implantation more frequently than in the bulk. They occur near the surfaces. In addition it seems that the largest defect clusters close to surfaces are vacancy in nature and have a Burgers vector $<100>$. We have used the cascade database obtained with MD for thin films and bulk samples as input for the OKMC code MMonCa [2] in order to compare directly to the experiments. In these type of experiments, $<100>$ and $1/2 <111>$ loops are always observed, but the way they evolve from smaller clusters is not clear. We test two different models for the evolution of these clusters. Comparing our simulation results with the experimental ones we are able to assess which of the models is the most accurate.

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Development of object kinetic Monte Carlo models for nanostructural evolution under irradiation in Fe-Cr alloys

Monica Chiapetto^{1,2}, Lorenzo Malerba¹, Charlotte S. Becquart², Giovanni U. Bonny¹

¹ SCK•CEN, Nuclear Materials Science Institute, Boeretang 200, B-2400 Mol, Belgium

² Unité Matériaux Et Transformations, UMET, UMR 8207, USTL, 59600 Villeneuve d'Ascq, France

High-chromium ferritic-martensitic steels are candidate structural materials for future fusion reactors, accelerator driven systems (ADS) and core components in Gen-IV reactors, thanks to their good resistance to irradiation-induced swelling and embrittlement. Starting from the already existing object kinetic Monte Carlo (OKMC) model for neutron irradiated Fe-C binary alloys [1], we developed physically-based sets of parameters able to consider the effects of Cr substitutional solutes and simulate the irradiation-induced nanostructural evolution and defect formation in Fe-Cr alloys. Our models proved to be able to describe the buildup of irradiation defect populations at the operational temperature of light water reactors (~ 300 °C), in terms of both density and size distribution of the defect cluster populations. Four Cr concentrations (2.5, 5, 9 and 12 wt.%Cr) were investigated up to ~ 0.6 dpa under both neutron and ion irradiation and specific reference irradiation experiments were simulated [2,3]. Different dose-rate and irradiation temperature ranges were also investigated.

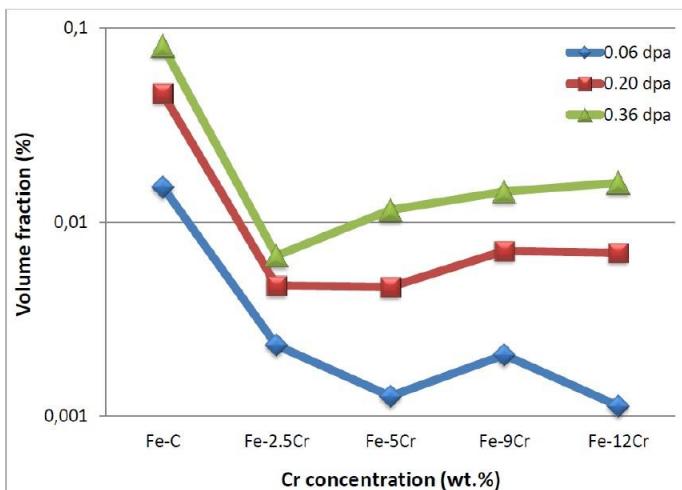


Fig. 1: Volume fraction of the total amount of vacancies after neutron irradiation for different Cr concentrations

observed void swelling suppression. The clustering of the vacancy population, when compared to Fe-C alloys, also appears to be significantly reduced already in the presence of limited Cr concentrations [Fig.1] and increases only slightly with Cr content.

Cr content has been shown to be a key parameter to determine the self-interstitial clusters diffusivity in Fe-Cr alloys, which proved to be strongly reduced in a non-monotonic way depending on both Cr content and cluster size when compared to "pure" Fe. This mobility reduction is the consequence of a relatively long-ranged, ~ 1 nm, attractive interaction between Cr atoms and SIA in the crowdion configuration [4] and exhibits the same non-monotonic dependence on Cr content of empirically

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PERFORM 60 - Prediction of the Effects of Radiation FOr Reactor pressure vessel and in-vessel Materials using multi-scale modelling – 60 years foreseen plant lifetime

A. Al Mazouzi¹, J. Sharples², M. Konstantinovic³, D. Moinereau¹, D. Feron⁴, C Domain¹

¹EDF R&D, Avenue les Renardières, Ecuelles, 77818 Moret sur Loing Cedex, France

²SERCO assurance, Walton House, Warrington Cheshire WA3 6GA, UK

³SCK.CEN, Boeretang 200, 2400 Mol, Belgium

⁴CEA, Saclay 91 191 Gif-sur-Yvette cedex, France

In nuclear power plants, materials may undergo degradation due to severe irradiation conditions that may limit their operational life. Utilities that operate these reactors need to quantify the ageing and the potential degradations of some essential structures of the plant to ensure its safe and reliable operation. So far, to take into account these degradations in the design and safe operation of the installations, the utilities and consequently the safety authorities rely mainly on in-field experience and on the experimental testing of surveillance materials in specialized hot cells.

Continuous progress in the physical understanding of the phenomena involved in irradiation damage and environmental effects, and in computer sciences encouraged the development of multi-scale numerical tools able to simulate the material behavior in nuclear field. Thus, recently, the FP7 Collaborative Project PERFORM 60 [1], has been launched to pursue the improvement of the developed tools under the previous FP6 PERFECT project [2], for reactor pressure vessel (RPV) steels and to initiate the development of similar multi-scale modeling tools to simulate the combined effects of irradiation and corrosion on the RPV internals.

To reach these objectives, twenty European organizations involved in the nuclear field are engaged to develop the necessary computer tools and their integration in a user friendly platform with the main concern to produce experimentally validated physical models to predict the lifetime of these components.

In this lecture, in addition to an overview of the project, the work that is being performed will be illustrated by examples to demonstrate the robustness and the complexity of the multi-scale modeling approach when applied to nuclear materials.

[1] www.perform60.net

[2] www.fp6-perfect.net

Stress and irradiation effects on solute diffusion to dislocations

Dallas R. Trinkle¹, Zebo Li¹, Thomas Garnier¹, Venkateswara Manga², Maylise Nastar³,
Pascal Bellon¹, Robert Averback¹

¹ Materials Science and Engineering, University of Illinois, Urbana-Champaign; Urbana,
IL

² Materials Science and Engineering, University of Arizona; Tucson, AZ

³ CEA, DEN, Service de Recherches de Métallurgie Physique, 91 191, Gif-sur-Yvette,
France

Study of creep under irradiation requires a quantitative description of diffusion of point defects such as vacancies, interstitials, and solutes to traps like dislocations. Prediction of dislocation creep rates involves consideration of diffusion under non-uniform, non-hydrostatic stress, the increased point defect density from irradiation, and the interaction of defects. We present calculations of the diffusion of Si in Ni, which has both vacancy- and mixed-dumbbell mediated diffusion under stress at dilute concentrations. First-principles calculations and self-consistent mean field method (SCMF) calculate the fluxes of various species under stress. Stress reduces the symmetry for hops in FCC Ni, and SCMF provides a direct calculation of phenomenological coefficients—including off-diagonal terms—for the lower-symmetry geometry. In particular, stress changes solute drag in particular directions, which affects the diffusion to sinks under irradiation and the resulting microstructure near dislocations. The final results are combined with the dislocation strain field to model these effects.

Inverse Relation between Strain Rate and Yield Strength of Dislocation-Obstacle Interaction in bcc Fe

Yue Fan¹, Akihiro Kushima¹, Sidney Yip^{1,2}, Bilge Yildiz¹

¹Department of Nuclear Science and Engineering, MIT, Cambridge, Massachusetts 02139

²Department of Materials Science and Engineering, MIT, Cambridge, Massachusetts 02139

Irradiation creep is an important long-term macroscopic degradation phenomenon in nuclear structural materials that involves dislocation interactions with irradiation induced obstacles. The yield strength of dislocation-obstacle interactions exhibit complex relations, for example an inverse relation to strain rate, that is decreasing of critical resolved shear stress while increasing strain rate. To quantitatively assess the dislocation-vacancy cluster interaction in bcc Fe at the time scale beyond conventional atomistic simulations, we combined a novel atomistic approach, the Autonomous Basin Climbing (ABC) method, with transition state theory. The directly simulated strain rates at the atomic level span a wide range from 10^8 s^{-1} down to 10^3 s^{-1} , the lower end of which is far beyond reach to traditional molecular dynamics (MD).

We examine the relation between the critical resolved shear stress (CRSS) and the strain rate, and demonstrate the origin of the inverse behavior between CRSS and strain rate below 10^5 s^{-1} . This behavior arises because of the competition of two driving forces: strain rate and thermal activation. At low strain rate, the obstacle has enough time to nucleate to a stable structure and thus has strong interaction with the dislocation. At high strain rate, however, the vacancy cluster is split into parts because of less time available for nucleation. The split vacancy cluster has larger surface area attached to the dislocation and yields a higher CRSS as well. Therefore the interaction leads to a “V” shape relation between the CRSS and strain rate (that is, decreasing at low strain rate and increasing at high strain rate) with the minimum at 10^5 s^{-1} . The interactions at high strain rates are directly benchmarked against MD simulations, and the results are well consistent with each other. This work shows that even a unit process can induce an inverse behavior, which complements the previous macroscopic models.

Interactions between mobile dislocations and radiation induced loops: a multiscale approach

L. Dupuy¹, X. Shi¹, L. Vincent¹, B. Devincre², D. Terentyev³, A. Etcheverry⁴, P. Blanchard⁴, O. Coulaud⁴, E. Ferrie⁵, M. Bletry⁶

¹SRMA, CEA-Saclay, 91191, Gif-sur-Yvette, France,

²Laboratoire d'Etude des Microstructures, CNRS-ONERA, 92322 Châtillon, France

³SCK-CEN, Nuclear Materials Science Institute, B-2400 Mol, Belgium

⁴HiePACS team, Inria Bordeaux Sud-Ouest

⁵Laboratoire SIMAP, CRNS-Grenoble-INP, 38402 St Martin d'Hères, France

⁶Institut de Chimie et des Matériaux Paris-Est, 94320 Thiais, France

The mechanical behavior of reactor pressure vessels steels and internals is affected by neutron irradiation, which induces the presence of defects such as Frenkel pairs, voids or loops. In this study, particular focus is given to interstitial loops. The modelling of this phenomenon requires a multi-scale approach going from the study of individual dislocation-loop interactions at atomic scale to the study of the collective behavior of dislocations at grain scale using dislocation dynamics simulations.

The interactions mechanisms between individual loops and gliding dislocations have been thoroughly studied at atomic scale using molecular dynamics within the Perform 60 project. Building on these results we show how it is possible to introduce these elementary mechanisms in our dislocation dynamics code Numodis [1], and to reproduce both qualitatively and quantitatively most of these hardening mechanisms. Various configurations are considered in both ferritic and stainless steels, with different dislocation characters (screw/edge) and different types of loops.

The good agreement between these two scales proves the validity of this multiscale approach, and opens the door to large scale simulations that are required to feed crystal plasticity models. Such simulations are currently made possible through the development of a new parallel code OptiDis based on a hybrid OpenMP/MPI paradigm. The performance of OptiDis will be demonstrated on a system containing a high density of radiation-induced loops involving about a million of interacting segments.

This work was partially performed in the framework of the EC-funded FP7/PERFORM60 project, under agreement 232612. OptiDis is a joint project between CEA Saclay, Inria, Paris-Est and Grenoble-INP funded by ANR COSINUS 2010.

[1] Numodis: <http://www.numodis.fr/>

Modeling of Tensile Deformation in Irradiated RPV steel

Pritam Chakraborty, S. Bulent Biner

Idaho National Laboratory, Idaho Falls, Idaho 83401, USA

The fracture behavior of Reactor Pressure Vessel (RPV) steels shows a strong dependence to temperature and irradiation. A transition from ductile (higher fracture toughness) to cleavage mode of fracture (lower fracture toughness) is observed with decreasing temperature. Also, due to the inherent statistical nature of cleavage fracture, large scatter in fracture toughness values is common in the ductile to brittle fracture transition (DBT) regime. Irradiation introduces additional lattice defects and precipitation/segregation of alloying elements, thus reducing the ductility of the material, and increasing the DBT temperature. To capture such variable fracture behavior of RPV steels, a combination of ductile damage and statistically based weakest link models has been successfully used in the past. Though these models provided satisfactory comparison of fracture properties with experiments, their accuracy strongly depends on the temperature and irradiation dependent flow stress (true stress-plastic strain) behavior obtained from tensile experiments. Under low dose irradiation or unirradiated conditions, significant strain hardening prior to onset of necking can be observed in the stress-strain behavior of tensile specimens. Hence the strain hardening behavior in the flow stress evolution can be clearly separated from damage initiation and growth. However with increasing irradiation level, a significant decrease in uniform elongation in conjunction with increase of yield stress are usually observed. The dislocation channeling has been considered to explain the strain softening behavior. Inverse methods using finite element (FE) simulations has been used to obtain the flow stress behavior under such situation [1]. However, ductile damage, which also contributes to strain localization and softening, has been neglected. In the present work, an attempt has been made using the GTN model [2] for ductile damage and, power law hardening and exponential softening for flow stress evolution, to identify their respective contribution on the engineering stress-strain behavior. Both stress and strain based void nucleation criterion are considered in the GTN model to investigate the effect of damage initiation on uniform and total elongation. Correlations between GTN and flow stress model parameters, and irradiation dose and temperature are also developed by simulating engineering stress-strain curves from the tensile tests. These model parameters will be used in a subsequent study to predict DBT in RPV steels under irradiated condition.

This work is funded through the Light Water Reactor Sustainability Program at Idaho National Laboratory.

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Multiscale simulation of strengthening induced by small dislocation loops

Ghiath Monnet

EDF, MMC

It is widely known that irradiation induces point defect clusters which grow to form Dislocation Loops (DLs) of different natures and sizes in addition to other defects as voids, stacking fault tetrahedrons, precipitates, etc. The evolution of the microstructure under irradiation is accompanied by a significant strengthening and a loss in ductility. The origin of these effects is still under debate and no physically-based quantitative theory is known to explain the basic features of radiation strengthening.

In this work we present a multiscale approach of strengthening induced by dislocation loops. Molecular Dynamics (MD) simulations have shown that dislocation interactions with DLs depend on the temperature, the loop nature and size and the dislocation character. In many cases, MD results revealed that small DLs of sizes less than 4 nm are often absorbed by the moving dislocation, forming super-jogs on edge dislocations and helical turns on screw dislocations. This feature has been implemented in Dislocation Dynamics (DD) simulations in order to compute the strengthening induced by the small DLs. In these simulations, we investigate the effect of the: loop size, dislocation character, friction stress and strain rate. In all simulation conditions, results show a large strengthening, substantially larger than the strengthening induced by impenetrable obstacles of equivalent size and density. Small dislocation loops are dragged by the moving dislocation creating a strong heterogeneity in the DL density and distribution.

Simulation for dislocation core structure of solute atom clusters using generalized stacking fault energy

- Dislocation core structure and shear modulus of ternary iron alloy of FeCuMn, FeSiMn, and FeNiMn -

Toshiharu Ohnuma, Kenichi Nakashima

Central Research Institute of Electric Power Industry
2-11-1, Iweado Kita, Komae-shi, Tokyo, 201-8511 Japan

Solute atom clusters enriched with Cu, Ni, Mn, and Si are formed in the reactor pressure vessel (RPV) steels of light water reactors irradiated by fast neutrons. The clusters become obstacles impeding the movement of dislocations, resulting in the embrittlement of RPV steels. Therefore, understanding the mechanism through which clusters of solute atoms interact with dislocations is important in order to correlate the changes in the microstructures of RPV steels with the mechanical property changes of RPV steels. Generalized stacking fault energy, which represents the total change in energy when a crystal that is partly in the slip plane rigidly shifts, is a key parameter used to determine the structure and mobility of dislocations that run through a given metal crystal. We calculated from first principles the generalized stacking fault energies and shear modulus for the FeCuMn, FeSiMn, and FeNiMn ternary-iron-alloy crystals and used the fractional dislocation model to calculate the dislocation core structures in the crystals.

Defect-induced plasticity in CuNb nanocomposites

Enrique Martínez¹, Alfredo Caro¹, Irene J. Beyerlein²

¹Material Science and Technology Division, MST-8, Los Alamos National Laboratory,
Los Alamos, 87545 NM, USA

²Theoretical Division, T-3, Los Alamos National Laboratory, Los Alamos, 87545 NM,
USA

Nanolaminate composites have been proven stable under light ion irradiation. In this paper we analyze the change in mechanical properties of model CuNb nanocomposites in vacancy supersaturated environments. We have performed compression tests using molecular dynamics for different defect contents. We have added different number of vacancies into the misfit dislocation intersections (where their formation energy is lower), and calculated the yield stress. We observe that for a small number of defects, the yield point hardly varies, while when the number of vacancies is large, the yield point substantially decreases, nucleating twins instead of partial dislocations. We have also tested the effect of heavy ion irradiation including different distributions of stacking fault tetrahedra (SFTs) in the Cu layer and voids in the Nb side. We see that dislocations nucleate at the SFTs at about 1/3 of the stress needed to nucleate dislocations at the interface in the pristine sample. In the Nb layer, vacancy loops nucleate at voids, and glide to be absorbed at the interface modifying considerably the nucleation stress compared to the pristine sample. We have analyzed in detail the dislocation-interface interaction mechanisms under different conditions, showing how dislocations react with the misfit dislocations present at the interface to modify the atomic structure of the boundary, which suggests that the interface could be designed to optimize its defect healing properties. We conclude that interfaces help in recovering materials subjected to heavy-ion irradiation.

Modelling of the effect of slip localization on grain boundary fracture in pre-irradiated austenitic stainless steels. Comparison with experimental data

Maxime Sauzay¹, Mohamed Ould Moussa¹, Boubakar Diawara², François Lebreau²

¹ CEA, SRMA, Bât. 455, 91191 Gif sur Yvette, France;

² Ecole Chimie Paris, 75005 Paris, France

Slip localization is a common feature in post-irradiated metallic poly-crystals undergoing tensile straining. This effect takes place for instance in the form of thin slip bands called channels or clear bands, formed after the local vanishing of irradiation defects induced interactions with gliding dislocations. Channel impingement towards grain boundaries (GBs) should induce local stress concentrations along GBs, in the quasi-elastic surrounding matrix. It has been shown extensively that this trigger GB crack initiation [1].

Since the fifties, the clear band stress fields have been modeled using the dislocation pile-up theory, which leads to stress singularities similar to the LEFM ones [2]. But such theory does not allow fair predictions of GB fracture, neither in inert or PWR environment [3]. In practice, channel thickness is at least 50 nm depending on material, temperature and loading conditions. As a matter of fact, many slip planes are plastically activated through the channel thickness. Numerous crystalline finite element (FE) computations have been carried out using microstructure inputs varying in broad ranges (slip band aspect ratio and spacing). Slip bands (low critical resolved shear stress) are embedded in a matrix or small aggregates (high CRSS). Microstructure inputs as well as plasticity parameters are evaluated based on TEM observations and dislocation dynamics computation results. High local stress fields are highlighted but they are nevertheless considerably lower than the ones deduced from the pile-up theory. Analytical formulae are deduced from the numerous FE results, accounting for channel thickness, grain size, channel density and crystal / GB orientations [6,7].

Grain boundary fracture is simulated using a double criterion based on both critical normal stress and fracture energy as deduced from atomistic computations of GB fracture [4]. The critical stress is deduced from the fracture energy using the universal-binding-energy relationship (UBER). In the case of brittle fracture, the fracture energy is defined as the two fresh free surface energy values minus the GB energy. A close-form expression giving the remote tensile stress to GB fracture is then deduced [6,7].

Finally, GB fracture of pre-irradiated SS (dose > 10 dpa) loaded in either inert or pressurized water reactor (PWR) environment is predicted for comparison with the existing experimental results obtained in similar conditions.

In the case of inert environment, free surface and GB energy values are easily found in literature. The predicted remote tensile stress to GB fracture is then equal to the yield stress in agreement with various experimental data.

In the case of PWR environment, GBs are assumed to be oxidized up to a depth of a few μm due to Cr depletion induced by the strong RIS observed at high irradiation dose [1]. Either literature data have been used (iron oxides [5]) or they have been computed by the DFT method for various GBs and by accounting for hydration / hydroxylation of the fresh free surfaces in PWR water (Cr_2O_3 oxide). Using the lowest fracture energies corresponding to the weakest GBs, the predicted remote tensile stress to oxidized GB fracture is about one-half of the yield stress, once more in fair agreement with many experimental data despite no parameter fitting is required. The influence of irradiation dose, strain rate and irradiation creep is finally quantitatively discussed.

This research work was supported by the european project PERFORM60 (FP7-232612).

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Multiscale cleavage fracture initiation model accounting for material microstructure and effects of irradiation

Anssi Laukkonen, Tom Andersson, Tapio Planman, Kim Wallin

VTT Materials and Manufacturing, Espoo 02044-VTT, Finland

Fracture initiation models typically contain limited information regarding material behavior at the mesoscale, especially with respect to polycrystalline microstructures. As a result, the methodologies and criteria can be quite phenomenological as far as their description of the micromechanical chain of events is concerned. This limits their use as far as being able to yield any exploitable predictive ability. One proposed solution has been the direct inclusion of microstructural deformation and anisotropic plasticity mechanisms on an aggregate scale in derivation of improved next generation cleavage initiation models, and as such, creating a multiscale cleavage fracture initiation model. This route is adopted also in current work to enrich the treatment of cleavage fracture and better incorporate the effects of irradiation in the fracture toughness predictions.

To that effect, crystal plasticity analyses founded on a dislocation dynamics based constitutive model are carried out for “Eurocurve Material A”. The crystal plasticity model is applied to a lath containing aggregate mesh over three differing states of imposed constraint in order to derive triaxial stress states ranging from those of uniaxial tensile tests to those indicative of near crack-tip plane strain conditions. The aggregate in question is founded on the microstructural morphology present in lower bainitic pressure vessel steels. Effects of irradiation are directly introduced to the crystal plasticity constitutive model via a defect density parameter, and as such influence the anisotropic deformation behavior of the material.

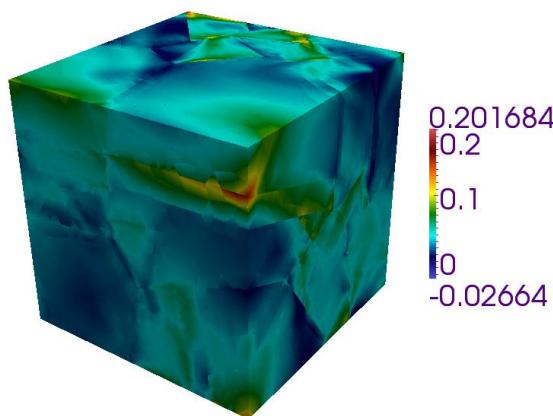


Figure 1: Contours of axial strain in a polycrystalline crystal plasticity aggregate of reactor pressure vessel steel.

The findings demonstrate the effects of temperature and crack-tip constraint on the distribution of stress and strain fields within the polycrystal aggregate, and are utilized further in the hierarchical multiscale modeling chain in development of a cleavage fracture model, a revised implementation of the micromechanically informed WST cleavage initiation model. The hierarchically upscaled crystal plasticity and cleavage fracture model is demonstrated to yield improved fracture toughness predictions within the ductile to brittle transition region.

White-noise quantum heat bath for MD and SLD simulations in magnetic materials

C. H. Woo, A. A. Semenov, Haohua Wen

Department of Physics and Materials Science, City University of Hong Kong, Hong Kong SAR, China

In both MD and SLD models, phase-space trajectories of activation processes are obtained by integrating classical equations of motion. Thermodynamic equilibrium/quasiequilibrium conditions among different parts of the system are maintained through temperature, which is controlled through the use of classical Boltzmann statistics. This route cannot produce sufficiently accurate results unless the atoms under consideration have wavelengths shorter than the interatomic spacing, and have vibrating frequencies corresponding to a Debye temperature much lower than the temperature of interest. In the former case, the classical particle picture breaks down and transition via quantum tunneling must be considered. In the latter case, quantum statistics have to be used to ensure that the correct thermodynamics conditions are kept in the simulations. Well known cases in MD simulations where quantum effects must be considered include light atoms such as hydrogen and helium. A similar, but even more serious, problem exists in SLD simulations of irradiation-generated lattice defects in magnetic materials. The quantization of the energy spectrum of the spin system is about an order of magnitude larger than that of the lattice and its effects cannot be neglected even for temperatures higher than the melting point of iron. Under such conditions the heat reservoir designed to control the spin temperature based on classical statistics fails. A quantum-physics based methodology is required to remove the restriction of the classical thermostat to solve this problem. In this paper, we will show that a white-noise temperature control can be reformulated based on the Langevin thermostat methodology. By recasting the scheme in an alternate form, using the Bose-Einstein statistics instead of the Boltzmann statistics, a quantum heat reservoir may be constructed from a simple modification of the classical fluctuation-dissipation relation. Development of the theory and associated numerical techniques for the quantum heat reservoir is considered in this presentation.

Effects of magnetism and strain relaxation on the phase stability of multi-component alloys

Jan Wrobel, D. Nguyen-Manh, M.Y. Lavrentiev, S.L. Dudarev

CCFE, Culham Science Centre, Abingdon, Oxon, OX14 3DB, UK

Fe-Cr-Ni alloys and austenitic steels form an important class of high temperature structural materials developed for nuclear and related applications. Fe-Cr-Ni alloys are among the most extensively studied ternary alloy systems, still the relation between their phase diagram, still the effect of magnetism on their phase stability and defect structures formed under irradiation is not known. We investigate Fe-Cr-Ni alloys by using a combination of several simulation methods. Density functional theory (DFT) and Cluster Expansion methods are combined in order to derive the cluster expansion parameters characterizing bcc and fcc crystal structures. DFT-based Monte Carlo (MC) simulations are then used for predicting the relative stability of fcc and bcc phases in Fe-Cr-Ni at elevated temperatures. Enthalpies of formation obtained from MC simulations at finite temperatures, as well as order-disorder temperatures and short-range order parameters predicted for a broad range of temperatures are compared with experimental data. Magnetic Cluster Expansion, a new method that extends the conventional Cluster Expansion to magnetic alloys, is applied to modelling magnetic phase transitions, with the emphasis on non-collinear magnetic configurations. We apply the above methodology to multi-component high-entropy alloys, exploring the effect of fluctuating microscopic strains and stresses, associated with the difference between volumes and electronegativities of the alloying elements, on the phase stability of crystalline versus amorphous phases of the alloys.

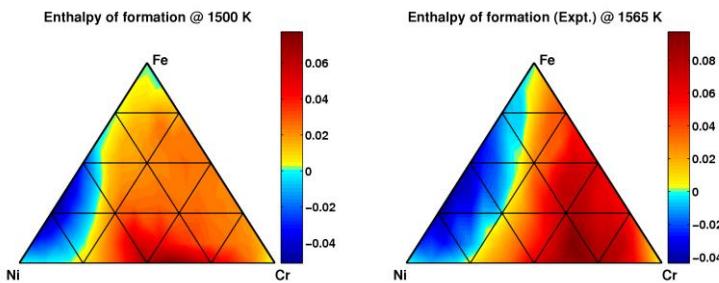


Figure 1: Enthalpies of formation (in eV) for the most stable crystal structures of Fe-Cr-Ni alloys computed using MC simulations at 1500 K (left). Experimental data from Ref. [1] are shown on the right.

This work was part-funded by the Accelerated Metallurgy Project, which is co-funded by the European Commission in the 7th Framework Programme (Contract NMP4-LA-2011-263206), by the European Space Agency, by the individual partner organisations, by the RCUK Energy Programme [grant number EP/I501045] and by the European Union's Horizon 2020 research and innovation programme. To obtain further information on the data and models underlying this paper please contact PublicationsManager@ccfe.ac.uk. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

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Effect of point defect sinks on irradiation-induced compositional patterning

Shipeng Shu, Pascal Bellon, Robert S. Averback

University of Illinois at Urbana-Champaign

The dynamical competition between the chemical mixing forced by energetic particle irradiation and thermally activated decomposition can lead to the stabilization of self-organized steady states in alloy systems comprised of immiscible elements. Continuum modeling and atomistic simulations predicted the stabilization of steady-state nanoscale compositional patterns for a well-defined range of ballistic mixing frequency normalized by the irradiation-enhanced thermal atomic jump frequency. While irradiation-induced compositional patterning has been observed experimentally, a quantitative comparison has been lacking because models and simulations had relied on a simplified treatment with a fixed point defect concentration. We have developed a novel kinetic Monte Carlo code that treats vacancies and interstitials as non-conserved species, including their production, recombination, and elimination on sinks. By controlling the sink density for the point defects to be in the sink dominated elimination regime, steady-state compositional patterns can be stabilized over a much larger temperature range than predicted before. These predictions are tested by comparing the characteristics of patterning in Cu-Ag and Cu-Ag-W alloys, and in particular the maximum irradiation temperature for Ag precipitates to maintain a stable size under irradiation. In addition, KMC simulations performed on systems with two planar sinks with different sink efficiency reveal that segregation and precipitation under irradiation offer a direct way to measure the relative sink efficiency of these two sinks.

Radiation induced grain boundary flow – Effects of grain boundary segregation

Yinon Ashkenazy¹, Amir Porat¹, Robert S Averback²

¹The Hebrew University of Jerusalem

²University of Illinois at Urbana Champaign

Irradiation of crystalline structure in conjunction with stress causes the materials to slowly deform (“creep”), resulting in changes to the material’s dimensions and strength. We recently demonstrated a new mechanism for irradiation-enhanced creep in nanocrystalline materials. The deformation is due to local atomic relaxations within the grain boundaries as they absorb point defects e.g., interstitials and vacancies, produced in the grain interior during irradiation. Similarities between these relaxation events and “strings” observed in flow of amorphous systems are discussed. We then use atomistic and analytic mean field model to establish the role of immiscible atoms on the grain boundary flow, discussing its effect on the localized relaxation events as well the integral macroscopic flow. We analyze the effects of various segregation scenarios, from isolated dilute gb solution to formation of immiscible precipitates, through their effect on the characteristics of the relaxation events.

Ion-Irradiation Induced Vacancy and Interstitial Clusters in Fe Investigated by X-Ray Diffuse Scattering and by Continuum and Molecular Dynamics Simulations

B. C. Larson¹, J. Z. Tischler², Yury Osetskiy¹, R. E. Stoller¹,
H. Bei¹, Y. Gao^{1,3}, Y. Zhang^{1,3}

¹Oak Ridge National Laboratory, ²Argonne National Laboratory
³University of TN-Knoxville

We have performed fundamental investigations of vacancy and interstitial defect clusters generated during room-temperature 15-MeV Ni-ion irradiation of Fe and Fe-Cr single crystals using x-ray diffuse scattering measurements near Bragg reflections. The measurements were analyzed using continuum anisotropic elasticity simulations of lattice distortions for vacancy and interstitial loops and by molecular dynamics simulations for voids and vacancy clusters as well as for vacancy and interstitial loops. Synchrotron x-ray diffuse scattering measurements were performed near the (002) reflection of <001> oriented Fe and Fe-Cr single crystals and analyzed within the so-called asymptotic regime using continuum and MD based scattering cross-sections. Measurements for irradiations corresponding to one displacement per atom (DPA) at ambient temperature will be presented and discussed in connection with determinations of the presence of vacancy and interstitial type clusters, determinations of the cluster types and orientations, and size distributions using the so-called local Bragg scattering interpretation. The method for calculating diffuse scattering cross sections directly from simulations of the atomic displacements around $a/2(111)$ and $a(100)$ vacancy and interstitial loops and around 3D vacancy clusters and voids.

Acknowledgement: Research supported by the US DOE, Basic Energy Sciences, Center for Defect Physics Energy Frontier Research Center. The Advanced Photon Source is supported by the US DOE, Basic Energy Sciences Facilities Division.

Modeling of swelling under electron, ion, and neutron irradiation

S.I. Golubov¹, A.V. Barashev^{1,2}, R.E. Stoller¹

¹Materials Science and Technology Division, ORNL, Oak Ridge, TN 37831- 6138, USA

²Department of Materials Science and Engineering, Center for Materials Processing,
University of Tennessee, East Stadium Hall, Knoxville, TN 37996-0750, USA

Development of radiation resistance materials requires understanding the controlling degradation mechanisms for structural materials, which can guide the development of a strategy for creating a new generation of the materials. To obtain these data using existing nuclear reactors requires keeping the materials in reactors for ~10-20 years, which is unfeasible. The only timely way to obtain the required data is to use charged particle irradiation since the high doses required can be reached in orders of magnitude smaller times because damage production rates are much higher than those in reactor irradiations. However, the utilization of such data to predict behavior under neutron irradiation, which is the main goal, is not straight forward. High dose rate ion irradiation conditions are qualitatively different from in-reactor irradiation. This situation has been considered in many papers but the analysis used there has been rather qualitative. The main objective of this presentation is to provide a quantitative comparison of damage accumulation in the form of swelling taking place under different types of irradiation. The computational method used here is based on a numerical integration of the master equation for the void size distribution. The calculations have been done using the RIME code developed at ORNL, which is based on a grouping method developed at ORNL as well. The implications of results for comparing data between ion and neutron irradiation is discussed.

Ductility and work hardening in nano-sized and irradiated metallic glasses

D.Z. Chen¹, D. Jang¹, X.W. Gu², K.M. Guan², Q. An³,
W.A. Goddard, III³, J.R. Greer^{1,4},

¹Division of Engineering and Applied Sciences, California Institute of Technology,
Pasadena CA, 91125

²Department of Chemistry and Chemical Engineering, California Institute of Technology,
Pasadena CA, 91125

³Materials and Process Simulation Center, California Institute of Technology, Pasadena
CA, 91125

⁴The Kavli Nanoscience Institute, California Institute of Technology, Pasadena CA,
91125

We report results of in-situ nano-tensile experiments performed on 70nm-diameter free-standing NiP metallic glass nanostructures made using a template electroplating technique. These samples exhibit tensile true strains of ~18%, an amount comparable to compositionally-identical 100nm-diameter samples made via focused ion beam (FIB) and ~3 times greater than 100nm-diameter samples produced via the same methodology. Simultaneous in-situ observations and stress-strain data during post-elastic deformation reveal necking and work hardening, features vastly uncharacteristic for metallic glasses. The evolution of free volume distribution within the sample during elastic and plastic deformation revealed by Molecular Dynamics simulations on two 30nm NiAl samples, irradiated and as-cast, shows evidence of a free surface-mediated free volume relaxation mechanism, leading to the observation of a new plasticity mechanism for nano-sized metallic glasses.

Modelling self trapping and trap mutation in tungsten using DFT and Molecular Dynamics with an empirical potential based on DFT

J. Boisse^{1,2}, C. Domain^{1,3}, A. De-Backer^{1,4}, C.S. Becquart¹

¹ Unité Matériaux et Transformations, UMET, UMR 8207, Université de Lille 1, F-59655 Villeneuve d'Ascq, France

² Laboratoire d'Energétique et de Mécanique Théorique et Appliquée, LEMTA , UMR 7563, Université de Lorraine, F-54504 Vandoeuvre-lès-Nancy, France

³ EDF-R&D, Département MMC, Les renardières, F-77818 Moret sur Loing, France

⁴ CCFE, Culham Science Centre, Abingdon, Oxon, OX14 3DB, UK

Being virtually insoluble in metals, but very mobile, He atoms can be trapped, associate with vacancies, forming platelets and bubbles. They have been shown to contribute to swelling, cause intergranular embrittlement and produce roughening and blistering at metal surfaces. Being repelled by the metal atoms, He atoms form stable clusters, which are also mobile. This tendency to form clusters is so strong that when too many He atoms are aggregated together it can be less costly to relieve the strain created by the interstitial elements by the ejection of one or more matrix atoms leading to the formation of one or more Frenkel Pairs (FP), i.e. vacancies and Self Interstitial Atoms (SIAs). When no vacancy is initially present, the He cluster will be trapped by the vacancy it created, in a self-trapping (ST) event; whereas when one or more vacancies are already associated with the He cluster, the same mechanism is referred to as trap mutation (TM) or loop punching, if more than one SIA is created. The metal studied in this work is tungsten, candidate for the divertor and currently under heavy investigations experimentally and theoretically. We have thus investigated the thermodynamics and kinetics of ST and TM using Density Functional Theory (DFT) calculations and Molecular Dynamics with a recently developed potential for W-He adjusted on DFT calculations. The stability of helium-vacancy clusters (He_nV_m) as well as pure interstitial helium clusters in tungsten results from a competitive process between thermal emission of vacancies, self interstitial atoms (SIAs) and helium, depending on the helium-to-vacancy ratio in mixed clusters or helium number in pure interstitial helium clusters and will be presented in this work.

Inert-gas defects and trapping of helium in bcc transition metals: *Ab initio* predictions and thermal desorption spectroscopy validation

Duc Nguyen-Manh, Sergei L. Dudarev

CCFE, Culham Science Centre, Abingdon, Oxfordshire OX14 3DB, United Kingdom

Modelling radiation effects formed through the bombardment of metals and alloys by inert gas ions is important because inert gas defects contribute to embrittlement and swelling of structural and plasma-facing materials, an issue of critical significance for fission and fusion power generation technologies. So far, experimental and theoretical effort has been focused primarily on the combined synergistic effects associated with the simultaneous accumulation of helium and hydrogen, and the effect associated with the incorporation of inert gases has not been systematically studied even though the agglomeration of noble gas atoms in metals and alloys is a well known phenomenon observed in multi-beam ion implantation irradiation experiments.

We investigate the structure and properties of defects resulting from the incorporation of noble-gas atoms (He, Ne, Ar, Kr, Xe) into all the bcc transition metals, including iron, using first-principles density functional theory (DFT) calculations. Helium is a relatively small atom and the scale of He defect energies is smaller than that corresponding to other noble gas atoms. The atom size effect changes the relative stability of tetrahedral and octahedral defects for Ne, Ar, Kr and Xe in comparison with He. There is a remarkable trend exhibited by the binding energy associated with interaction between inert-gas atoms and vacancies, where a pronounced and colossal size effect is observed when going from He to Ne, Ar, Kr, Xe. The origin of this trend can be explained by electronic structure calculations that show that p-orbitals play an important part in distinguishing the last four inert-gas elements from helium, which contains only $1s^2$ electrons in the outer shell. Figure 1 shows DFT predicted binding energies, validated by experimental thermal desorption spectroscopy measurements, of a helium atom trapped by five different defects (the substitutional He atom defect HeV, Ne, Ar, Kr, Xe) in Tungsten [1]

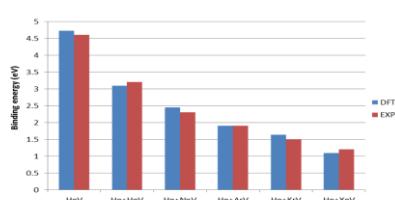


Figure 1: Comparison of predicted values of binding energies between He and various defects (HeV, Ne, Ar, Kr and Xe) with experimental measurements derived from thermal desorption spectrometry of bcc tungsten.

We have also investigated the attachment of He clusters to inert gas impurity atom traps in all the bcc transition metals. The results form a trapping energy database required for modeling helium bubble nucleation in bcc metals and alloys.

This work was part-funded by the RCUK Energy Programme [grant number EP/I501045] and by the European Union's Horizon 2020 research and innovation programme. To obtain further information on the data and models underlying this paper please contact PublicationsManager@ccfe.ac.uk. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

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Multiscale Modeling of Defect Cluster Evolution in Irradiated Structural Materials

Brian D. Wirth, D. Xu, A. Kohnert

Department of Nuclear Engineering, University of Tennessee

Irradiation effects impact structural materials performance in nuclear environments. Irradiation effects initiate from displacement cascades, and are ultimately determined by the diffusional transport and fate of point defects and their clusters, along with solute and impurity re-distribution. This presentation will introduce the inherently multiscale nature of irradiation effects in materials and describe a multiscale research paradigm based on close integration of materials modeling and experimental characterization. Results will be presented from in-situ ion irradiation studies of thin film materials in the transmission electron microscope of molybdenum and ferritic/martensitic steels. In this effort, spatially dependent cluster dynamics models, which are informed by lower length scale understanding of cascade dynamics and defect cluster behavior, are shown to be in good agreement with the fine details of the dose, dose rate and sample dimension dependencies of the defect density and size distribution observed experimentally for low dose irradiation.

Prediction of material behavior after irradiation for reactor pressure vessel steels and reactor internals : modeling aspects and implementation in the PERFORM platform

Félix Latourte¹, Jean-Michel Proix², Gilles Adjancourt, Ghiath Monnet¹

¹EDF R&D, MMC Department, Ecuelles, 77818 Moret-sur-Loing Cedex, France

²EDF R&D, AMA Department, 92 Clamart, France

In the frame of FP7 PERFORM60 European project [1,2], a main objective is to establish multi-scale models to predict the behavior of reactor pressure vessel steels and reactor internals. Once the models are proposed and validated, they are implemented in a numerical platform aiming at providing simple tools to both researchers and industrial users to conduct a wide range of calculations crossing length-scales from ab-initio to molecular dynamics, dynamics of dislocations, crystal plasticity and fracture mechanics. These different calculations will be briefly introduced, as well as the possible chaining between these calculations. The original methods introduced in the platform to take advantage of time consuming small scale simulations like molecular dynamics used to obtain atomic displacement cascades will be introduced, as well as specific and efficient methods like Object Monte-Carlo methods to predict longer term microstructure evolution once the cascade database is available. Larger scale simulations will be also discussed, and more specifically the introduction of irradiation in crystal plasticity laws and the calculation of the material fracture toughness and its change with irradiation. A live demonstration of the platform will allow future potential users to realize the possibilities of use and appreciate the calculation efficiency.

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The necessary initial conditions for simulation of damage cascades under neutron irradiation

Mark R. Gilbert, Jean-Christophe Sublet

CCFE, Culham Science Centre, Abingdon, Oxfordshire OX14 3DB

A key requirement for the accurate prediction of the damage accumulation due to neutron irradiation is a full description of the nuclear events, resulting from interactions with neutrons (for example, generated in fusion plasmas or fission fuel rods), which produce the primary knock-on atoms (PKAs) that initiate the cascades. This is a more relevant transfer of information between complex calculations of neutron irradiation fields and the modelling and experiment of materials to investigate radiation damage, than the simple integrated quantities such as ‘displacements per atom’ (dpa) used normally. The need to use the data from neutron transport calculations more fully has become more urgent due to recent work that identified the large variation in neutron field and integrated dpa values as a function of position within the latest conceptual designs for the DEMO fusion reactor [1,2].

In this work, we have developed a computational methodology to enable the complete distribution of PKA energies for all atomic species (either pre-existing or those created by nuclear reactions) in a material subjected to a given neutron field. This involves taking data from the latest nuclear cross section data files to produce PKA cross section matrices, combining these with an appropriate neutron energy spectrum, and processing the results to produce output that is most applicable for subsequent statistical analysis of damage accumulation (perhaps using the results of extensive cascades simulations).

We present results for several important materials, with an emphasis on fusion materials, and, in particular, consider how the results vary with neutron field in DEMO. We find that the assumed PKA energies often used in displacement cascade simulations are in no-way representative of the complex picture observed in full PKA spectra. For instance, while the average PKA energy of Fe atoms in Fe may be of the order of a few 100s of keV, the full spectrum shows that recoils are produced with energies ranging from a few eV (where cascades would not be produced) right up to 1 MeV. Additionally, there are a significant proportion of recoils associated with transmutation nuclear reactions (such as neutron capture followed by proton or alpha-particle emission – producing, in Fe, Mn and Cr, respectively). While the probability of these reactions is lower than the dominant, simple scattering reactions, their PKA energies are generally higher (Cr atoms can be generated in Fe with recoil energies of more than 2 MeV). Furthermore, the energies of the secondary emitted (light) particles from these inelastic reactions can be much higher, with alpha-particles in Fe generated at 10 MeV or more. Such species are likely to produce markedly different damage compared to the lower-energy “standard” recoils of atoms identical to the host lattice.

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This work was part-funded by the RCUK Energy Programme [grant number EP/I501045] and by the European Union’s Horizon 2020 research and innovation programme.

Elastic trapping of dislocation loops in ion-irradiated tungsten foils

Daniel R Mason¹, Xiaoou Yi^{1,2}, Marquis A Kirk³, Sergei L Dudarev¹

¹ CCFE, Culham Science Centre, Abingdon, Oxfordshire OX14 3DB, United Kingdom

² Department of Materials, Oxford University, Oxford OX1 3PH, United Kingdom

³ Materials Science Division, Argonne National Laboratory, Argonne, WI, USA

We have investigated the role played by the elastic interaction between defects produced in radiation damage cascades with a joint experimental and modelling approach. Using in situ transmission electron microscopy, we have observed the nanoscale dislocation loops formed when ultra-high-purity tungsten foil is irradiated with a low fluence of self ions at a range of irradiation temperatures. The loops seen are predominantly of prismatic $1/2<111>$ type, of vacancy character, and formed close to the surface. Concurrently we have performed object kinetic Monte Carlo simulations of the evolution of self ion damage in tungsten foil. The simulations have been seeded with the best available cascade morphology statistics derived from molecular dynamics; with loops, clusters and vacancies treated entirely equivalently, and with no parameters tuned to improve the fit to experiment.

We find that the number density and size distribution of loops observed is reproduced only if the elastic interaction between loops is taken into account. Our simulations show how important residual defect statistics one nanosecond after a cascade are for understanding experimental observation one second later, and our analysis highlights the profound effect of elastic interaction between defects on the microstructural evolution of irradiated materials.

This work was part-funded by the RCUK Energy Programme [grant number EP/I501045] and by the European Union's Horizon 2020 research and innovation programme. To obtain further information on the data and models underlying this work please contact PublicationsManager@ccfe.ac.uk. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

Defect Interaction and Evolution in Iron and Its-based Alloys

Haixuan Xu¹, G. Malcolm Stocks² Yury Osetsky², Roger. E. Stoller²

Department of Materials Science and Engineering, The University of Tennessee,
Knoxville, TN, 37996, USA

Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge,
TN 37831-6114, USA

The evolution of defects governs the microstructure and properties of materials for various energy applications. Since defect evolution usually involves processes at very different time scale, *e.g.*, the defect production in cascades occurs over picoseconds while defect accumulation in reactors is up to forty years, the span of more than twenty orders of magnitude creates tremendous challenges for both experiments and simulations and there is a significant gap in the accessible time scale between them. To bridge this gap and to computationally model and predict the defect evolution over a long period while maintaining the desired fidelity, an accelerated kinetic Monte Carlo (KMC) approach, self-evolving atomistic KMC (SEAKMC), has been developed for simulating complex defect structures. In contrast to the conventional KMC models that require all reactions to be predetermined, this method incorporates on-the-fly determinations of transition states with a new scheme for defining active volumes in an off-lattice (relaxed) system and any physically relevant motion or reaction may occur. Applications of SEAKMC for simulating defect evolution are demonstrated through three selected problems for BCC iron: (i) $<100>$ -loop formation, (ii) annealing of cascade damage and (iii) long-term evolution vacancy clusters and their growth. The formation mechanism of $<100>$ loop in BCC iron is revealed using SEAKMC. For cascade annealing, a comparative study using SEAKMC and object KMC is performed. For the multi-vacancy case, the results are compared with those obtained using the autonomous basin climbing method, kinetic activation-relaxation technique, and molecular dynamics (MD). It is found that SEAKMC possesses the atomistic fidelity that is similar to the MD but on a much longer time scale. The differences between SEAKMC and other methods are discussed. In addition, the unique predictive capabilities and the limitations of SEAKMC as well as its potential applications to a wide range of problems are elaborated.

This material is based upon work supported as part of the Center for Defect Physics, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

Diffuse interface modeling of void growth in irradiated materials. Mathematical, thermodynamic and atomistic perspectives

Anter El-Azab¹, Karim Ahmed¹, Srujan Rokkam², Thomas Hochrainer³

¹Purdue University, ²Advanced Cooling Technologies, ³University Bremen

We present an assessment of the diffuse interface models of void growth in irradiated materials. Since the void surface is inherently sharp, diffuse interface models for void growth must be constructed in a way to make them consistent with the sharp-interface description of the problem. Therefore, we first present the sharp-interface description of the void growth problem and deduce the equation of motion for the void surface. We also compare two existing phase field models to determine which one corresponds to the sharp-interface analysis. It was shown that a phase field model of type C, which couples Cahn-Hilliard and Allen-Cahn equations, is the most adequate since this type of model can take into account the reaction of point defects at the void surface via an Allen-Cahn equation. Fixing the model parameters in the diffuse interface model is discussed from the points of view of asymptotic matching. Sample results for void growth in a single component metal based on sharp and diffuse interface models are presented. Finally, a perspective on the use of atomistic modeling in both constitutive and nucleation modeling within the phase field approach for void formation in irradiated materials is presented.

This material is based upon work supported as part of the Center for Materials Science of Nuclear Fuel, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Basic Energy Sciences under award number FWP 1356, through subcontract number 00122223 at Purdue University.

Constrained ab initio method for non-collinear magnetic excitations

Pui-Wai Ma, S. L. Dudarev

Culham Centre for Fusion Energy, Abingdon, Oxfordshire, OX14 3DB, United Kingdom

Magnetic excitations determine the finite temperature phase stability of the most important class of structural nuclear materials, such as iron alloys and steels. They influence production, migration and evolution of defects in such materials. *Ab initio* calculations are a powerful tool for the investigation of defects on the atomic scale. However, it is intrinsically incapable of treating excited states, including spin excitations. In order to consider the effect of non-collinear magnetic excitations in ferromagnetic iron, we develop a constrained method involving the use of Lagrange multipliers. Some of the methods developed earlier involve various sophisticated procedures for calculating vector Lagrange multipliers iteratively, and all of them do not guarantee numerical convergence.

We propose a new constrained method for the *ab initio* treatment of non-collinear magnetism. The method involves using a fixed scalar Lagrange multiplier λ and does not require re-calculating Lagrange parameters on the fly. We prove analytically that the method guarantees convergence if a sufficiently large value of λ is used. The penalty energy or the penalty potential are inversely proportional to λ . The method is simple and straightforward, and can be readily implemented in a DFT code, including VASP. Both the atomic and magnetic configuration can be relaxed using our method.

In this work, we describe applications of the new method. Firstly, we study a 2 atom configuration in BCC Fe using constrained orientations of magnetic moments. The energy change as a function of orientations compares well with literature data. Variation of energy for the 2 atoms case with magnetic moments at 90 degrees confirms the predicted relation between the penalty energy and the choice of λ . Secondly, we study a 54 atom amorphous system with magnetic moments pointing in random directions, showing that the method applies also to large magnetically disordered configurations. Lastly, we investigate the case of a <110> dumbbell SIA defect that shows how magnetic excitations induce extra forces acting on atoms. We find that the local volume in the core of a dumbbell increases when the magnetic configuration changes from antiferromagnetic to ferromagnetic.

This work was part-funded by the RCUK Energy Programme [grant number EP/I501045] and by the European Union's Horizon 2020 research and innovation programme. To obtain further information on the data and models underlying this paper please contact PublicationsManager@ccfe.ac.uk. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

***Ab initio* study of threshold displacement energies in tungsten**

P. Olsson¹, C. Domain²

¹KTH Royal institute of Technology, Reactor Physics, Roslagstullsbacken 21, 106 91
Stockholm, Sweden

²EDF-R&D, Department of materials and mechanics of components, Les Renardières, 77
250 Moret-sur-Loing, France

The most fundamental parameter in phenomenological radiation damage theories, such as the Kinchin-Pease- or the NRT models predict a damage dose that depends on the average threshold displacement threshold of the material. We here present an *ab initio* molecular dynamics study of the angular dependent threshold displacement threshold surface in the refractory metal tungsten. W is the strongest candidate material for the plasma divertor in nuclear fusion tokamaks. We present a detailed study of the anisotropy of the energy surface and an average value that can be used as a more reliable input in damage dose assessments. We compare our results to predictions made using semi-empirical interaction potentials, as well as available experiments for tungsten. We also compare to other bcc metals such as iron, where a similar study has been recently performed [1]. In order to improve the short range part of stiffened interatomic potentials, we also predict the energy loss in replacement collision sequences and discuss the implications of the here performed quantum mechanical simulations.

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Role of Microstructure on Fuel Performance: Macroscale Insights from Atomic-resolution Simulations

Simon R. Phillpot

Department of Materials Science and Engineering University of Florida

Nuclear fuel in service is a unique environment of high temperature, high stress, irradiation and ever changing chemistry and microstructure. The insights that can be obtained by atomic-level simulation into the complex chemical and microstructural phenomena that take place in both the fuel pellet and the clad are illustrated.

With respect to fuel the issues, we illustrate insights from atomistic simulations of defect energetics, evolution and thermal transport properties. Specifically, we have used atomic-level simulation methods to determine the interaction of metallic fission products with the core of edge dislocations in UO₂. Detailed analysis shows that the trends in segregation energy can be understood in terms of bulk behavior and continuum elasticity, opening up an efficient method for rapidly generating databases of segregation properties for input to mesoscale codes. We also analyze the results of molecular dynamics simulation of void formation in UO₂ in the bulk and close to a grain boundary. The microstructural evolution during burnup, results in a progressive degradation in the thermal transport properties. We present the results of thermal conductivity calculations within the lattice dynamics framework in UO₂ using electronic-structure calculations for the interatomic force constants. Comparison of the phonon lifetimes with the recently measured lifetimes is provided. We have also performed large scale molecular dynamics (MD) simulations to determine the effects of microstructure – grain boundaries and dislocations - on the thermal conductivity of UO₂. We show how insight from such simulations can be integrated into the FRAPCON fuel performance code

Finally, in the context of clad, we have developed a charge-optimized many-body (COMB) potential for the Zr-ZrO₂-ZrH_x system. We perform classical molecular dynamics simulations showing the initial corrosion behavior of three low-index zirconium surfaces via the deposition of O₂ and H₂O molecules. The basal (0001) surface shows greater resistance to oxygen diffusion than the prismatic surfaces. Nanoindentation simulations on both basal and prismatic Zr and ZrO₂/Zr provide insights into unit mechanisms associated with the deformation of clad.

Interatomic potentials accuracy: how do they bridge the scales? U-Mo fuel case

Vladimir Stegailov, Karen Fidanyan, Alexey Kuksin, Daria Smirnova,
Sergey Starikov, Alexey Yanilkin

Joint Institute for High Temperatures of Russian Academy of Sciences

Perspective reliable multiscale models of radiation damage in nuclear fuels should bridge a gap between atomistic level dynamics and kinetic rate theory (or phase field theory) at mesoscopic level. Radiation defects evolution models comprised of millions of atoms are required to resolve essential physical effects (point defects clustering, interaction with dislocation loops, grain boundaries etc). Empirical potential models are the main tool for transferring to the meso-level the peculiarities of atomic interactions that can be captured only using sophisticated quantum methods. That is why the accuracy of the interatomic potentials is of utmost importance for predictive modelling and simulation of nuclear fuels.

We have built a set of interatomic potential models targeted at the description of U-Mo fuels. The developed central symmetric EAM many-body potential models have been shown to provide decent accuracy for pure Mo [1], pure U [2] and U-Mo alloys [3]. Recently an angular dependent ADP model for the U-Mo alloy has been built as well. All potentials are constructed using force-matching method and fitted to the values of ab initio interatomic forces, energies and stresses. As a question of verification we discuss the loss of information at the corresponding “data transfer” between quantum and classical levels. The validation and application of the resulting models include the following issues:

1. Structure of α -U, γ -U, bcc Mo, U_2Mo compound and U-Mo alloys.
2. Elastic constants, melting temperatures, thermal expansion and isotherms of U-Mo and the Grüneisen parameter for liquid and solid U.
3. Point defect formation energies, diffusion mechanisms and diffusivities.

We discuss a consistent way to include FPs in the U-Mo model and present the simulation results on Xe diffusion and bubble formation. We also consider how the resulting MD models bridge the gap to the level of rate theory [4].

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Atomistically-informed cluster dynamics modeling of void and loop nucleation in irradiated UO₂

Sarah Khalil¹, Todd Allen¹, Anter El-Azab²

¹UW-Madison, ²Purdue University

A novel Cluster Dynamics (CD) model that describes the nucleation and evolution of defect clusters in oxides systems has been developed. The model has been used to predict clustering of vacancies and interstitials into voids and dislocation loops, respectively, in irradiated UO₂. The model reproduces well a range of experimental data on nucleation and growth behavior and its temperature dependence. A very important feature of this model is its ability to predict the off-stoichiometry (or composition) of defect clusters, allowing, in turn, for the tracking of off-stoichiometry of the matrix. The effect of migration energy of point defects on the concentration and average size of voids has been studied. Also, the effect of irradiation conditions such as irradiation temperature, irradiation dose and dose rate on clusters concentration and composition has been investigated. The preliminary results show that Frenkel defects, as opposed to Schottky defects, dominate the nucleation process in irradiated UO₂. Vacancy clusters tend to grow mainly by absorbing oxygen vacancies and the migration energy of uranium vacancies is the rate limiting energy in nucleation and growth of voids. The results also show that, in a stoichiometric UO₂ under irradiation, vacancy clusters (voids) tend to have both hypo- and hyper-stoichiometric composition with a higher fraction of hyper-stoichiometric composition clusters. A hyper-stoichiometric cluster composition indicates that the matrix would become oxygen rich even if the initial state is perfectly stoichiometric.

Radiation growth in Zr under Frenkel-pair produced irradiation

Y.N. Osetsky¹, A.V. Barashev^{1,2}, S.I. Golubov¹, G.D. Samolyuk¹, R.E. Stoller¹

¹ Materials Science and Technology Division, ORNL, Oak Ridge, TN 37831- 6138, USA

² Center for Materials Processing, Department of Materials Science and Engineering,
University of Tennessee, East Stadium Hall, Knoxville, TN 37996-0750, USA

Existing theory explains radiation growth of hcp Zr under 1 MeV electron irradiation by the diffusion anisotropy of self-interstitial atoms (SIAs), assuming isotropic diffusion of vacancies. Recent density functional theory (DFT) study suggests preferential in-basal-plane diffusion for both vacancies and SIAs. Kinetic Monte Carlo calculations of the point defect diffusion at temperatures from 200 to 1100K, performed using the DFT data on the migration, are presented. The ratio of diffusion coefficients parallel and perpendicular to the basal planes, i.e. the diffusion anisotropy, is found to be higher for vacancies than SIAs at temperatures below ~900K. With these data the theory predicts existence of a crossover temperature somewhere between 600 and 800K, depending on the dislocation bias (which is defined by the relative strength of point defect interaction with the dislocation stress field), below which the diffusion anisotropy difference between point defects does not account for observations. It is speculated that small SIA clusters with higher diffusion anisotropy may determine the observed growth in Zr.

Challenges in energy applications of non-stoichiometric complex perovskites

E.A. Kotomin^{1,2}, M.M. Kuklja³, Yu.A. Mastrikov², R. Merkle¹, J. Maier¹

¹Max Planck Institute for Solid State Research, Heisenbergstr. 1, Stuttgart, Germany

²Institute for Solid State Physics, University of Latvia, Kengaraga str. 8, Riga, Latvia

³Materials Science and Engineering Dept, University of Maryland, College Park, USA

Two ABO_3 -type perovskite solid solutions (BSCF: $\text{Ba}_{1-x}\text{Sr}_x\text{Co}_{1-y}\text{Fe}_y\text{O}_{3-\delta}$ and LSCF: $\text{La}_{1-x}\text{Sr}_x\text{Co}_{1-y}\text{Fe}_y\text{O}_{3-\delta}$), mixed ionic – electronic conductors, recently have attracted a lot of attention because of a wide range of potential applications in modern technologies, e.g. gas separation membranes, solid oxide fuel cells (SOFC), etc. The use of SOFC for electricity supply in space stations poses a question of materials radiation stability. Clearly, radiation defects, first of all oxygen vacancies and antisite defects in perovskites, affect many properties and worsen performance of the perovskite materials in specific applications.

In this study, we present results of first principles calculations of the perfect BSCF and LSCF crystals, the crystals containing basic point defects (cation and anion vacancies, cation exchange, and antisite defects), disorder (Frenkel and Schottky), and a set of relevant solid-solid solution reactions [1,2]. Our DFT modeling reveals that oxygen Frenkel defects, full Schottky disorder and partial Schottky disorder accompanied by the growth of a new phase (e.g. a parent perovskite) all have relatively low formation energies and are favorable. The obtained cation exchange energies are very low for both the A- and B- sublattices of the perovskite structure; this leads to a formation of new phases or interphases.

We explored and analyzed in great detail the oxygen vacancy formation energies in the cubic and hexagonal phases of BSCF and demonstrated that a high concentration of vacancies (oxygen non-stoichiometry), in fact, serves as a stabilizing factor that governs the preference of the cubic phase over the hexagonal phase. We also discuss peculiarities of the oxygen vacancy diffusion in BSCF and LSCF. We established that the A/B-site cation size mismatch in BSCF leads to the unusually low oxygen vacancy formation energy, which causes a considerable non-stoichiometry, and facilitates vacancy migration with a prominent charge transfer at the transition state. The smaller mismatch between A- and B-site cations in LSCF results in twice higher vacancy formation energy and higher migration activation barrier, which give rise to a smaller oxygen vacancy concentration and thus a slower oxidation reaction, as compared to BSCF.

Based on the above-discussed results of first principles calculations of the defect formation and migration energies, as well as oxygen atom and molecule adsorption on perovskite surfaces, we calculated the diffusion-controlled kinetics of oxygen reduction reaction (ORR) as a function of adsorbed oxygen and surface vacancy concentrations [3]. This allowed us to determine *the rate-determining steps* (which is important for improvement of fuel cell and permeation membrane performances) and suggest interpretation of available experimental data.

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First principles study of anisotropy of point defect diffusion barriers in HCP Zr

G.D. Samolyuk¹, A.V. Barashev^{1,2}, S.I. Golubov¹, Y.N. Osetsky¹, R.E. Stoller¹

¹ Materials Science and Technology Division, ORNL, Oak Ridge, TN 37831- 6138, USA

² Center for Materials Processing, Department of Materials Science and Engineering,
University of Tennessee, East Stadium Hall, Knoxville, TN 37996-0750, USA

The radiation growth of Zr is observed not only under neutron irradiation but also under ~1 MeV electron irradiation and the neutron. To explain this it is natural to assume that the diffusion anisotropy of single self-interstitial atoms (SI) (preferentially along the basal planes) is higher than that for vacancies. We used density functional theory (DFT) approach to find the lowest in energy SI configuration of SI and analysed large set of possible transition barriers between these configurations together vacancy transition barriers. We demonstrated that the lowest barrier corresponds to two transitions 1) between basal octahedral (BO) and basal split (BS) configurations, and 2) BO and octahedral (O) configuration. Between the last two barriers the in basal one (BO to BS) is slightly lower and corresponds to longer “jump”. Thus, it was demonstrated that in-basal plane jumps are the most favorable for both vacancies and SIAs, so that both defects exhibit anisotropic diffusion, predominantly parallel to the basal planes.

Radiation damage evolution in nanostructure materials

Blas Pedro Uberuaga

Los Alamos National Laboratory

As the materials in nuclear reactors, both fission and fusion, experience ever increasing radiation damage due to a desire to maximize efficiency, the need to design materials that can withstand that damage becomes ever more pressing. One proposed avenue for mitigating that damage is through the use of nanostructure materials where the high density of interfaces can enable the enhanced recombination of the defects. Here we present combined experimental and theoretical studies of radiation damage evolution within nano composites, focusing on composites containing oxide phases. We first examine how the defect kinetics and thermodynamics within the constituent phases influence the damage evolution in the composite, independently of the structure of the interfaces themselves. Atomistic results are used to parameterize reaction-diffusion models of the composite under irradiation. We find that the damage evolution is very sensitive to the defect properties within these phases with different damage evolution regimes possible depending on the relative kinetics and thermodynamics of defects. We then examine how the atomic structure of the interfaces in oxide/ oxide composites further modifies the evolution of radiation damage within these materials. We find that there can be a complex interplay between the structure of the interface and the evolution of defects produced under irradiation. Finally, using a combination of atomistic and phase field simulations, we examine the evolution of the chemistry of a multicomponent nanocomposite under irradiation and how factors such as the interfacial structure, the characteristic length scale, and the chemistry of the alloy itself can be used to control the redistribution of the various chemical species under irradiation. Together, these studies elucidate the effect of nanocrystalline microstructure on the overall radiation damage response of the composite and provide insights into the design of advanced radiation tolerant materials.

***Ab initio* prediction of point defect properties in materials for energy production**

F. Bruneval, G. Roma, G. Petretto

CEA, DEN, Service de Recherches de Métallurgie Physique, 91191 Gif-sur-Yvette,
France

In materials science, defects may be unintentionally created and have detrimental effects, e.g. during crystal growth or in harsh environments found in electronic devices in satellites, optical fibers in nuclear plants. They can also be introduced deliberately into a material to engineer its electrical, transport, or optical properties (e.g. semiconductor junctions ensuring charge separation in photovoltaic cells or transparent conducting oxides used as electrodes. Despite their technological importance, defects are difficult to characterize experimentally. Quantum mechanical first principles calculations offer a complementary description. However, first principles calculations for defects are still challenging for several reasons: The structural models required for a converged description of a defect contain a large number of atoms and therefore make a quantum mechanical calculation computationally very expensive. Furthermore, the point defect properties are strongly affected by the exchange-correlation approximation employed in the calculations.

In this presentation, I will present recent advances on the effect of the exchange-correlation approximation choice on the defect properties. The talk will focus on hybrid functionals and on the so-called GW [1] and Random-Phase [2] approximations of the many-body problem.

The results will be exemplified with two relevant materials for the energy production: SiC for the nuclear industry [3] and ZnO for the photovoltaic applications [4].

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Void Dynamics in Phase Field Modeling

Z.H. Xiao¹, S.Q. Shi¹, A.A. Semenov², C.H. Woo³

¹Department of Mechanical Engineering, The Hong Kong Polytechnic University

²Institute for Nuclear Research, Russian Academy of Sciences, Moscow, Russia

³Department of Physics and Materials Science, City University of Hong Kong

Void growth in Mo and Cu is studied in the phase-field framework. The void-metal diffuse interface is customarily modeled by a Ginzburg-type gradient energy term with a parameterized coefficient. Following the previously obtained results, the latter is treated as a constant independent of void size. Realistic vacancy supersaturations, as well as the real time and real length scales are used in the simulations. This allows us to make a direct comparison between the results obtained in the phase-field model and those derived from the sharp boundary approach. It is found that the developed phase-field model reproduces reasonably well the dynamical behavior of an individual void, well-known from the rate-theory treatment of void evolution. The ultrafine characteristic spatial scales of the void-metal diffuse interface present a challenge to numerically efficient modeling of the evolution of a void ensemble under irradiation.

Key words: Phase-field modeling, sharp boundary approach, rate theory, void evolution

Vacancy assisted diffusion and clustering of interstitial solutes in α -Fe from first principles

Caroline Barouh¹, Chu-Chun Fu¹ and Thomas Jourdan¹

¹CEA, DEN, Service des Recherches de Métallurgie Physique, F-91191 Gif-sur-Yvette Cedex, France

Under irradiation, a large amount of vacancies (V) are produced. They strongly interact with interstitial solutes (X) such as carbon (C), nitrogen (N) and oxygen (O) atoms, which are always present in steels, either as alloying elements or as impurities. The V-X attraction influences the mobility of both the solutes and the vacancies. On one hand, a decrease of the vacancy mobility has been revealed experimentally in the presence of carbon and nitrogen, most likely due to the trapping of vacancies at small vacancy-solute complexes [1, 2]. On the other hand, however, it is not clear whether vacancies always reduce the mobility of the interstitial elements.

Density Functional Theory (DFT) calculations have been performed to study the energetic and kinetic properties of V_nX_m clusters. Low-energy configurations of small V_nX_m have been determined. It has been revealed that vacancies enhance the clustering of solutes. Moreover, a systematic comparison of C, N and O - neighbors in the Periodic Table – shows different behaviors of the solutes in the neighborhood of vacancies as a function of the electronic band filling. For instance C atoms tend to decorate the surface of V clusters whereas O atoms will preferentially gather inside the V clusters.

The mobility of the V_nX_m clusters has been carefully studied. We especially focused on the V_nX clusters as it has been shown that V_2 and V_3 are even more mobile than a monovacancy in α -Fe [3]. As a result, all the V_3X have been found to be very mobile. In particular, some clusters can be as mobile as the isolated solutes. Therefore, vacancies may be efficient to drag the interstitial solutes towards sinks such as grain boundaries, dislocations and free surfaces. Also, the result found on the mobility of small V_nN clusters may explain the apparent discrepancy between the resistivity recovery experiments and the DFT data [2].

The interpretation of such experiments may be worth revisiting in the light of the present DFT prediction.

The obtained DFT data have been used to parameterize a Cluster Dynamics model, based on the Rate Theory, which allows to predict the time evolution of the clusters concentration. The consequences of small highly mobile clusters on the kinetic properties of vacancies and solutes under various irradiation conditions have been explored using this model.

This work is supported by the joint program "CPR ODISSEE" funded by AREVA, CEA, CNRS, EDF and Mécachrome under contract n°070551.

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Study of hydrogen behavior on beryllium surfaces from the first principles

Dmitry V. Bachurin, Pavel V. Vladimirov

Institute for Applied Materials – Applied Materials Physics, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

Presently beryllium and its alloys are considered as a material for fusion reactor blanket and plasma facing first wall. The interaction of hydrogen and its isotopes with beryllium surfaces leads to a significant change of the surface properties of the material. However, this phenomenon is not yet well investigated in the literature.

Static *ab-initio* calculations of surface energies were performed for five various close-packed beryllium planes: basal, prismatic (types I and II), pyramidal (types I and II). In order to achieve the convergence of the results, different sizes of the simulation cell were used (72–128 atoms). The free surfaces were separated by a 17–23 Å thick vacuum region. The volume and the shape of the simulation cell were rigidly fixed during relaxation. No restrictions on the motion of atoms were imposed.

The calculations have shown that the basal plane is the most energetically favorable. The energy of prismatic (type I) and pyramidal (type I) planes are almost equal and they are found to be the second energetically favorable planes in beryllium. The other planes have noticeably higher surface energies. Usually up to 5 outmost atomic layers are involved in surface relaxation. The largest change from the interlayer spacing occurs near the free surfaces (up to 25% with respect to ideal hcp lattice).

A behavior of a single hydrogen atom on the different beryllium surfaces was studied. Hydrogen atom was placed in all nonequivalent positions within each considered plane. Stable positions of the hydrogen were found. Almost in all possible configurations the presence of hydrogen atom leads to a noticeable reduction of the surface energy.

Increase of hydrogen coverage of the beryllium surfaces results in reduction and thereafter to an increase of the surface energy while coverage proceeds. At high coverage the basal plane is not the most energetically favorable anymore. Stable positions of the hydrogen are somewhat different in contrast to the case of a single hydrogen atom. Interplanar relaxation at higher hydrogen coverage was analyzed as well.

Molecular dynamics study on interaction between an edge dislocation and a Frank loop in Fe-10%Ni-20%Cr alloy

Akiyoshi Nomoto¹, Ghiath Monnet², Jean-Baptiste Baudouin³, Christophe Domain²

¹Central Research Institute of Electric Power Industry, Tokyo, 201-8511, Japan

²EDF, Moret sur Loing, 77818, France

³Université de Lyon, INSA Lyon, MATEIS, Villeurbanne, F69621, France

Inhibition of dislocations motion by irradiation-induced defects, such as dislocation loops, is one of the main mechanisms of irradiation hardening of austenitic stainless steels. In this work, Molecular Dynamics (MD) simulations of interaction between an edge dislocation and Frank loops in Fe-10%Ni-20%Cr ternary alloy mimicking austenitic stainless steels are carried out to investigate and model dislocation behavior. An empirical interatomic potential developed recently for a ternary FeNiCr system is used for the MD calculations. The interactions are calculated at different temperatures, loop orientations, loop size and solute atom configurations. The results show that the loop strength and the interaction processes depend on the solute atom configuration, the geometrical configurations between the dislocation and the loop and temperature. It is also demonstrated that a small Frank loop is not so weak obstacle in the alloy. The interaction leads microstructural change such as loop shearing, loop unfaulting and loop absorption in the dislocation. In the former two cases, the loop remains after the interaction, however in some cases absorption of the remaining loop by subsequent interactions with successive dislocations is observed.

Stability of SIA clusters in Fe: the role of substitutional atoms – ab initio study

C. Domain^{1,3}, C.S. Becquart^{2,3}

¹ EDF-R&D, Département MMC, Les renardières, F-77818 Moret sur Loing, France

² Laboratoire commun EDF-CNRS Etude et Modélisation des Microstructures pour le Vieillissement des Matériaux (EM2VM), France

³ Unité Matériaux Et Transformations, UMET, UMR 8207, Villeneuve d'Ascq, France

The ageing and the evolution of mechanical properties of pressure vessel steels under radiation has been correlated with the formation of more or less dilute solute clusters. Point defect produced under irradiation can form clusters and these clusters interact with solute atoms.

We have used DFT calculations to investigate the impact of substitutional atoms representative of the alloying elements of pressure vessel steels (e.g. Cu, Ni, Mn, Si, P, Cr) on the stability of Self Interstitial Atom (SIA) clusters. All the solute atoms studied were found to interact with isolated SIAs as well as SIA clusters. Different small SIA clusters can be formed with non parallel $\langle 110 \rangle$ SIAs which are found to be the most stable configurations, compared to small $\langle 111 \rangle$ loops. The solute interactions with small SIA clusters (consisting of several non parallel $\langle 110 \rangle$ SIAs) is most often at least 0.4 eV. The most attractive configuration depends on the solute size, chemistry and magnetism. The same trends were found for C15 Lave phase based SIA clusters and small $\langle 111 \rangle$ loops. In that later case, the most attractive sites are found at the periphery of the loop. These fine scale calculations are important to assess the validity of coarse grained approaches (Kinetic Monte Carlo or Molecular Dynamics) which rely on more empirical cohesive models.

This work is part of the PERFORM project.

Nucleation of point defect clusters in displacement cascades near edge and screw dislocations in fcc metals subjected to fast particle irradiation

Alexander E. Volkov¹, Roman Voskoboinikov²

¹Russian Research Centre ‘Kurchatov Institute’, Kurchatov Sq., Moscow 123182 Russia

²Institute of Materials Engineering, Australian Nuclear Science and Technology Organisation, New Illawarra Road, Lucas Heights 2234 NSW, Australia

Along with grain boundaries, free surfaces, secondary phase interfaces and other structural defects, dislocation network constitutes an essential part of the microstructure of advanced structural materials for demanding engineering applications. Being a key factor that determines the yield strength, fracture toughness, plasticity, creep and fatigue resistance and other materials' service properties, dislocations can also contribute to elemental partitioning, facilitate segregation of impurities and alloying elements or change the balance of residual point defects in materials exposed to fast particle irradiation. Existing phenomenological models implement thermodynamic or kinetic approaches to describe the interaction of dislocations with radiation defects. In the undertaken study we have considered athermal coupling of collision cascades with screw and edge dislocations in aluminium and nickel at the timescale of the order of cascade lifetime.

The velocity-Verlet molecular dynamics simulations have been applied to study the radiation damage created in collision cascades in aluminium and nickel crystals harbouring an isolated screw or edge dislocation with $1/2[110]$ Burgers vector and in the two defect-free metals for comparison. The total of more than 2000 displacement cascades formed by the recoil of primary knock-on atoms (PKA) with energy, EPKA, ranging from 5 to 20 keV in crystals at temperatures $100\text{K} < T < 600\text{K}$ (aluminium) or $100\text{K} < T < 1200\text{K}$ (nickel) were simulated to get statistical reliability of the results.

We evaluated the number of residual vacancies and self-interstitial atoms created in displacement cascades as a function of (EPKA, T) and compared the obtained data with the number of Frenkel pairs formed in collision cascades in the pristine materials under the same conditions. The conditions that control dislocation climb by absorbing point defects from the displacement cascade region were revealed and a few visualisations were prepared in order to illustrate point defect redistribution in the two considered materials. Special attention was paid to studying governing factors that determine formation of point defect clusters in collision cascades near edge and screw dislocations in aluminium and nickel exposed to fast particle irradiation. Preliminary results of the undertaken research were published in [1, 2].

Partial support from the Russian Foundation for Basic Research under grant # RFBR-14-08-00859a is gratefully acknowledged.

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Mesoscale simulation of phonon mediated thermal transport in UO₂: Perturbation theory based Monte Carlo solution of Boltzmann Transport EquationAhmed Hamed, Anter El-Azab

School of Nuclear Engineering, Purdue University, West Lafayette, IN, United States

Safety of nuclear reactors depends on the reliability of materials under harsh radioactive conditions inside the core of the reactor. The worst part originates from radiation induced damaging effects that lead to microstructural and compositional changes and ultimately can cause material failure. To design materials with enhanced radiation resistant properties, the behavior of materials under irradiation need to be well understood and reliable predictive theoretical models need to be established along with experimental verification techniques. As it is the most widely used nuclear fuel, the advancement of the nuclear technology passes necessarily through a complete understanding of uranium dioxide's properties on every aspect. The revival of vigorous research in the nuclear energy field had instigated a wide interest in UO₂ in an attempt to study its mechanical, thermal and electronic properties, among others. Fuel thermal conductivity controls the fuel operating temperature, and hence affecting nuclear fuel performance and many important processes. There are several factors that can contribute to the change of thermal conductivity under irradiation, most significantly are the change of oxygen-to-metal ratio and defects concentrations. Studying phonon transport represents an adequate paradigm to understand heat transfer phenomena in crystalline semiconductor and insulator materials at the nanoscale level. Unlike phenomenological heat diffusion models, which can not be applied at this length scale, phonon transport theory can capture the microstructure and nanostructure effects on the thermal conductivity. Boltzmann Transport Equation (BTE) provides the capability of tracking phonon evolution in phase space, however solving BTE exactly is not possible in most of the realistic cases. We present a Monte Carlo solution of BTE for phonons in uranium dioxide with various levels of defects. BTE is linearized by introducing the Relaxation Time Approximation (RTA). Individual phonon relaxation times, timescale measure of the scattering strength of each phonon interaction processes (causing transition between phonon states), are calculated by Fermi's Golden Rule under time dependent perturbation theory approximation. Total relaxation time, for each phonon, is calculated by adding individual phonon relaxation times (by all possible mechanisms) together using Matthiessen's rule. The simulation scheme accounts for all acoustic and optical branches of the dispersion relationships and considers the 3D representation of the actual shape of the UO₂ Brillouin zone (truncated octahedron). Experimental dispersion data of UO₂ in high symmetry directions were employed to model phonon anisotropic dispersions. Unlike most other works on solving this equation by Monte Carlo method, the momentum and energy conservation laws for phonon-phonon interactions in uranium dioxide are treated exactly by considering only the interactions that obey the pertinent conservation laws. Using periodic boundary conditions, our results illustrate the diffusion limit of phonon transport in uranium dioxide, and make possible the prediction of thermal conductivity. A simple kinetic theory model is also implemented in which conductivity is calculated using phonon heat capacity, velocities, and scattering time-scales. The effect of temperature and defect concentration on conductivity is predicted with both models and the results are compared with experimental data available in the literature.

This research was supported as a part of the Energy Frontier Research Center for Materials Science of Nuclear Fuel funded by the U.S. Department of Energy, Office of Basic Energy Sciences under award number FWP 1356, through subcontract number 00122223 at Purdue University.

Examination of multiscale concept for swelling description of metals and alloys

Vladimir Khlebnikov, Alexey Kuksin, Ivan Novoselov, Mikhail Romashka, Alexey Yanilkin

All-Russia Research Institute of Automatics, Moscow 127055, Russia

The multiscale concept for material under irradiation has the long history and started from the description of point defects and small clusters by the atomistic simulations and finished at macroscopic description for a long time of irradiation. For the moment there are a lot of atomistic simulations of materials behavior under irradiation in literature, a lot of theoretical models of defects evolution (growth, nucleation). The time and spatial bridges between atomistic simulation and rate theory are covered by kinetic Monte-Carlo (KMC) and cluster dynamics (CD). So it seems that the multiscale concept is filled to methods and materials parameters. The main goal of our work is to examine the today's possibility of quantitative description by the multiscale concept of materials under irradiation. The examination is carried out in order to emphasize present-day problems: large uncertainties in constants, unreasonable physical models, insufficient computational methods, codes and resources.

The multiscale concept consists of atomistic simulations, KMC, CD based on KMC solver and rate theory. Two different tests are considered: irradiation of thin foils by ion beams [1,2,3], irradiation of bulk sample by neutron beam in reactor. The conditions of irradiation in these two experiments differ from each other by dose rate (about three orders of magnitude), production bias (average PKA energy under neutron beam is smaller than ion beam energy), sink strength (the influence of the surface for thin foil experiments is very sufficient). We consider pure Fe and Mo, FeCr alloy, and alloys based on Mo and FeCr. These metals are better investigated than others and have the real application today. At low doses we compare the calculated dislocation loop or cluster concentrations and radius distribution with experimental results. At high doses the swelling rate is compared. Based on the comparison the conclusions of sufficiency of material constants and models are made.

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Assessment of the influence of elastic anisotropies on dislocation loops sink strength: a phase-field approach

Hadrien Rouchette¹, Ludovic Thuinet^{1,3}, Alexandre Legris^{1,3}, Antoine Ambard², Christophe Domain^{1,3}

¹Unité Matériaux Et Transformations (UMET), UMR CNRS 8207, Université Lille 1, 59655 Villeneuve D'Ascq, France

²EDF R&D MMC, Électricité de France, 77810 Moret-sur-Loing, France

³Laboratoire commun EDF-CNRS Étude et Modélisation des Microstructures pour le Vieillissement des matériaux (EM2VM), France

Long term prediction of irradiated materials ageing relies on proper comprehension of microstructural defect behaviour. Evolution of those irradiation defects (dislocation loops, voids) is responsible for dimensional instabilities and embrittlement of metals. Particle irradiation of a metallic crystal leads to the production of vast amounts of point defects (PDs) – vacancies and self-interstitial atoms (SIAs) – which diffuse in the material and are absorbed by various sinks, such as dislocations, grain boundaries, voids, surfaces, etc. The sink efficiencies depend on the migrating mechanism, the sink geometry (cylinder, spherical, toroidal) and the intensity of the long range elastic interactions between defects and the sink. These quantities are crucial parameters in long time scale rate-theory predictions.

Most of analytical models rely on simplifying assumptions to calculate those sink efficiency: (i) the sink is generally isolated in a defect-free region with arbitrary geometry, (ii) a concentration is fixed on the outer boundary of the sink-free region instead of uniformly produced PDs, (iii) the point defects are considered as pure dilatation centres in an isotropic crystal when elasticity is accounted for.

As a consequence, more accurate models must be developed to rigorously calculate sink efficiencies in complex microstructures. For this purpose, a 3D phase-field (PF) model is proposed to include the anisotropic microelasticity theory coupled to the diffusion of PDs in any dislocation network.

Numerical results on benchmark cases have been compared with analytical solutions, when available. This preliminary step allowed to validate the method. Nevertheless, calculations show that for dislocation loops, capture efficiencies have been significantly underestimated by existing models, even in the simplest cases.

As an application, we computed the anisotropic properties of PDs in zirconium by atomic scale *ab initio* method, and used them as input data in the PF model, to calculate the sink efficiencies of dislocation loops with different Burgers vectors and habit planes. Results show a preferential absorption of SIAs by prismatic loops due to the strong deformation of SIAs in the basal plane. This effect tends to promote the growth of experimentally observed basal vacancy loops.

Towards a quantitative modeling of radiation induced segregation in alloys

M. Nastar¹, F. Soisson¹, L. Messina², P. Olsson², T. Garnier^{1,3}, D. Trinkle³, P. Bellon³

¹ CEA, DEN, Service de Recherches de Métallurgie Physique, F-91191 Gif-sur-Yvette, France

² Reactor Physics, KTH, Albanova University Centre, 106 91 Stockholm, Sweden

³ Department of Materials Science and Engineering, Univ. of Illinois, Urbana-Champaign, USA

Recent developments of the Self-Consistent Mean Field (SCMF) kinetic theory provide the exact phenomenological coefficients L_{ij} of dilute alloys, starting from vacancy and split interstitial jump frequencies calculated ab initio [1]. Binding energies between solute atom and point defect at distances beyond the first nearest neighbor site distance are considered. The effect of a strain field on the migration energies and the resulting transport coefficients L_{ij} can be considered as well [2]. Kinetic correlations are accounted for through a set of time-dependent effective interactions within a non-equilibrium distribution function. In the case of strong binding energies between vacancy and solute atom, the kinetic correlations may lead to a solute drag by the vacancies from the bulk towards grain-boundaries. Starting from a Master Equation written at the atomic scale, generalized diffusion equations for alloys under irradiation are derived. They are applied to the modeling of radiation-induced segregation at grain boundaries in dilute Fe-based model alloys and radiation-enhanced spinodal decomposition in Fe-Cr alloys.

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Point defect modeling in materials : coupling *ab initio* and elasticity approaches

Céline Varvenne¹, Fabien Bruneval², Mihai-Cosmin Marinica², William A. Curtin¹

¹Laboratory for Multiscale Materials Modeling, EPFL, Lausanne CH-1015, Switzerland

²Service de Recherche de Métallurgie Physique, CEA Saclay, 91191 Gif-sur-Yvette,
France

Point defects in crystalline solids play a crucial role in controlling material properties and their kinetic evolution. This is true for both intrinsic defects such as vacancies, self-interstitials, and their small clusters, and extrinsic defects such as impurities and dopants. As a consequence, a proper understanding and modeling of material properties require a precise knowledge of point defect characteristics, in particular their formation and migration energies. To this end, *ab initio* calculations based on density functional theory and performed with periodic boundary conditions have become a valuable tool. But they are technically limited to a few hundred atoms, so the long-range elastic fields of the defect induce a spurious interaction energy with the periodic images. Convergence of point defect properties can therefore be out of reach, especially for clusters.

Here, we propose to couple *ab initio* calculations and linear elasticity to get rid of this limitation [1]. We use elasticity theory to model the interaction of the defect with its periodic images so as to withdraw it from the *ab initio* results. Properties of the isolated defect are then accessible with reduced supercell size. The reliability and benefit of our approach are demonstrated for three problematic cases: the self-interstitial in hcp zirconium, clusters of self-interstitials in bcc iron and the neutral vacancy in diamond silicon. In all cases, our coupled approach allows a more accurate description of point defects than what could be achieved with a simple *ab initio* calculation. The extension of our corrective scheme to the case of charged point defects will be discussed.

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Multiscale modeling of dislocation-precipitate interactions: implementing precipitate pinning in Discrete Dislocation Dynamics

Artru Lehtinen¹, Lasse Laurson¹, Fredric Granberg², Dmitry Terentyev², Kai Nordlund², Mikko Alava¹

¹Department of Applied Physics, COMP center of excellence, P.O. Box 11100, FIN00076 Aalto University, Espoo, Finland

²Department of physics, P.O.Box 43, FIN-00014 University of Helsinki, Finland Nuclear Materials Science Institute, SCK-CEN, Boeretang 200 B-2400 Mol, Belgium

Plasticity in crystalline materials is due to motion of crystal defects known as dislocations. Dislocations create an anisotropic stress field around themselves which can be quite complex giving rise to rich variety of possible interactions. Discrete Dislocation Dynamics (DDD) is method where the dislocation segments are modeled as straight lines connected by discretization points. The stress field is obtained from linear elasticity theory. The reactions related to the dislocation core, such as junction formation and pinning to defects, are beyond the reach of linear elasticity theory and thus require input from more microscopic approaches.

When dislocation encounters an impenetrable precipitate it will become pinned. If the external stress is high enough the dislocation moves past the precipitate and leaves a loop around it. This is called the Orowan process and the loop Orowan loop [1]. New dislocations need more stress to move past the obstacle because they must overcome the old loop in addition to the precipitate. This leads to work hardening of the metal which is important phenomena to understand in the context of building structural parts for nuclear reactors.

Here we combine atomistic simulations to DDD in order to model carbide precipitates interactions with dislocations in BCC-iron. We implement spherical precipitates into ParaDis [2] simulation code by adding a normal force to the segments which come into contact with it. This results in the formation of the aforementioned Orowan loops. The shearing strength of the precipitate is obtained from a molecular dynamics simulations.

This work is part of the SIRDAME project funded by the Academy of Finland.

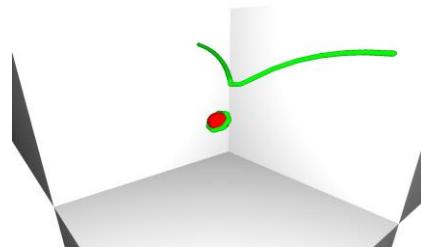


Figure 1: A mixed dislocation has unpinned and left an Orowan loop around a carbide precipitate

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Multiscale modeling of helium-induced nano-fuzz formation on tungsten surfaces

Satoshi Numazawa, Marcel Sluiter, Barend J. Thijssse

Department of Materials Science and Engineering, Delft University of Technology,
The Netherlands

Although tungsten is a promising candidate for the surface material of the divertor in a Tokamak type fusion reactor, fuzz-like structure growth on the tungsten surface is reported at high temperature under low-energy (60 eV) He ion irradiation. The detailed mechanism of this surface reaction is still not well understood on an atomistic level. Molecular dynamics (MD) simulation has revealed several basic atomistic events, such as migration of interstitial He and bubble formation resulting in W interstitial creation. However, due to the restriction of the time scale, surface topography changes simulated by MD alone are quantitatively far from the experimental conditions (Fig. 1, left).

In order to take into account the effects from events much rarer than those at ns intervals, we have developed a direct combination model of MD and lattice kinetic Monte Carlo simulations, in which the two techniques alternate continuously (Fig. 1, right). For the atomic interactions the Juslin-Wirth EAM potential was used, supplemented by the ZBL potential for small distances. The He concentration, stress from He bubbles, and mobility of W surface adatoms are evaluated, and the surface structure evolution is found to agree closely with the experimentally observed evolution speed under the same condition. The details of atomistic events and the novel multi-timescale simulation model are discussed.

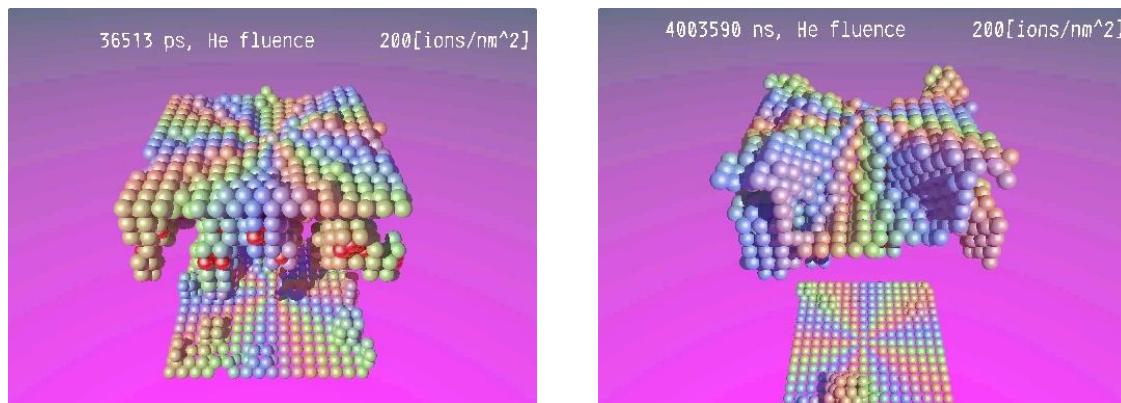


Figure 1: Geometry of a W (100) surface after bombardment by 60 eV He ions with a fluence of 200 ions/nm². Left: MD simulation. Right: Alternating MD and lattice kinetic MC simulation. Note the difference in time allowed by these two simulation methods for the evolution of the surface topography and the resulting difference of roughness ('fuzz').

Only W atoms with fewer than 8 neighbors are shown. Bright red atoms are He. Pale colors are used only to differentiate between sectors in the horizontal planes.

Molecular dynamical investigation of the interaction of edge dislocations with carbides in BCC Fe; Parametrization for DDD-simulations

Fredric Granberg¹, Artuu Lehtinen², Dmitry Terentyev³, Lasse Laurson², Mikko Alava², Kai Nordlund¹

¹Department of Physics, P.O. Box 43, FIN-00014 University of Helsinki, Finland

²COMP center of excellence, Department of Applied Physics, Aalto University School of Science, P.O. Box 11100, FIN-00076 Aalto, Espoo, Finland

³Nuclear Materials Science Institute, SCK-CEN, Boeretang 200 B-2400, Mol, Belgium

Steels are not only a homogeneous alloy of Fe and alloying elements but they also, in almost all cases of practical interest, have a complex micro- and nanostructure of grains, different phases, dislocations and inclusions. One of the most common classes of phases is carbide precipitates. These have a strong effect on the mechanical properties of steels. Since the mechanical properties of metals are dominated by dislocations, it is hence important to understand the interactions of dislocations with carbide precipitates. In particular, the effect of carbides is important for structural parts in nuclear reactors, where controllable elongation is crucial.

In this work, we use molecular dynamical simulations to investigate the interaction between edge dislocations and carbide precipitates. This nanoscale phenomenon, simulated by molecular dynamics, can be parametrized to be able to simulate similar properties on a larger scale with discrete dislocation dynamic, DDD, simulations.

A simulation technique proposed by Ossetsky and Bacon[1] was utilized on a simulation cell of BCC Fe. In earlier studies either impenetrable infinitely hard obstacles, like fixed atoms, or penetrable obstacles, like voids or loops, were considered. In this study impenetrable obstacles with a finite strength, which is more close to real systems, were investigated. The obstacles were of M_3C -, cementite, and $M_{23}C_6$ -type. The effect of size and temperature on the unpinning stress was studied. Identification of different unpinning mechanisms like Orowan loop formation and climb was done. This knowledge is important for the understanding of how realistic impenetrable obstacles interact with edge dislocations.

How the critical stress depends on the temperature and on the size of the precipitate can be parametrized to calibrate the strength of obstacles in DDD simulations. In this modeling method we can get the atomically correct interaction from molecular dynamics to be used in a simulation method, capable of simulating millisecond and micrometer scales.

This research was funded by the Academy of Finland project SIRDAME (grant no. 259886). We thank the IT Center for Science, CSC, for granted computational resources.

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Mesoscopic Investigation of Homogeneous to Heterogeneous Deformation Transitions in Irradiated BCC Crystals

A. Arsenlis, J. Marian, M. Rhee, G. Hommes, R. Cook and N. R. Barton

Lawrence Livermore National Laboratory, Livermore, CA U.S.A.

Low temperature irradiation of crystalline materials is known to result in strengthening and loss of ductility, which limits the usefulness of candidate materials in harsh nuclear environments. In bcc metals, this mechanical property degradation is caused by the interaction of in-grown dislocations with irradiation defects, particularly small prismatic dislocation loops resulting from the microstructural evolution of displacement cascades. In this work, we present a multi-length scale investigation including dislocation dynamics (DD) simulations, and finite element simulations using a novel set of continuum constitutive equations for the response of irradiated bcc single crystals based on the dislocation dynamics simulation results. Simulations of the response of the material with varying concentrations of prismatic loops are conducted to investigate changes in the mesoscopic and macroscopic flow behavior. The study is motivated by experimental observations of plastic flow localization and softening in a variety of structural materials for nuclear applications. At the mesoscopic scale, the simulations reveal a transition from homogenous to highly localized deformation as the prismatic loop density increases. In the heterogeneous deformation regime defect-depleted channels are created as a principal signature of softening. The mechanism of defect depletion observed in the simulations is the translation and clustering of loops defects into larger structures that no longer act as effective obstacles to glissile dislocation motion. The results of the dislocations dynamics simulations are used to construct and augment a single crystal plasticity constitutive law with a tensorial irradiation damage state variable and evolution equations capable of reproducing the flow behavior observed in the dislocation dynamics simulation and of reaching strains in excess of 10% for linkage with the engineering scale. The calibrated crystal plasticity model is used as the constitutive relation in FE simulations of polycrystalline irradiated Fe systems, and the results compared to experiments for different levels of irradiation damage.

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Modeling of a Ni-based superalloy: From micro-pillar compression tests to polycrystalline models

J. Segurado^{1,2}, A. Cruzado², H. Chang², B. Gan², S. Milenkovic², J. M. Molina-Aldareguia², J. Llorca^{1,2}

¹Department of Materials Science, Polytechnic University of Madrid, E.T.S. de Ingenieros de Caminos, 28040 Madrid, Spain

²IMDEA Materials Institute, C/Eric Kandel 2, 28906 Getafe, Madrid, Spain

A microstructure based crystal plasticity (CP) model is developed to simulate the elasto-visco-plastic behavior of Inconel 718 grains containing γ' and γ'' precipitates and δ phase. The CP model is an elasto-visco-plastic physically inspired model [1] that accounts for the effect of temperature, softening due to cyclic loading and tension-compression strength differential (when present) at the grain level.

The parameters defining the CP behavior were fitted from tests at the microscale on grains of wrought and cast materials with different contents of γ' and γ'' and δ . The testing at the grain level consisted first on the identification of grain orientations using EBSD and then micromechanical testing at different temperatures by micro-pillar fabrication inside a grain and uniaxial compression. Tests were made using several pillar diameters, strain rates and temperatures. In addition, testing of small polycrystalline samples inside the SEM were done to complement the crystallite characterization. The resulting CP parameters where finally linked with the corresponding microstructure.

The CP plasticity model was finally used to simulate the elastic-plastic and creep behavior of polycrystalline alloys at different temperatures. The polycrystalline behavior was obtained by the finite element simulation of a periodic representative volume element (RVE) of the microstructure [2]. The RVE contained information about grain size, shape and orientation distribution. The resulting behavior was compared with macroscopic tests of alloys with different microstructures to verify the validity of the model.

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Simulating the brittle-ductile transition using discrete dislocation plasticity

Edmund Tarleton¹, Daniel S. Balint²

¹Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH, UK

²Department of Mechanical Engineering, Imperial College London, London, SW7 2AZ, UK

At a given strain rate, metals fracture at low temperatures in a brittle manner characterized by little or no plasticity. As the temperature is raised dislocation nucleation and motion occurs in the highly stressed region surrounding the crack-tip and the material exhibits a more ductile fracture behavior. The dislocations generate a back stress on the crack-tip which acts to shield the crack causing an increase in the fracture toughness. The temperature at which this brittle-ductile transition occurs increases with increasing strain rate. We have studied the relation between applied deformation, governed by the applied loading rate, and dislocation plasticity and crack-tip shielding, where the time scale is determined by Frank-Read source nucleation time and dislocation drag coefficient. Micro-cantilever bending was simulated in plane strain with a discrete dislocation plasticity (DDP) model utilizing cohesive elements to model the crack propagation. The micro-cantilever DDP simulations will be presented and compared to corresponding experiments to investigate rate and size effects in the brittle-ductile transition.

Mesoscale modeling of dislocation mechanisms and the effect of nano-sized carbide morphology on the strengthening of advanced lightweight high-Mn steels

S.M. Hafez Haghigat, E. Welsch, I. Gutierrez-Urrutia, D. Raabe

Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany

The development of high performance lightweight steels for structural applications in the automotive industry is currently one of the main targets of steel industries. The FeMnAlC system is a promising low density steel grade that offers a combination of outstanding mechanical properties and specific weight reduction. The addition of Al promotes the precipitation of L'1₂ ordered (Fe, Mn)₃AlC carbides, the so-called κ -carbides. In the austenitic FeMnAlC steels, κ -carbides are nano-sized cuboidal precipitates that control the dislocation assisted plasticity of these materials. It is thus important to understand the interaction mechanisms between dislocations and κ -carbides and to investigate the influence of precipitates morphology that arises from spinodal decomposition on the mechanical behaviour. Here we provide new insights into κ -carbide strengthened high-Mn steels by employing TEM observations [1] and simulating comparable microstructure using discrete dislocation dynamics (DDD) simulations. The DDD simulations of this study are based on the previous model developed for cuboidal γ' strengthened Ni base superalloys [2]. To investigate the effect of the κ -carbides morphology we established a similar particles arrangement as indicated by TEM images, concerning particle size and position along <100> directions. In order to get more insight into the bowing of dislocations into the channels between the particles and the subsequent mechanical response theirs size and geometry are varied at a fixed κ -carbide fraction. In connection with TEM observations this gives us the opportunity to understand how the geometrical arrangement of these particles induces the plastic deformation of these materials. This provides new guidelines in the alloy design of advanced lightweight steels based on the underlying dislocation mechanisms at different κ -carbide geometrical arrangements.

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Mechanisms of Plastic Deformation of Polycrystalline Sodium Chloride at room temperature and at 350°C :2D and 3D observations and modeling

Jean L. Raphanel¹, Alexandre Dimanov¹, Mathieu Bourcier², David Picard¹,
Ababacar Gaye³, Michel Bornert³

¹LMS Ecole polytechnique, 91128 Palaiseau, France

²MSSMAT, Ecole Centrale, 92430 Chatenay Malabry, France

³Laboratoire Navier, Ecole des Ponts ParisTech, 77420 Champs sur Marne, France

Synthetized sodium chloride polycrystals have been deformed at room temperature and at 350°C by uniaxial compression a) in a Scanning Electron Microscope, b) for 3D Xray analysis (absorption) on a synchrotron beam line. 2D and 3D markers have allowed the use of Digital Image Correlation to compute the strain fields through an ad-hoc software (CMV). For large grained samples, both intracrystalline plasticity (CP) and grain boundary sliding (GBS) are recorded from the start of the permanent deformation and at both temperature. There is some indication that the orientation of the boundary with respect to the applied uniaxial loading plays a critical part for GBS, as well as the relative crystalline orientations as measured by EBSD (Electron Back Scattered Diffraction). GBS is also found on the samples deformed at high temperature, even though CP is easier in this case than at room temperature. Studies on halite single crystals have indeed determined that this ionic crystal, with a centered cubic lattice, may deform plastically on three potential families of slip systems, which have in common the <110> directions associated to the {110}, {100} and {111} planes respectively. The initial critical shear stresses (CSS) are very different for each family of systems with a strong temperature and strain rate dependence. At room temperature, it is generally recognized that the {110}<110> systems have the lowest CSS. They do not however provide enough independent systems to accommodate any local strain state, so that systems with higher initial CSS or other plastic deformation mechanisms have to be activated as well. At a higher temperature, the initial critical shear stresses of the different families decrease and tend to a common value, which should provide enough active slip systems to accommodate any plastic strain. However, GBS is still a component of the material response.

If direct observations or DIC computations may give some clues about the local activity of slip planes, they are not sufficient to get a complete description of CP. An approach is then to use crystal plasticity finite element methods (CP-FEM) with a careful selection and assessment of the underlying assumptions. Three main hypotheses are reviewed: the choice of a 3D structure based on 2D observations, the boundary conditions and the constitutive equations at the single crystal level. For this last part, we compare results from the literature with experiments that we have performed on single crystals. We thus identify and improve the hardening model used in the computations. Classical CP-FEM models do not account for GBS but allow the estimate of normal or tangential stresses along perfect grain boundaries. In a first step, we use these results to analyze regions where GBS has been observed. In a second step, we enrich the classical model by adding a specific behavior in the vicinity of boundaries allowing some localized displacements.

A massively parallel level-set approach for the modelling of 3D anisotropic grain growth in polycrystalline materials

Christian Mießen, Luis Barrales-Mora, Günter Gottstein

Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University,
D-52056 Aachen, GERMANY

Microstructure evolution during heat treatment is of primary relevance because the properties of metallic materials are determined basically by their microstructure. During heat treatment, mainly three phenomena are triggered that modify the microstructure: recovery, recrystallization and grain growth. Grain growth is the enlargement of the crystallites of a polycrystal that takes place in order to minimize the free energy of the system. This phenomenon is controlled by the motion of grain boundaries, which in turn is driven by the local curvature of the grain boundaries and influenced by the mobility and energy of the grain boundaries and their junctions. In the present contribution, we present a model based on the level-set approach that is capable to consider all the factors that affect grain boundary migration and thus, grain growth. A statistically relevant 3D polycrystal was simulated and compared to theoretical expressions for the growth of 3D grains for validation of the model.

The authors gratefully acknowledge the financial support from the Deutsche Forschungsgemeinschaft (DFG) within the Reinhard-Koselleck project GO 335/44-1, in which frame this work is settled.

The work is related to my PhD studies, which I would like to present preferentially in the form of an oral talk.

Investigations of the effect of grain boundaries shape modeling in three-dimensional actual polycrystalline aggregates

Edouard Pouillier¹, François Curtit¹, Loïc Signor², Félix Latourte¹

¹EDF R&D, Département Matériaux et Mécanique des Composants, Avenue des Renardières, 77818 Moret-sur-Loing Cedex, France

²Institut Pprime, UPR 3346 CNRS ENSMA Université de Poitiers, France

The aim of the present study is to investigate the consequences of assumptions on the grain boundaries shape provided in the simulations of polycrystalline aggregates.

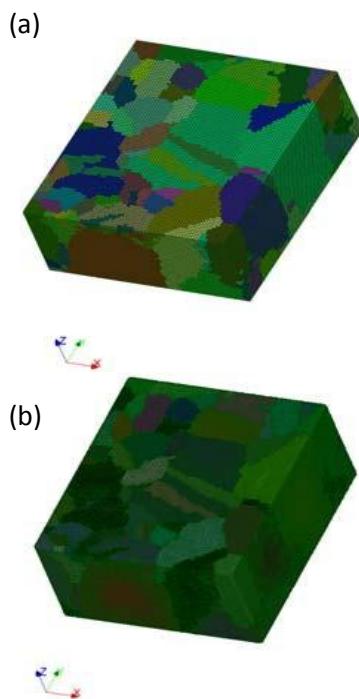


Figure 1: Polycrystalline aggregate made of 130 grains meshed with (a) hexahedron elements and (b) tetrahedron elements based on a Laplacian smoothing applied to grain boundaries.

The framework of this study is the fatigue crack initiation in ductile alloys like austenitic stainless steels that is mainly due to the occurrence of localized deformation in persistent slip bands (PSB) [1]. The study is made on a 316 stainless steel where PSB is classically related to microstructural features such as grain boundaries and neighborhood of the crystallographic grain orientations [2].

To determine the role of the grain boundaries shape on the behavior of polycrystal aggregates, a crystal plasticity model was used to describe the constitutive behavior of each grain in the finite element model of a 3D microstructure submitted to cyclic loadings. From the same initial 3D EBSD map, three polycrystals meshes were generated with different assumptions on the modeling of the shape of grain boundary shape: (i) a mesh based on EBSD measurement points considered as voxels and mesh with hexahedron elements (Fig. 1.a), (ii) a mesh based on a marching cube algorithm and, (iii) a mesh where the microstructure generated by the marching cube algorithm was smoothed with a Laplacian smoothing (Fig. 1.b). A statistical analyze of the FE results is carried out to highlight influences of grain boundaries shape on the local stress and local strain fields and on the macroscopic behavior of the material.

This work was supported by Agence Nationale pour la Recherche and EDF R&D division, in the framework of the project AFGRAP. The authors acknowledge institut Pprime for provided experimental data.

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Microstructure-sensitive modeling of void nucleation in polycrystalline materials

Evan Lieberman¹, Anthony Rollett¹, Edward Kober², Ricardo Lebensohn²

¹Carnegie Mellon University, Pittsburgh, Pennsylvania 15213, USA

²Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

We present the implementation of a model for void nucleation in a Fast-Fourier Transform (FFT)-based elasto-viscoplastic formulation. The latter produces full-field solutions for the stress and strain in voxelized polycrystalline microstructures[1]. Utilizing the knowledge of which voxel belongs to which grain, the local first order Cartesian moments of the grain structure are used to calculate the grain boundary normal vectors of the voxelized microstructure. [The first order moments are equivalent to the gradient of the grain character within the volume of calculation and the direction of the maximum gradient is the surface normal.] Combining these, the grain boundary tractions can be calculated. We identify “traction hotspots”, i.e. regions with tractions that are significantly above the mean, and use them to predict void nucleation sites in copper polycrystal. The proposed methodology can be separately implemented in a dilatational FFT-based model that simulates porosity evolution. The results are compared to both experiments and molecular dynamics (MD) simulations to improve the accuracy of the model[2]. The MD model provides additional insight into other factors to incorporate beyond grain boundary tractions, and with the experiment results used to confirm the models’ predictions. There are two paths of the experimental comparison. One path is to compare morphologic trends in the traction hotspots to the experimentally measured morphological trends of voided grain boundaries. The other path utilizes near field high-energy diffraction microscopy (nf-HEDM) to obtain microstructure images of a copper polycrystal before and after shock loading is applied. Traction hotspots derived from the pre-shocked state are then compared to void locations in the post-shocked state.

A second aspect is to use some of these techniques to characterize experimental data obtained from nf-HEDM. Normally, the samples are characterized by the local crystallographic orientation at about 1 micron resolution. Currently, grains are identified by thresh-holding differences in the misorientation angle between neighboring voxels. As above, it is difficult to characterize the grain boundary normal from these voxelized images. The first order moment technique above can be used to define interfaces by looking at the maximum in the gradients; only here it is applied to either the misorientation angle or the quaternion vector that describes the crystallographic orientation. This same analysis can be applied to the simulations, ignoring the grain identities and focusing only on the local orientation, and achieves similar results. Because the grain boundaries and their normals are defined analytically, the results of the simulation and experiment can be directly compared even though they come from meshes with differing resolutions.

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Synergies between experiments and simulations: mapping and modelling of LiFePO₄ electrodes

Bernardo Orvananos¹, Fiona C. Strobridge², Clare P. Grey², Katsuyo Thornton¹

¹Department of Materials Science and Engineering, University of Michigan, Ann Arbor,
Michigan 48109, USA

²Department of Chemistry, University of Cambridge, Cambridge, Cambridgeshire CB2
1EW, UK

Electrochemical systems are difficult to analyze, both experimentally or by modeling, because of the complex interplay of electrochemistry, thermodynamics, and transport (diffusion and phase transformations). The interpretation of experimental data is challenging due to the involvement of multiple materials (e.g., electrolyte, electrode particles, and conducting additives). Thus, the combination of experiments and simulations is essential in elucidating the processes underlying experimentally observed phenomena.

This collaborative work is based on an *in situ* energy dispersive X-ray diffraction (EDXRD) that is used to measure the inhomogeneous electrochemical reaction of LiFePO₄ particles within a coin cell. Profiles of the state of charge in two dimensions are obtained throughout the process. To understand the evolution of the state of charge during the discharge process, we simulate the dynamics using a cell-scale model parameterized with experimental measurements. We use simulations to extract the effective material parameters and use the results to hypothesize their changes from a cycle to another. These hypotheses then inspire additional simulations at microstructure-level and experiments, which will be discussed.

This work was supported as part of the Northeastern Center for Chemical Energy Storage, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award # DE-SC0001294.

Defect Character at Grain Boundary Facet Junctions: A Combined HRSTEM and Atomistic Modeling Study of a $\Sigma=5$ Grain Boundary in Fe

D.L. Medlin¹, K. Hattar², J. Zimmerman¹, F. Abdeljawad², and S.M. Foiles²

¹Sandia National Laboratories, Livermore, California 94551, USA

²Sandia National Laboratories, Albuquerque, New Mexico 87185, USA

A fundamental challenge for understanding the structure and behavior of grain boundaries is to establish physically meaningful links between the atomic-scale interfacial configurations, which can often be described in terms of sets of characteristic structural units [1], and the more macro-scale descriptors of the interfacial geometry, e.g., grain misorientation and boundary inclination. A useful approach for establishing such linkages is to identify and characterize the sets of interfacial line defects that accommodate departures from low-energy singular reference configurations [2].

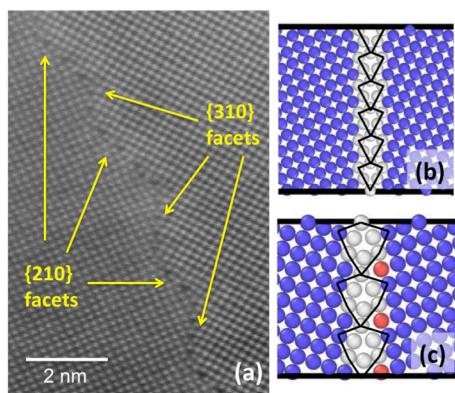


Figure 1: (a) HAADF-STEM image of a $\Sigma=5<001>$ boundary in Fe. The boundary has adopted an asymmetric inclination with nanoscale facets on $\{310\}$ and $\{210\}$ type planes. Calculations for the symmetric $\{310\}$ and $\{210\}$ inclinations, computed using the Mendelev potential [3] are shown in (b) and (c), respectively.

Here, we consider such approaches in the context of atomic resolution experimental observations and theoretical calculations of the structure of $\Sigma=5<001>$ tilt boundaries in BCC iron, focusing in particular on the analysis of facet junctions and grain boundary dislocations present at the interface. Figure 1a shows a high angle annular dark field (HAADF) scanning transmission electron micrograph (STEM) of such a boundary observed in a pulsed-laser-deposited thin film of Fe. Two symmetric inclinations, $\{210\}$ and $\{310\}$, are geometrically possible for $\Sigma=5<001>$ boundaries. Figures 1b,c show simulations for these inclinations computed using the Mendelev potential for Fe [3]. The observed boundary has adopted an asymmetric inclination, but accommodates the departure by forming nanoscale facets aligned with these two symmetric inclinations. As we will

discuss, a full description of this interface requires consideration of the geometric incompatibility at the junctions, which can be represented by dislocation-like defects, as well as the incorporation of additional dislocation content due to departure from the exact $\Sigma=5$ orientation relationship. We will also discuss how the finite facet size affects the structure relative to an unconstrained, planar geometry.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Using Atomistic Reconstructions of 3D Atom Probe Tomography Data to Study the Interactions of Dislocations with γ' -Precipitates in a Ni-base Superalloy

Erik Bitzek¹, Aruna Prakash¹, Juan Wang¹, Julien Guénolé¹,
Ivan Povstugar², Pyuck-Pa Choi², Dierk Raabe²

¹Department of Materials Science and Engineering,
Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU),
91058 Erlangen, Germany

²Department of Microstructure Physics and Alloy Design,
Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany

Single crystalline Ni-base superalloys are key materials for turbine blades in modern gas turbines. The microstructure of these alloys consists of cubic γ' -precipitates of Ni_3Al in the $\text{L}1_2$ crystal structure embedded in the fcc γ -matrix. The interaction of dislocations in the γ -channels with the γ' -precipitates is a main factor for the superior strength of these alloys even at high temperatures. Processes at the atomic scale govern the cutting of the dislocations from the γ -channels into the precipitates. However, only few atomistic simulations of the dislocation behavior at the γ/γ' -interface have so far been performed. Up to date, all simulations made furthermore use of highly idealized simulation set-ups with straight dislocation lines interacting with perfectly planar interfaces.

Here we report on a new method to create realistic three-dimensional atomistic samples based on geometrical information and the local concentrations of chemical elements obtained from atom probe tomography. We applied this method to recreate the γ/γ' -microstructure of CMSX-4 and to study the influence of temperature and gradients in the local Al and Re concentration on the structure of the γ/γ' -interface. Simulations of tensile tests were subsequently used to study the influence of the interface and the misfit dislocation network on the mechanical properties of realistic γ/γ' -microstructures. Finally, the interaction of carefully inserted channel dislocations with the fully 3D microstructure was studied in detail. The results of these studies are juxtaposed to simulations performed using a classical, quasi-2D simulation set-up with planar interfaces and straight dislocation lines and discussed in the framework of a multiscale modeling approach to study the mechanical behavior and stability of Ni-based superalloys.

The authors acknowledge support by the Deutsche Forschungsgemeinschaft (DFG) through projects C3 and A4 of Collaborative Research Center SFB/Transregio 103 (Single Crystal Superalloys).

Measuring and Modeling Strain Fields in High Angle Graphene Grain Boundaries

Colin Ophus¹, Haider Rasool^{1,2}, Zi-Ang Zhang³, Boris Yakobson³, Alex Zettl^{1,2}

¹Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

²University of California Berkeley, Berkeley, California 94720, USA

³Rice University, Houston, Texas 77005, USA

Some chemical deposition processes of graphene can produce highly polycrystalline films containing a high density of grain boundaries (GBs) [1]. The local structure and strain at these boundaries can strongly affect their mechanical properties [2,3]. In this work, we use a combination of high-resolution transmission electron microscopy (HRTEM) and molecular dynamics (MD) simulations to measure and model the structure of high angle graphene GBs.

Exit wave reconstructions of graphene GBs were performed using the algorithms described in [4], along with a new method for numerical aberration correction in crystal lattices. From this data we can understand the local structure of high angle graphene GBs and measure strain distributions, shown in Figure 1.

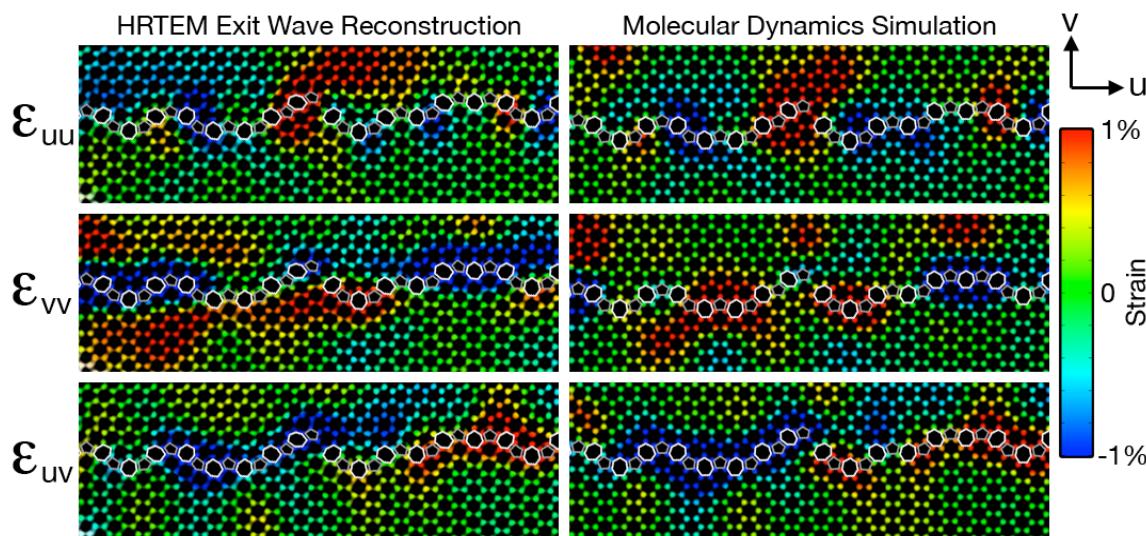


Figure 1 – Comparison of strain fields from HRTEM experiment and MD simulation.

We have used the measured atomic positions as inputs for MD simulations. We then compare the strain distributions from the relaxed MD simulations and determine how the local 3D structure of the boundary affects these distributions. Figure 1 shows a direct comparison between the experimental and simulated strain distributions [5].

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Atomistic Determination of Grain Boundary Mobility in Fe-He Alloys

A. T. Wicaksono, C. W. Sinclair, M. Militzer

Department of Materials Engineering, The University of British Columbia, Canada

The addition of even small amounts of solute is known to drastically reduce the mobility of grain boundaries. This fact is widely made use of in order to control microstructure in engineering alloys, where solute drag can be used to control the velocity of a migrating grain boundary (see e.g. [1]). While atomistic simulations have provided new insight into the mechanisms governing grain boundary motion, these studies have focused on pure materials rather than technologically important alloys. Atomistic studies on the mobility of solid-liquid interfaces have, on the other hand, shown significant effects arising from solute trapping [2].

One factor that restricts studies of grain boundary migration by molecular dynamics in the presence of solute is the large boundary velocities required relative to the typical diffusivity of solute atoms. In the work presented here, we have sought to overcome this limitation by studying the Fe-He system where He atoms diffuse rapidly at the temperatures of interest. Moreover, He tends to form clusters, these clusters having a different character at the boundary compared to within the bulk of a material. The effect

of such solute clustering is not well captured in classical mean-field solute drag or precipitate drag models. The mobility of select boundaries in pure Fe was determined for a driven boundary using a synthetic driving force method [3] as well as for a stationary boundary using a random walk analysis [4]. Following this, the random walk analysis was used to obtain the mobility of the boundaries in the presence of He atoms. Results show that the presence of solute and solute clusters lower the mobility of the grain boundaries, in qualitative agreement with experiments.

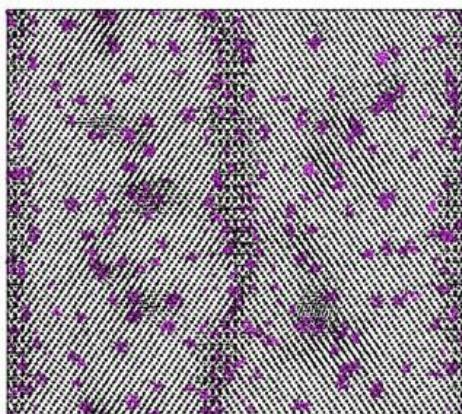


Figure 1: Cluster formation in an incoherent $\Sigma 3$ grain boundary in an Fe-1at%He alloy

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Ultrafast melting of laser-excited gold nanofilms: Combining experiment and atomistic modelling

S. L. Daraszewicz², Y. Giret^{1,2}, N. Naruse¹, Y. Murooka²,
J. Yang¹, D. M. Duffy², A. L. Shluger², K. Tanimura¹

¹ The Institute of Scientific and Industrial Research (ISIR), Osaka University,
8-1 Mihogaoka, Ibaraki, Osaka 567-0047, Japan,

² London Centre for Nanotechnology, Department of Physics and Astronomy,
University College London (UCL), Gower Street, WC1E 6BT, London, UK

The ability to model and ultimately predict the sub-picosecond atomistic dynamics in laser-excited matter is an essential step in future structure and function control of nanomaterials. We present state-of-the-art transmission ultrafast electron diffraction (UED) measurements of laser-excited gold nanofilms. We have used relativistic electron pulses (3.0MeV), which allowed us to perform single shot measurement without any multiple diffraction or possible inelastic effects. We quantitatively combine the measured temporal evolution of the Bragg peaks with the two-temperature molecular dynamics (2T-MD) model and thereby directly expose the atomistic dynamics of gold nanofilms during a photo-induced solid-to-liquid phase transition. Notably, the equivalent spatiotemporal scales of the experiment and the model, which encompasses both ultrafast changes in the interatomic potential and the electron-phonon relaxation process, have enabled a direct prediction of the atomistic behaviour behind the UED signals. We used a wide range of laser fluences and observed transition between slow heterogeneous melting, rapid homogeneous melting and ultrafast non-thermal melting at very high fluence, where electronic excitation effects on the interatomic potential are non-negligible. We discuss the latter case in terms of a shift of equilibrium lattice volume leading to rapid surface expansion accompanied by bond softening. An excellent agreement between the 2T-MD model and experiment enables us, for the first time, to expose the sub-picosecond timescale atomistic behaviour of the melting dynamics and demonstrates that 2T-MD is a reliable characterisation tools for structure determination from UED measurements.

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Modeling of nanocalorimetry experiments of damage evolution in self-implanted silicon

Manuel Ruiz, Lourdes Pelaz, Luis Marqués, Pedro López, Iván Santos, María Aboy

Universidad de Valladolid, 47011 Valladolid, Spain

Ion implantation cascades in crystalline Si generate different damage configurations going from isolated point defects and point defects clusters to amorphous pockets and continuous amorphous layers if the implanted fluence is high enough. Schietekatte's group has performed extensive experimental work on nanocalorimetry of ion implanted thin films [1]. This technique provides information about the kinetics of damage annealing by monitoring the rate of heat released during annealing of ion beam induced defects [2]. However, since many different damage configurations may coexist it is difficult to unravel the mechanisms and energetics controlling the process.

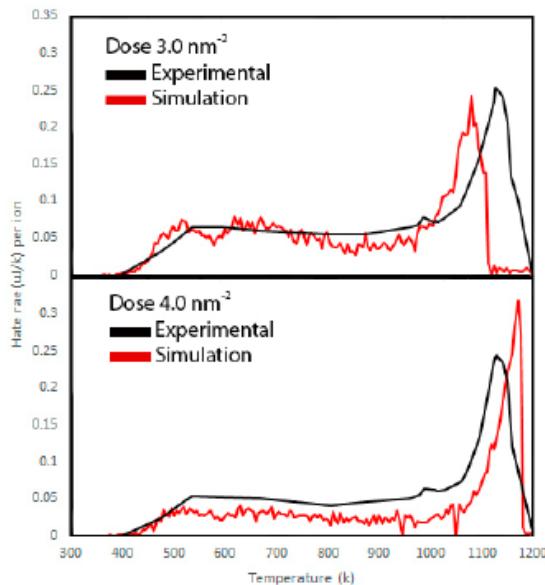


Figure 1: Heat release during damage annealing after implantation at 10 keV for different doses.

results are shown in Fig. 1. At low temperatures the heat is mostly released by small amorphous pockets that recombine, while the peak that appears at higher temperatures is associated to the regrowth of extensive amorphous regions, and eventually a full amorphous layer when it is formed during the implantation.

This work was funded by Ministerio de Ciencia e Innovación under project TEC2011-27701.

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In this work we use a Kinetic Monte Carlo atomistic model on defect generation and annealing to follow the evolution of ion beam induced defects at temperatures, time and space scales of experiments. The model includes the energetics associated to self-interstitial and vacancy clusters, and describe amorphous regions as bond defect agglomerates [3]. Some parameters are obtained from fundamental calculations, while others are obtained from indirect experiments or interpolation. Although the model simplifies the complex atomic relaxation scenario by reducing the number of possible defect configurations to a small finite set, it reproduces and disentangle the main features of experimental nanocalorimetry scans under different implant conditions. Obtained

Molecular-dynamics simulations and experimental investigation of the migration of tilt and mixed grain boundaries in pure Aluminum

L A Barrales-Mora, J E Brandenburg , D A Molodov

Institut für Metallkunde und Metallphysik, RWTH-Aachen University, Aachen, Germany

Grain boundary migration is determinant for numerous physical processes in materials science such as recrystallization and grain growth. Despite extensive investigations on grain boundaries, little is still known about the migration mechanisms of general grain boundaries because most of the studies have been conducted in either pure tilt or twist grain boundaries. In the present contribution, we present experimental findings of the migration of tilt and mixed grain boundaries in pure aluminum. Additionally, we made use of molecular-dynamics simulations to study comprehensively the migration mechanisms and kinetics of these boundaries. The results showed that low angle grain boundaries of mixed character are definitely more mobile than those of tilt character, a fact that might change the way grain boundary mobility is considered in mesoscopic models of phenomena controlled by grain boundary migration.

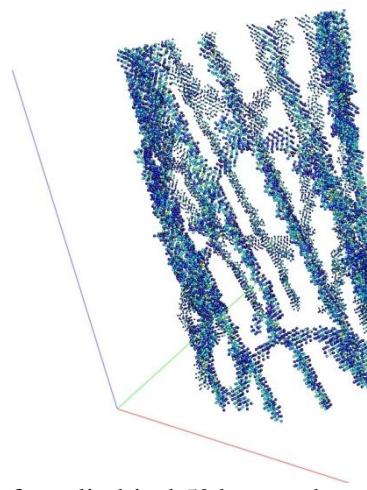


Figure 1. Dislocation structure of a cylindrical 5° low angle grain boundary of mixed character in Al as revealed by the central-symmetry parameter.

This work was founded by the German Research Foundation within the framework of a Reinhard-Koselleck Project (No. GO 335/44-1) and grant (MO 848/14). The simulations were performed at the high-performance computing cluster of the RWTH-Aachen University.

Modeling and experimental characterization of {311} defects in silicon

Luis A. Marqués¹, K.J. Dudeck², G.A. Botton², L. Pelaz¹, I. Santos¹,
P. López¹, M. Aboy¹, M. Ruiz¹

¹Departamento de Electrónica, Universidad de Valladolid, E.T.S.I. de Telecomunicación,
47011 Valladolid, Spain

²Department of Materials Science and Engineering, McMaster University, 1280 Main
Street West, Hamilton, Ontario L8S 4L7, Canada

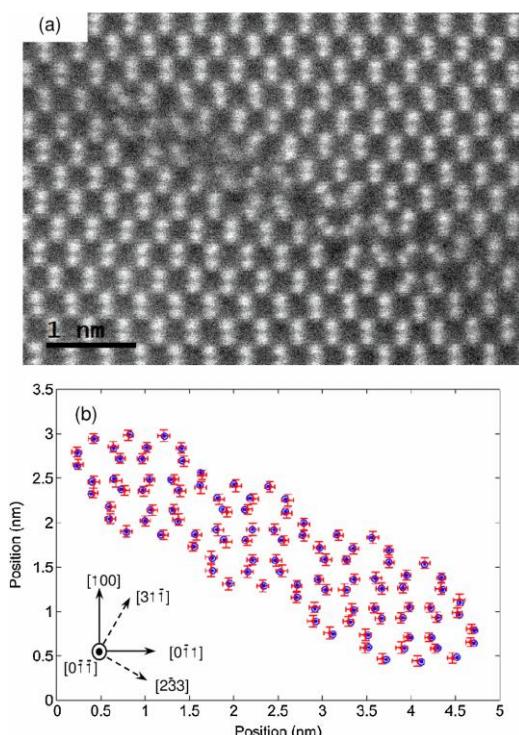


Figure 1: (a) Unprocessed HAADF STEM image of a planar {311} defect. (b) Structural units associated with the defect as obtained from the image (red squares) and from the MD simulations (blue circles).

TEM images. Agreement between experiment and theoretical atomic positions is better than ± 0.05 nm. We find that the shape of five-, six-, seven- and eight-member rings in 311s varies as a function of position within the defect, and that is perfectly reproduced in the simulations. This excellent agreement validates the simulation results and, at the same time, it demonstrates that HAADF scanning TEM image analysis techniques can be used to extract precise quantitative information at the atomic scale.

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Ion implantation and annealing are key processing steps used for the fabrication of PN junctions within the manufacturing industry of Si electronic devices. Besides the introduced dopant atoms, excess self-interstitials above equilibrium conditions are generated in the lattice. They form aggregates that, as sizes of several hundred interstitials, become visible in transmission electron microscopy (TEM) images [1]. Among them, the so-called {311} defects (311s) have received much attention because they act as a reservoir of interstitials that are slowly released during subsequent thermal treatments, causing the unwanted transient enhanced diffusion of interstitial-diffusing dopants [2].

Here we propose an atomistic model based on chains of self-interstitials and bond defects, able to describe the formation and structure of 311s. By the use of molecular dynamics (MD) simulations, we show that these chains spontaneously transform into planar 311s when annealed. MD results are compared with experimental measurements obtained by high-angle annular dark-field (HAADF) scanning

Molecular dynamics modelling of mechanically loaded interfaces of single-walled carbon nanotubes and palladium

Steffen Hartmann¹, Ole Hölk², Bernhard Wunderle¹

¹Technische Universität Chemnitz, Reichenhainer Str. 70, D-09120, Germany

²Fraunhofer IZM Berlin, Gustav-Meyer-Allee 25, D-13355, Germany

The interface of a single-walled carbon nanotube (CNTs) and an embedding metal is of particular interest for the design of future mechanical sensors. Certain species of single-walled CNTs exhibit very high intrinsic piezoresistive gauge factors and it is pursued to integrate them as a new sensing material into macroscopic sensor devices [1]. To evaluate their piezoresistivity, single-walled CNTs have to be connected to metal electrodes (e.g. palladium [2]) to provide an electrical connection and a mechanical clamping. In application the CNT can be elongated and its change in resistance be evaluated. In fact, the force to elongate the CNT is also acting on its interface to the embedding metal electrode and the assessment of interface strength and critical loading conditions is an important issue for the sensor design and its layout to prevent damage or failure.

We investigated the interface of a single-walled CNT and a palladium matrix by means of molecular dynamics and performed accompanying nano scale experiments inside a scanning electron microscope. We set up a model in which one single-walled CNT is embedded in a single crystalline matrix and a pull-out test can be simulated (see figure 1). With this model we can obtain force-displacement relations and energy evolutions for a quasi-static displacement controlled test. Furthermore, we are able to investigate the influence of CNT type, embedding length, temperature, intrinsic defects and functional side groups on the interface behaviour.

For defect free models of uncapped and chiral single-walled CNTs we found depending on the

CNT diameter pull-out forces in the nano to tens of nano Newton range. Due to the incommensurate interface of the CNT and the metal, the embedding length has no influence on the maximum pull-out force and the failure mode is an interface fracture with the mechanism of a dry sliding detachment. The situation is different when alcohol groups are attached onto the CNT. We found that alcohol groups act as small anchors in the palladium matrix and significantly enhance the resisting forces opposing the pull-out. By comparing our computational and experimental results of maximum pull-out forces (also several tens of nano Newtons) and the predicted failure mode we conclude a very good agreement.

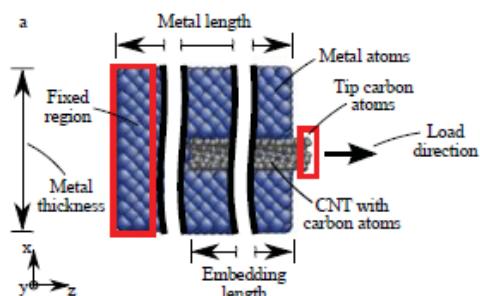


Figure 1: Representative geometry of pull-out test setup. Shown is the cross-section of a (6,3) CNT embedded in a palladium block.

With this contribution we focus on the potential of molecular dynamics simulations (i) to reasonably predict maximum pull-out forces of single-walled CNTs embedded in a palladium matrix and (ii) to provide valuable input to understand the underlying mechanisms of failure.

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Investigating the limits of discrete dislocation descriptions of inclined twin boundaries in the presence of hydrogen

Christopher J. O'Brien¹, Douglas L. Medlin², Stephen Foiles¹

¹Sandia National Laboratories, Albuquerque, New Mexico, USA

²Sandia National Laboratories, Livermore, California, USA

Low mobility twin boundaries dominate the microstructure of grain boundary engineered materials and are critical to understanding their plastic deformation behavior.

Furthermore the presence of solutes, such as hydrogen, has a profound effect on the thermodynamic stability of the boundaries. In order to develop a more complete mesoscale model of the interfacial behavior, we are developing analytical expressions modeling boundary energy and hydrogen segregation dependence on inclination and misorientation from low energy singular configurations. We start by considering a $\Sigma 3$ grain boundary at inclinations from $0^\circ \leq \Phi \leq 90^\circ$. The angle Φ corresponds to the rotation of the $\Sigma 3(111)\langle 110 \rangle$ (coherent) into the $\Sigma 3(112)\langle 110 \rangle$ (lateral) twin boundary. To this end, atomistic models utilizing empirical potentials are applied to determine the validity of modeling the inclination and misorientation of the boundary by incorporating arrays of discrete $\frac{1}{3}\langle 111 \rangle$ and $\frac{1}{6}\langle 112 \rangle$ disconnections. After establishing the model, this study investigates the angular range of inclination and hydrogen concentration over which the superposition of such disconnections may serve as an accurate representation of grain boundary energy and interstitial segregation behavior. The predictions of this model will be compared with detailed microscopy of inclined $\Sigma 3$ grain boundaries.

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Simulation analysis of stress and strain partitioning in dual phase steel based on real microstructures

F. Roters, M. Diehl, P. Shanthraj, C. Zambaldi, C. C. Tasan, D. Yan, D. Raabe

Max-Planck-Institut für Eisenforschung,
Max-Planck-Straße 1, 40237 Düsseldorf, Germany

The mechanical response of alloys consisting of multiple phases is governed by microscopic strain and stress partitioning among the various phases, crystals and subgrains. Yet, due to the limitations that are inherent in the experimental characterization of the stress-strain partitioning that takes place at the micro-scale, microstructure optimization of such alloys is typically based on the averaged macro-scale response (e.g. engineering stress-strain curve). To strengthen the connection between microstructure and mechanical properties, a novel methodology is introduced in this work that enables the joint simulation and experimental based analysis of the deformation- induced evolution of heterogeneous materials with multiphase microstructures.

This is achieved through a combined numerical-experimental approach, i.e. relying on crystal plasticity (CP) simulations and in-situ deformation experiments both initiated from the same electron backscatter diffraction (EBSD) mapped representative microstructural area of interest. 2D full-field crystal plasticity simulations are run employing a recently developed spectral solver suitable for high-phase contrast materials [1, 2] implemented in the crystal plasticity simulationkit DAMASK [3]. The model is created directly from high resolution EBSD based crystal structure, phase, and orientation maps. The individual phase properties are obtained by additional inverse CP simulations of nanoindentation experiments carried out on the original microstructure [4]. The simulated local strains are compared to experimental results obtained by a recently developed, digital image correlation-based, high-resolution, 2D strain mapping methodology [5].

The methodology is demonstrated here on the example of martensite-ferrite dual phase (DP) steel, for which promising correlation between the simulations and experiments is achieved, despite the complex micro-mechanics of this material. Obtained strain maps reveal significant strain heterogeneity arising from martensite dispersion, ferrite grain size, and defect densities effects; and early damage nucleation at notch-like irregularities in martensitic zones that cause high stress triaxiality. Deviations between simulations and experiments can be explained in terms of known limitations of the involved techniques. The presented integrated engineering approach provides a high dimensional set of micro-mechanical output information that can enhance the understanding and further development of complex bulk multiphase alloys.

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- [3] <http://damask.mpie.de>
- [4] C. Zambaldi, Y. Yang, T. R. Bieler, D. Raabe: Journal of Materials Research 27 (2012), 356-367
- [5] see talk by C. Tasan in Symposium A

Resolving the evolution of pore structures in 304-L laser welds

James W. Foulk III¹, Michael G. Veilleux¹, John M. Emery², Jonathan D. Madison²,
Helena Jin¹, Jakob T. Ostien¹, Alejandro Mota¹

¹Sandia National Laboratory, Livermore, California 94550, USA

²Sandia National Laboratory, Albuquerque, New Mexico, 87185, USA

The failure of partial-penetration Nd:YAG laser welds in 304-L stainless steel have been investigated through the direct incorporation of pore structures at the specimen level.

Micro-computed tomography (μ CT) is employed to characterize multiple weld schedules and develop idealized representations of the size, shape, and spacing of the pores. Pore growth and the subsequent necking are natural outcomes of the simulation.

The large deformations between pores require a robust mapping scheme for the remeshing and mapping of internal state variables [1]. We employ higher-order tetrahedral elements to resolve strong gradients and ease the burden of discretizing complex and evolving pore structures.

Through our ability to idealize, resolve, and evolve pore structures, we can investigate the performance of candidate weld schedules.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Understanding how oxidized grain boundaries fail: A combined experimental and crystal plasticity finite element approach

Judith Dohr¹, Edmund Tarleton¹, David E.J. Armstrong¹,
Thierry Couvant², Sergio Lozano-Perez¹

¹Department of Materials, University of Oxford, Oxford, United Kingdom

²Électricité de France R&D, Écuelles, France

Stress Corrosion Cracking (SCC) of Alloy 600 in the primary loop of Pressurized Water Reactors (PWRs) represents one of the most challenging forms of materials failure the nuclear industry has faced. Over the last decades many mechanisms have been proposed to explain this complex localized sub-mode of corrosion but experimental evidence in favour of one of them is still unavailable. Although Alloy 600 is known to suffer from cracking along grain boundaries (intergranular SCC) under PWR primary water conditions, information about the stress necessary to induce cracking and the link between the specific grain boundary (GB) microstructure, degree of oxidation and deformation behaviour is still unknown.

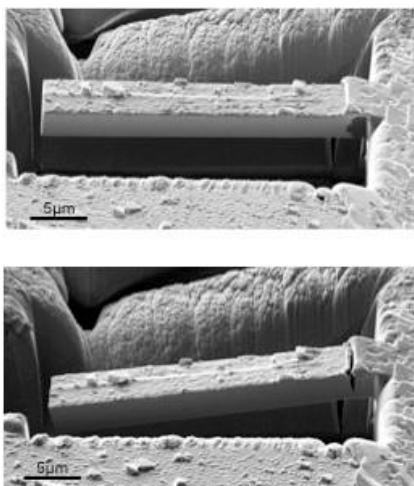


Figure 1: SEM images of a FIB-machined cantilever, before (top) and after (bottom) the micromechanical test. The bottom image shows how the oxidized portion failed (intergranular) along the grain boundary after testing.

of the metal/oxide interface, allowing our model to reproduce the different fracture modes observed in experiments, and the interaction between plasticity and fracture. We aim to use our calibrated model to predict the fracture behaviour of different types of GBs, including variations in misorientation and carbide coverage. This could reveal which oxidized GBs are harder to fracture, which is relevant to the field of GB engineering.

The authors want to thank INSS (Japan) and EDF (France) for the provision and autoclaving of the samples. EDF is further acknowledged for the financial support of this work.

A novel approach, combining extensive experimental work and modelling through the crystal plasticity finite element method (CPFEM), now enables the quantification of the stress necessary to fail individual oxidized GBs. This approach involves the micromechanical testing of cantilevers containing the GB of interest (Figure 1), to obtain information about the elastic modulus, yield stress and fracture toughness, as well as a detailed characterization of the fracture region via 3D FIB-Slicing and (S)TEM to correlate the measured mechanical response to the specific (3D) microstructure and degree of oxidation. Selected Area Diffraction (SAD) is used to identify grain orientations and active slip directions. With this information, a realistic crystal plasticity model of the cantilever is built, employing a user element (UEL) for Abaqus [1]. Previous work [1-2] has highlighted the dependence of local stress and slip accumulation on grain orientation. In this work we are able to incorporate the crystallographic orientations and sample geometry into our model very accurately

We also use cohesive contact to simulate the fracture of the metal/oxide interface, allowing our model to reproduce the different fracture modes observed in experiments, and the interaction between plasticity and fracture. We aim to use our calibrated model to predict the fracture behaviour of different types of GBs, including variations in misorientation and carbide coverage. This could reveal which oxidized GBs are harder to fracture, which is relevant to the field of GB engineering.

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Cyclic deformation experiments and plasticity modeling of three Ti microstructures

Benjamin D. Smith^{1,2}, Donald S. Shih¹, David L. McDowell²

¹The Boeing Company, St. Louis, Missouri 63134, USA

²Georgia Institute of Technology, Atlanta, Georgia 30332, USA

The performance of titanium alloys is strongly dependent on their microstructure formed during thermo-mechanical processing. Accurate modelling of the microstructure-sensitive deformation for titanium alloys is crucial for future materials design and development. The current state-of-the-art for modelling polycrystalline deformation is through the crystal plasticity finite element method (CPFEM). In the present work, a crystal plasticity framework based on a Kocks-type of flow rule has been calibrated to data acquired from cyclic deformation experiments performed on three different titanium microstructures: 1) Ti-64 in a beta-annealed condition; 2) Ti-18 in a solution-treated, age hardened (STA) condition; 3) Ti-18 with a beta-annealed, slow-cooled, age-hardened treatment (BASCA).

The crystal plasticity model employs physically based parameters to determine the simulated mechanical response, many of the parameter values have been obtained from materials characterization as well as from literature sources. The remaining parameters have been estimated such that the simulated macroscopic stress-strain response closely agrees with the experimental results. The robustness of all the calibrated model parameter sets were evaluated by comparing simulation results to additional experimental data. The simulated plasticity model was able to accurately capture the stress-strain response of each microstructure while maintaining the relative strength trends presented in the literature for the estimated parameters (see Fig. 1) [1].

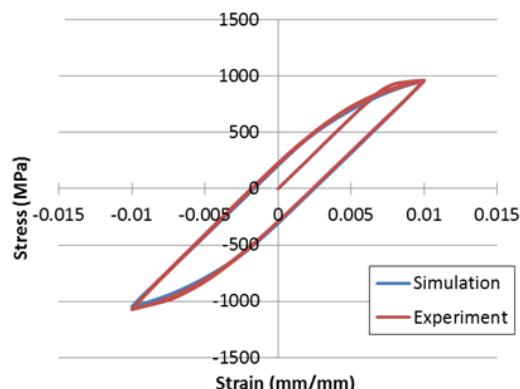


Figure 1: Calibrated results for the initial five cycles of loading of the Ti-64 β -annealed microstructure at room temperature with fully reversed, $\epsilon_a=1\%$, and $5 \times 10^{-4} \text{ s}^{-1}$ loading. [1]

The present work demonstrates the process of model development and calibration necessary to simulate the cumulative deformation mechanisms which cooperatively produce the observed experimental results. These calibrated models have great potential for future utilization in microstructure sensitive studies which can expedite the materials design process by identifying ideal microstructure morphologies for specific applications.

This work was accomplished with financial support of the Boeing Company. The Carter N. Paden Chair in Metals Processing at Georgia Tech also provided supplementary support.

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The Deformation Induced Martensitic Transformation of Metastable Austenite

Chad W. Sinclair¹, Loic Malet², Michel Perez³, Stephane Godet², David Marechal⁴

¹Dept of Materials Engineering, University of British Columbia,
Vancouver, BC V6T 1Z1, Canada

²Université Libre de Bruxelles, 4 MAT, Ave F.D. Roosevelt 50,
CP 194/ 03, 1050 Brussels, Belgium

³INSA Lyon, MATEIS, UMR CNRS 5510, 25 Ave. Capelle,
F69621 Villeurbanne, France

⁴Institut de Mécanique et Ingénierie de Bordeaux,
UMR CNRS 5295, 33607 PESSAC Cedex, France

Metastable austenitic steels are valued for their high strength and uniform elongation. This unusual combination of properties arises from the progressive transformation of the microstructure from austenite to α' -martensite during deformation. Unsurprisingly, the success of any model for the bulk mechanical response is tied to successfully modelling the dependence of martensitic transformation on deformation. Lacking a fundamental understanding of the processes that control nucleation and growth of the martensite phase in this case, models must rely on empirical descriptions of the transformation kinetics. Recent work on the role of stress and plastic strain on crystallographic variant selection has raised the question of the relative importance of plasticity versus local stress state in governing the transformation kinetics[1-3]. In this work, we have attempted to study a simplified situation by examining the martensitic γ to α' -BCC transformation via molecular dynamics and molecular statics simulation using an empirical potential that mimics many of the characteristics of pure Fe. These results are examined in conjunction with experimental work on the martensitic transformation in γ -Fe precipitates in model alloys as well as the martensitic transformation in stainless steels. In particular, the role of local stress state is emphasized in the process of nucleation. The resulting orientation relationship between a confining FCC matrix and martensite is discussed in terms of

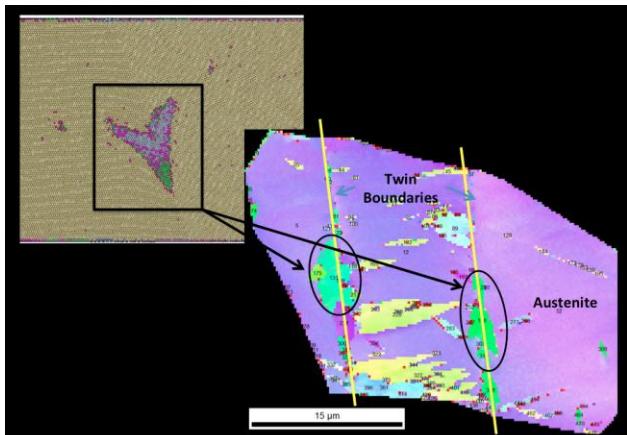


Figure 1: Comparison of the morphology and crystallography of martensite formed during deformation at a twin boundary in an FCC matrix by molecular dynamics simulation (top, left) and experimentally (by EBSD) at annealing twin boundaries in a metastable austenitic stainless steel (bottom right).

the pathway followed during the γ to α' -BCC martensitic transformation.

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Microstructure based continuum modeling of highly anisotropic metals

R.J. McCabe¹, M. Knezevic², L. Capolungo³, A.W. Richards¹, K.D. Clarke¹, R. A. Lebensohn¹, C.N. Tome¹

¹Los Alamos National Laboratory

²University of New Hampshire

³Georgia Tech

We present our methods for incorporating deformation physics and microstructure evolution into continuum level simulations of highly anisotropic metals. This involves a combination of modeling efforts and experimental validation at length scales ranging from the micro-scale to continuum level.

Our micro-scale constitutive law accounts for a dislocation- based hardening law for multiple slip systems and experimentally characterized twinning modes at the grain level. We incorporate the micro- scale deformation laws into a viscoplastic self-consistent (VPSC) polycrystal homogenization scheme that is calibrated with mechanical tests and experimental measures of texture and twin volume fraction evolution. These experiments include compression and tension tests in multiple orientations for three different starting textures. We included strain rate and temperature effects through thermally-activated recovery, dislocation substructure formation, and slip-twin interactions that are calibrated to experiments at multiple strain rates and temperatures. The VPSC based polycrystal model is implemented into an implicit finite element (FE) framework. In this approach, a finite element integration point represents a polycrystal material point and the meso-scale mechanical response of each integration point is obtained by the mean-field VPSC homogenization scheme. We demonstrate the accuracy of the FE-VPSC model by analyzing the mechanical response and microstructure evolution of α -uranium samples under simple compression/tension and four-point bending tests. Predictions of the FE-VPSC simulations compare favorably with experimental measurements of geometrical changes and microstructure evolution. The model accurately captures the tension–compression asymmetry of the material associated with twinning, as well as the rigidity of the material response along the hard-to- deform crystallographic orientations. We apply this method to predict strain heterogeneities that occur during rolling and forming operations of α -uranium parts.

Strain Gradient Crystal Plasticity Modelling – An Efficient Approach to Capture Experimental and Discrete Dislocation Dynamics Observations?

Eric Bayerschen, Stephan Wulffinghoff, Thomas Böhlke

Karlsruhe Institute of Technology, Karlsruhe 76131, Germany

Size effects are commonly observed in the elastic-plastic deformation of micro-specimen in experiments, e.g. in tensile tests (for a recent work see e.g. [1]). One major contribution to this phenomenon in the mechanical response stems from the resistance of grain boundaries against plastic flow [2].

It is shown that this experimentally observed behavior can be reasonably captured with a single-crystal strain gradient plasticity theory for small deformations. This theory is extended by a grain boundary yield criterion [3]. For numerical efficiency the use of an equivalent plastic strain and its gradient are emphasized.

The theory is implemented in weak sense with Finite Elements. Tensile test simulation results of oligocrystals are shown. Further comparison to an experiment and a comparison to Discrete Dislocation Dynamics (DDD) simulations are presented.

Discussion of the latter comparisons and an outline of further possible refinement of the theory at hand conclude the talk.

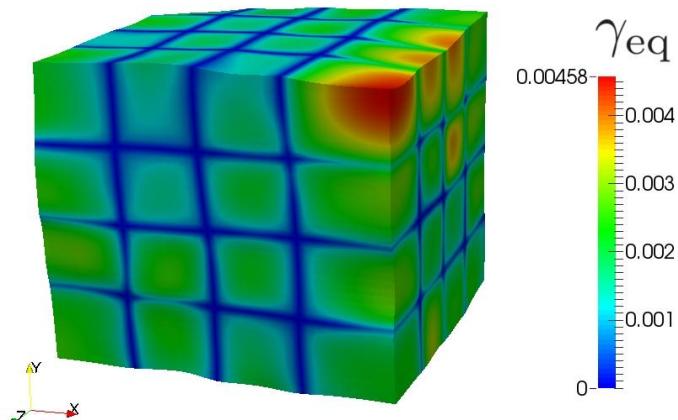


Figure 1: 64-grain tensile test simulation, equivalent plastic strain field distribution at the onset of plastic deformation

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Intermittent and heterogeneous plasticity in hcp alloys: correlations between experimental results and multiscale models

A. Marchenko¹, H. Jousset², M. Mazière¹, S. Forest¹, J. L. Strudel¹

¹Centre des Matériaux ; Mines-ParisTech - 91003 EVRY Cedex-03 (France)

²Altis Semiconducteurs 91830-CORBEIL-ESSONNES (France)

Zirconium and titanium alloys exhibit, in a wide domain of temperatures and strain rates, a strongly heterogeneous spacio-temporal distribution of plasticity at scales that vary across the domain and also with their microstructure, their texture, the amount of plastic strain and the load path. Various slip systems are observed to generate arrays of dislocations including pile-ups, tangles and subgrains.

Throughout the temperature and strain rate domain where negative strain rate sensitivity and its associated strain localization phenomena are observed, Ti base alloys exhibit two radically different *eigen-modes* of plasticity: 1- the *friction mode* that leads to intermittent plasticity in strain localization bands that are usually mobile. 2 – the *solute drag mode* of plasticity akin to creep and that can eventually lead to complete « arrest » due to the cumulative effects of strain- and time- hardening.

Creep bifurcation phenomena, observed as prevailing in the lower temperature part of the domain, can adequately be modeled by simply combining KEMC equations with FEM. When bifurcation takes place “within the structure” (test piece, part in service), the contrast in flow stress level of neighboring zones increases and results in local accumulation of damage and finally enforces fracture. These detrimental strain localization phenomena are enhanced when the structure is exposed to “Fatigue with dwell time” or “creep-fatigue” mode.

The shortcoming of this simple approach lies in the formation of strain rate bands, the size, distribution and velocities of which are not observed experimentally. The spacial distribution of strain localization in hcp structures appears to be strongly dependent on grain orientations and local combinations of plastically compatible grain associations. A polycrystalline model was therefore developed which includes “a” basal, prismatic and pyramidal slip systems, “c+a” pyramidal slip systems, realistic values of their CRSS and their potential strain and time hardening abilities. The results compare well with the experimental observations of tensile curves exhibiting Portevin-Lechâtelier serrations and the corresponding distribution of grain orientation sensitive strain and strain rate localizations. This model also provides detail information regarding the strain burst patterns eventually leading to creep arrest.

Grain-scale Experimental Validation of Crystal Plasticity Finite Element Simulations of Tantalum Oligocrystals

H. Lim¹, J. D. Carroll¹, C. C. Battaile¹, B. L. Boyce¹, C. R. Weinberger²

¹Sandia National Laboratories, Albuquerque NM, 87185, USA

²Drexel University, Philadelphia, PA, 19104, USA

Quantitative comparison of experiments and simulations of polycrystalline deformation behavior at the grain scale is challenging due to the heterogeneous subsurface grain morphology. To mitigate this effect of unknown subsurface microstructure, we used tantalum tensile specimens with a pseudo-two-dimensional grain structure with grain sizes on the order of millimeters. The deformation of tantalum oligocrystals (less than 20 grains in the gage section) was characterized using various experimental techniques and quantitatively compared with predictions using a novel BCC crystal plasticity finite element (CP-FE) model.

An experimental technique combining in-situ electron backscatter diffraction (EBSD), high-resolution digital image correlation (HR-DIC), and profilometry, was used to map intergranular crystal rotation, surface strain fields and out-of-plane topographic distortion, respectively, at various applied strains. The CP-FE predictions of deformation agreed reasonably well with experimental measurements. Possible causes of localized disagreements and the influence of model parameters will also be discussed, such as the mesh dependence, the assignment of initial crystal orientations and the choice of the slip planes and hardening laws.

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Integrated experimental-numerical methodology to map microstructural strain and stress evolution in bulk nanostructured alloys

C.C. Tasan, D. Yan, M. Diehl, F. Roters P. Shanthraj, C. Zambaldi, D. Raabe

Max-Planck-Institut für Eisenforschung,
Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Microscopic strain and stress partitioning among the present phases govern the macroscopic mechanical response of multi-phase alloys. However, these phenomena are challenging to probe due to the multiple scales involved, dynamic nature of the deformation process, and lack of dedicated methodologies. The challenge is even more enhanced for multi-phase alloys with features smaller than micrometer scale.

A novel approach is introduced in this work that strengthens the connection between microstructure and mechanical properties in such alloys. To this end, numerical simulations and experiment analyses are carried out in an integrated manner to investigate the microstructural deformation mechanisms in multiphase microstructures.

For the experiments, a novel, *in-situ* SEM imaging and digital image correlation (DIC) based methodology is developed that allows concurrent microstructure and strain mapping at sub-micron resolution. Strain mapping is achieved by the application of a layer of nanoparticles on the sample surface (as the DIC pattern) that are selectively imaged during deformation. Concurrent microstructure mapping is achieved by optimization of imaging conditions to minimize the interference of the DIC pattern nanoparticles.

For the simulations, the electron backscatter diffraction (EBSD) map of the undeformed state of the same *in-situ* investigated microstructural patch is used to create the model. 2D full-field crystal plasticity simulations are run employing a recently developed spectral solver suitable for high-phase contrast materials [1, 2] implemented in the crystal plasticity simulation-kit DAMASK [3, 4]. The individual phase properties are obtained by additional inverse CP simulations of nanoindentation experiments carried out on the original microstructure [5].

The methodology will be demonstrated here on the example of martensite-ferrite dual phase (DP) steel, for which promising correlation between the simulations and experiments is achieved, despite the complex micro-mechanics of this material.

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Microstructure-sensitive modeling of the mechanical behavior of polycrystalline materials with direct input from emerging 3-D characterization methods

Ricardo Lebensohn, Reeju Pokharel

Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Emerging characterization methods in experimental mechanics pose a challenge to modelers to devise efficient formulations to permit exploitation of the massive amount of data generated by these novel techniques. In recent years, we have developed Fast Fourier Transform (FFT) based methods for polycrystals (e.g. [1]), which can efficiently use voxelized microstructural images of heterogeneous materials as input to predict their micromechanical and effective response.

Furthermore, models based on polycrystal plasticity are increasingly used in engineering applications. These models require a proper consideration of the single crystal plastic deformation mechanisms, a representative description of the microstructure, and an appropriate scheme to connect the microstates with the macro response. FFT-based methods are ideal candidates to fulfill these requirements, albeit at the expense of numerically very demanding computations.

In this talk, we will discuss the latest numerical implementations of the FFT-based formulation for complex constitutive behaviors [2,3] and amenable to input and validation from 3-D characterization methods [4], as well as our recent efforts to embed this kind of models in Finite Elements, to solve complex boundary-value problems with microstructure-sensitive material response.

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Computational Process-Structure-Properties Modeling of Thermal Sprayed Coatings

Tatu Pinomaa, Anssi Laukkanen, Kenneth Holmberg, Erja Turunen, Tarja Laitinen

VTT Technical Research Centre of Finland, Espoo, Finland

We present a predictive multiscale model for microstructure formation and evaluation of material properties in thermal spray coatings. The model is linked to a multiscale nano-microstructure based continuous material model to predict material properties and wear resistance of powder metallurgy based end products.

The studied coating technique is called high velocity oxygen-fuel spray (HVOF). In this process, oxygen and fuel is ignited inside a nozzle, leading to a high temperature exhaust gas flow that – due to the high combustion pressure – accelerates to supersonic velocities. Coating powder is injected into this gas stream, which is dragged into high velocity, and is partially or fully molten in flight. The powder particles hit the surface, and during several microseconds, simultaneously deform into disk-shaped "splats". Subsequent particle impacts lead to a lamellar coating microstructure. Based on specified process parameters, we use computational fluid dynamics (CFD) to describe a reacting and supersonic gas flow inside the nozzle, followed by a lagrangian particle model for the propagation and heating of injected coating particles. This model provides particle velocities and temperatures upon impact, which are used as input for a phase field simulation of coating particle impact and rapid solidification. Subsequent particle impact simulations can be used to model the coating formation.

This process-structure model, complemented with metallurgical and thermodynamical information yields the microstructure for a structure-property computational model. The process analysis results are coarse grained to yield a statistically representative model of the thermal spray coating, the structure being explicitly included in the imaging based property computation utilizing a finite element approach. The nano-microstructural model is subjected to simulated testing for its mechanical and wear responses, and a feedback loop to the coating processing model is presented for material tailoring. The microstructure can be linked to a multiscale representation of material response on larger spatial scales using methods such as the Arlequin method, which provide the basic material properties of the coating in a product and component environment, e.g. porosity, splat-substrate adhesion, and splat-splat cohesion and their effects can be evaluated and quantified. The methodology can also be used to link the coating response to specific external environments – for example degradation due to wear, high temperatures, or erosion-corrosion.

An inverse optimization strategy to determine single crystal mechanical behavior from polycrystal tests: application to Mg alloys

V. Herrera-Solaz¹, Javier Segurado^{1,2}, Javier LLorca^{1,2}

¹Department of Materials Science, Polytechnic University of Madrid, 28040 Madrid, Spain

²IMDEA Materials Institute, 28906 Getafe, Madrid, Spain

An inverse optimization strategy was developed to determine the single crystal properties from experimental results of the mechanical behaviour of polycrystals. The optimization method is based on computational homogenization of the polycrystal behavior by means of crystal plasticity finite element simulations of a representative volume element of the microstructure in which the dominant slip and twinning systems were included in the constitutive equation of each grain [1-2]. The inverse problem was solved by means of the Levenberg-Marquardt method, which provided an excellent fit to the experimental results. The iterative optimization process followed a hierarchical scheme in which simple representative volume elements were initially used and successively by more realistic ones to reach the final optimum solution, leading to important reductions in computer time.

The new strategy was applied to identify the initial and saturation critical resolved shear stresses and the hardening modulus of the active slip systems and extension twinning in Mg alloys. It was found that if only two stress-strain curves were used as input in the optimization procedure, the parameters obtained from optimization were not able to accurately predict the mechanical behaviour of the polycrystal under different loading conditions. Thus, a minimum of three independent stress -strain curves was necessary to determine the single crystal behaviour from polycrystal tests in the case of highly textured Mg alloys.

This methodology was applied to study the critical resolved shear stresses (CRSS) of two magnesium alloys, MN10 and MN11 containing 0.5wt.% and 1wt.% Nd, respectively. The initial CRSSs were observed to change drastically with increasing RE content. In particular, the CRSSs of basal and twinning modes increased while the CRSSs of pyramidal and prismatic systems decreased to an extent that all values become similar for alloying additions of 1wt.%. This is consistent with the isotropic yielding behaviour observed in the MN11 alloy. The changes in CRSS with RE addition lead to the promotion of twinning at the expense of basal slip and to enhance the activity of non-basal systems.

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Identification of constitutive parameters by inverse simulation of indentation in single crystals and close to grain boundaries

Claudio Zambaldi¹, David Mercier¹, Yang Su², Philip Eisenlohr², Thomas R. Bieler², Martin A. Crimp², Dierk Raabe¹, Franz Roters¹

¹Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

²Michigan State University, East Lansing, MI, USA

We present findings based on a recently introduced method [1,2] to extract critical resolved shear stresses and hardening parameters from quasi single crystal indentation. Individual grains of known orientation were probed by nano- or microindentation far away from the grain boundaries for their single crystal mechanical response. The resulting pile-up topographies were characterized by atomic force microscopy or confocal microscopy. In this way the orientation dependent activation of different deformation systems was analyzed by comparing the measured pile-up topographies against crystal plasticity finite element simulations of the indentation process.

Non-linear optimization of the constitutive parameters for the underlying crystal plasticity model, allowed us to extract a single set of parameters which represents the experimentally observed data for all indented orientations. In this way the relative activation of plastic deformation modes could be quantified based on simple indentation experiments.

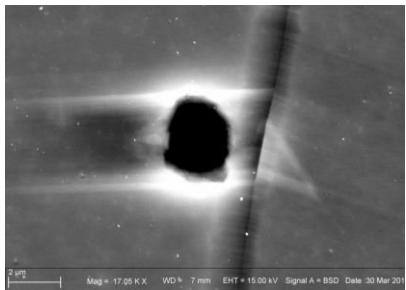


Figure 1: Nanoindentation close to a grain boundary in magnesium. Twinning is initiated in the adjacent grain.

After the initial development of this method on pure titanium [1] it has been applied to a number of metals and alloys with hexagonal (titanium alloy, magnesium [3]) and bcc (ferrite phase [4], tantalum, molybdenum) structure. The specific findings for the relative activation of different mechanisms in each phase will be presented and discuss.

Furthermore, the approach to quantify micromechanical effects by evaluating the anisotropic pile-up profile was extended to characterize the micromechanical effect of grain boundaries. In this case the possibility to efficiently probe many locations on a sample was important since it enabled the rapid acquisition of experimental data. Again the topographic data was compared to crystal plasticity finite element simulations of the deformation during indentation of a bicrystal. From the observed level of agreement between experimental data and simulation results, the slip transfer through the different types of grain boundaries was assessed.

This work was performed under the NSF/DFG Materials World Network initiative under Contracts NSF-DMR-1108211 and ZA523/3-1.

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Building realistic atomic models of kerogen using Hybrid Reverse Monte Carlo simulations

Colin Bousige^{1,2}, Benoît Coasne^{1,2}, Franz-Josef Ulm¹, Roland Pellenq^{1,2}

¹Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge MA 02139, USA

²<MSE>2, UMI 3466 CNRS-MIT, 77 Massachusetts Avenue, Cambridge MA 02139, USA

Gas and oil shale are unconventional deposits of hydrocarbons that represent important reserves worldwide. Organic-rich shales are natural composites as they consist of different inorganic minerals and a disordered porous carbonaceous material, called kerogen. Understanding and predicting the adsorption, transport, and mechanical properties of such disordered carbons requires having realistic atomistic models that can be used to establish reliable structure – property relationships. Such models can be obtained using Hybrid Reverse Monte Carlo (HRMC) simulations [1,2] in which a numerical atomic model having a structure factor identical to the experimental structure factor is built while using a force field to describe the chemistry of the material.

In this presentation, we will report realistic models of various kerogens obtained using HRMC. We will first show that this HRMC procedure can be computationally accelerated and, hence, applied to much larger systems by combining it with Molecular Dynamics simulations [3]. Thanks to the use of the REBO force field [4], these HRMC can be used to generate numerical models of kerogens with different chemical compositions and maturities. After standard characterization of the different structures in terms of pore size distributions and chemical analysis, the atomistic models of kerogen will be tested against a panel of measurements, accessible to both experiments and molecular simulations, such as nitrogen and water adsorption isotherms, vibrational density of states, and mechanical properties. These refined atomic models will also be used to test the importance of heteroatoms on the hydrophilicity of kerogen.

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Integrated Computational and Experimental Structure Determination for Nanoparticles

Min Yu, Andrew B. Yankovich, Amy Kaczmarowski, Dane Morgan, Paul M. Voyles

University of Wisconsin - Madison, Madison, Wisconsin 53706, USA

Advanced experimental techniques, such as scanning transmission electron microscopy (STEM) provide structural images of materials at atomic resolution. However, a single image provides only a two-dimensional projection of the structure, and three-dimensional tomographic imaging at atomic resolution and single-atom sensitivity remains extremely difficult. Experimentally driven structural refinement approaches typically rely on minimizing the error between forward simulation from atomic models and the experiment data. Such optimizations are challenging with limited data and rely on knowing good initial guesses for the ground state, which may be insufficient for predicting metastable, out of equilibrium states. Such optimizations also typically make no direct use of information about the energy of the potential structures. Genetic algorithms (GAs) have proven to be extremely effective in structure prediction for a wide range of complex structures, including clusters, crystals, and grain boundaries, and have also been used to accelerate matching STEM data to a nanoparticle of known structure. We will discuss development of an integrated GA optimization tool that can reverse engineer the 3D structure of a nanoparticle by matching forward modeling to experimental STEM data and simultaneously minimizing the energy. This tool integrates the power of GAs for complex optimization and utilizes both available experimental and energetics data simultaneously. We demonstrate this nanostructure determination tool on STEM data of Au nanoparticles.

Towards efficient fatigue simulation and parameter identification using models with multiple time scales

Guillaume Puel, Denis Aubry

Laboratoire MSSMat (Ecole Centrale Paris/CNRS UMR8579), Grande voie des vignes,
92290 Chatenay-Malabry, France

When dealing with the numerical prediction of material fatigue, classical life estimation methods, such as those described in [1], can give poor results as far as one is interested with complex loading histories (such as a loading with a slow-evolving average) or inertia effects (for high frequency loadings). It seems indeed more relevant for such cases to use time transient models describing how internal variables, such as plastic strain, or isotropic damage, change with respect to time. However, the computational cost associated with such simulations can become prohibitive if each individual cycle has to be computed.

Therefore a specific method is proposed here to drop the calculation cost by factors up to several thousands: it relies on periodic time homogenization, which is similar to what is usually developed in space homogenization. Moreover, the method is based on a sound mathematical framework, which can guarantee the accuracy of the derived equations and solutions. A first formulation of this method has been proposed in [2]: it is based on the assumption that two different time scales (a fast one, associated with the fast cycles, and a slow one) can be defined and decoupled. Using asymptotic expansions of the scale ratio, it then allows to solve the different equations at the slow time scale only, by taking into account the averaged effect of the fast cycles in the homogenized solution. Since this reference, several extensions have been studied, such as the dynamic framework [3] or how to describe an isotropic damage evolution [4,5].

Moreover, it is possible to address the parameter identification process for such time-homogenized problems. This latter is solved by minimizing a misfit function defined as a norm quantifying the discrepancy between the available measurements and the associated quantities derived from the model [6]. Work is in progress to address the main questions arising when one tries to use in the identification process the time-homogenized model rather than the reference problem.

Eventually, this should lead to a suitable strategy for addressing accurate fatigue predictions and associated parameter identification for arbitrary cases of study, whereas the computational cost remains affordable.

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A coupling method for stochastic polycrystalline models at different scales

Régis Cottereau

Laboratoire MSSMat, École Centrale Paris, CNRS, F-92295 Châtenay-Malabry, France

In this study, we present an approach that allows to couple two stochastic continuum models [1]. In particular it allows to couple a homogeneous (or slowly fluctuating) continuum mechanics model with random constitutive tensor and a polycrystalline model with stochastic anisotropic grains. The latter model represents the micro-scale model while the former would be its upscaled (or homogenized) version. The coupling strategy is performed in the Arlequin framework [2], which is based on a volume coupling and a partition of the energy between two models. The main interest of this framework is that it allows to couple models that are different in nature: discrete vs. continuous, deterministic vs. stochastic, linear vs. nonlinear, with vs. without defects or cracks.

A suitable functional space is chosen for the weak enforcement of the continuity between the two models. The choice of this space ensures that the ensemble average of the two stochastic solutions are equal point-wise in the coupling area, and that appropriate boundary conditions on the stochastic dimension are passed from one model to the other. However, it does not impose any strong continuity, that would induce undue strength localization from one model onto the other. The proposed coupling approach is an extension of a previous work dealing with the coupling of a stochastic model with a deterministic one [3]. It leads to a mixed problem. This choice of functional spaces and coupling operator ensures that the mixed problem has a unique solution that can be approximated by spectral finite elements or a Monte Carlo technique.

This presentation will be focused on showing the interest of such an approach for identification of polycrystalline models when the information comes from experiments performed at different scales. This is for instance the case when measuring concurrently elastic strains through X-ray diffraction during in situ mechanical tests coupled with image correlation. In general, different models are identified at different scales using different experimental information. However, using all the information concurrently and making sure that models at the different scales are compatible (in the sense of homogenization [4]) is a key to relieving some numerical difficulties encountered in the identification process.

Extension to the coupling of dynamics of dislocation models and polycrystalline models will be highlighted if time permits.

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Dislocation-induced elastic distortion fields in deformed FCC crystals: Discrete dislocation dynamics simulations and experimental measurements

Mamdouh Mohamed¹, Ben Larson², Anter El-Azab³

¹Physical Science and Engineering Division, KAUST, Jeddah, Saudi Arabia

²Oak Ridge National Laboratory, Oak Ridge, TN, United States

³School of Nuclear Engineering, Purdue University, West Lafayette, IN, United States

The statistical characteristics of dislocation-induced elastic distortion fields in deformed FCC crystals are investigated both experimentally and theoretically. Discrete dislocation realizations are generated by the discrete dislocation dynamics method and the induced elastic distortion fields are computed by solving the corresponding boundary value problem. Moreover, sample three-dimensional X-ray measurements for the lattice misorientation are also presented to address the corresponding statistical features and to highlight the possibility to conduct a comparison between experiments and dislocation dynamics simulations.

The current analysis addresses critical issues related to the similarities and differences, in terms of the spatial characteristics, between the elastic strain and lattice rotation fields induced by the same dislocation structure. Moreover, the significance of the elastic strain field contribution to the dislocation density tensor, which is usually considered insignificant during the experimental detection of the dislocation density tensor, is also investigated quantitatively. Finally, we present a preliminary comparison between the elastic distortion fields computed based on discrete dislocation simulations and those measured experimentally through 3D X-ray microscopy.

This work was supported by the U.S. DOE Office of Basic Energy Sciences, Division of Materials Science & Engineering.

Metal-rich Ceramic Phase Stability and Microstructures in Group IV and V Carbides and Nitrides

Xiao-Xiang Yu¹, Christopher R. Weinberger², Gregory B. Thompson¹

¹Department of Metallurgical and Materials Engineering, the University of Alabama,
Tuscaloosa, AL 35487

²Mechanical Engineering and Mechanics Department, Drexel University, Philadelphia,
PA 19104

Phase stability and phase transformation pathways are critical in determining the morphology of a material's microstructure. For example, in the group V carbides and group IV nitrides, similar metal-rich crystallographic phases are observed between the two systems. Yet the morphology of these phases in the microstructure varies. These microstructures include equiaxed grains of single phases, equiaxed grains with a crisscross pattern of laths, or acicular grains with parallel laths of different phases along the major axis of the grain. In this talk, we investigate the inter-relationship between material microstructure and phase stability in the transition metal carbides and nitrides using experimental characterization of diffusion couples coupled with electronic structure density functional theory (DFT). The combination of these two tools provides unique insight into the interrelationships between equilibrium stability and meta-stability for each specific phase observed in the diffusion couples. Using DFT, the energy of formation for the vacancy ordered rock-salt carbide variants (such as Me_6C_5) and stacking fault variants (such as Me_4C_3 and Me_3C_2) have been investigated. For example, the stability of the Ta_4C_3 or zeta phase has been in question for some time and we now demonstrate that this is because the zeta phase as well as the eta phase (Ta_3C_2) are metastable and likely only exist if the vacancy ordered Me_6C_5 phase cannot form. In addition, the energy of formation for vacancies in the group V carbides reveal why the vacancy ordering Me_6C_5 phase is readily present in some group V carbides and not others. The carbide computational results for the metal rich carbide phases are compared to their equivalent crystallographic structures in the metal-rich nitrides, e.g. Me_4N_3 and Me_3N_2 phases, which have been found to be thermodynamically stable. These computational results provide insights into why certain metal-rich ceramic phases are seen to coarsen within the experimentally observed microstructures. Collectively, the comparison of the computational and experimental findings provides new insight into why specific phases form and its consequences on the morphologies observed within these carbide and nitride microstructures.

Computational multiscale modeling and experimental characterization of martensitic transformations in CoNiAl alloys

V. I. Yamakov^{1,2}, T. A. Wallace¹, J. A. Newman¹, J. D. Hochhalter¹, V. K. Gupta^{1,2},
G. P. Purja Pun³, Y. Mishin³

¹NASA Langley Research Center, Hampton, VA 23681, USA

²National Institute of Aerospace, Hampton, VA 23666, USA

³George Mason University, Fairfax, VA 22030, USA

The concept of utilizing ferromagnetic shape memory alloys as embedded sensory particles in aluminum alloys for real time damage detection is discussed. The modeling effort employs molecular dynamics and Monte Carlo atomistic simulations together with finite element modeling at the particle level with developed shape memory alloy constitutive models. The atomistic simulations are performed with a recently developed embedded-atom interatomic potential to study the effect of chemical composition and uniaxial mechanical stresses on the martensitic phase transformation in CoNiAl alloys. The transformation is analogous to the martensitic transformation in Ni-rich NiAl alloys. The martensitic phase has a tetragonal crystal structure and can contain multiple twins arranged in domains of different orientations in a crystal. The predicted martensitic transformations are compared to experimental data obtained from CoNiAl arc-melted buttons of various compositions. Specimens were machined from these buttons, solution-treated and quenched to lock in the shape-memory behavior, and then the martensitic transformation was characterized using differential scanning calorimetry and electron microscopy. The simulation model shows similarities, but also some differences with the experimental data. The temperature and the hysteresis of the transition in the simulation model tend to be higher than the experimental values and are shown to depend strongly

on the configurational entropy of the system, which is estimated by using grand-canonical Monte Carlo simulations. The simulation model also indicates a decrease in the transition temperature with increase in the Co concentration, which is in agreement with the experimental data. The technology of embedded sensory particles will serve as the key element in an autonomous structural health monitoring system that will constantly monitor for damage initiation in service, which will enable quick detection of unforeseen damage initiation in real-time and during on-ground inspections.

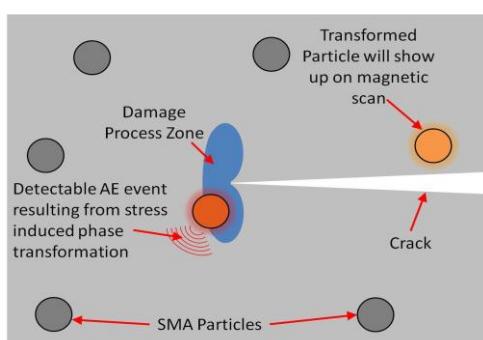


Figure 1: Embedded sensory particles, which undergo a detectable phase transformation in the presence of a crack.

Stagnation of microstructure features in simulated grain growth

Jonathan Lind¹, Jeremy Mason², Bryan W. Reed¹, Shiu F. Li¹,
Vasily V. Bulatov¹, Mukul Kumar¹

¹Lawrence Livermore National Laboratory, Livermore, California 94550, USA

²Boğaziçi University, Bebek, Istanbul 34342, Turkey

The mechanical properties of polycrystalline materials depend on microstructure properties such as grain size, texture, grain boundary character distribution (GBCD) as well as higher order correlations in the topological networks [1]. Coarsening of these microstructures through thermal treatment can vary depending on the anisotropy of the material and the network of special and random boundaries. Owing to the properties of the material being directly related to the microstructure, it is important that simulation methods agree with experimental results on a statistical and phenomenological level.

A new approach to the traditional 2D Potts model will be introduced which is combined with a grain boundary energy function [2] to study anisotropic grain growth systems. This method relieves several problems inherent with meshed simulations. We apply this approach to experimentally obtained 2D EBSD data and synchrotron-generated 3D

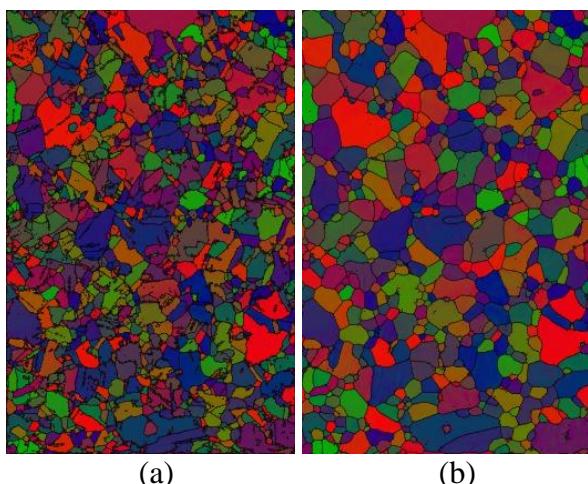


Figure 1: Simulated annealing (b) of a grain boundary engineered Cu specimen obtained experimentally via EBSD (a)

HEDM data as inputs. Comparison of microstructure energy evolution is performed and stability of microstructure features (boundaries, triple junctions) between experiment and simulation performed. This type of validation allows us to analyze the dynamics of boundaries and triple junctions of purely simulated microstructures. Chains of triple junctions that promote growth (and those that hinder it) will be studied. These results can help to guide experimental efforts in searching for salient features in measured microstructures and reliably predict its evolution.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. This work was supported at LLNL by US DOE Office of Basic Energy Sciences, Division of Materials Science and Engineering.

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Massively Parallel Cellular Automata Algorithms for the Simulation of Primary Recrystallization

Markus Kühbach, Luis A. Barrales-Mora, Günter Gottstein

Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, D-52074 Aachen, Germany

Primary recrystallization is a softening mechanism used during industrial annealing in order to regain formability after forming operations and to tailor the final properties of metallic materials. Microstructural evolution along this process is basically determined by grain boundary motion and its interaction with various microstructural defects such as dislocations and particles. This interaction however, occurs atomistically in a complex manner. Owing to this complexity, the development of cost-efficient and sustainable annealing treatments can particularly benefit from 3D computer modelling.

In this regard, classical mesoscopic modelling approaches, such as cellular automata, are advantageous because they combine accurate spatial representation of microstructural features with real-time scaling, enabling a direct comparison with experimental data. Nevertheless, the limitation of cellular automata models is their computational efficiency. In this contribution, two fundamentally different 3D cellular automata models for recrystallization are presented and contrasted. These models were designed and optimized for their execution in parallel computing architectures.

The first model is based on a classical 3D domain decomposition scheme to evolve accurately and efficiently large microstructures. As expected from such approach, this model is computationally constrained by sub-domain communication. To overcome this limitation in the second approach, large simulations domains are partitioned and executed as separate entities, whose evolution is corrected statistically by the introduction of impingement on a local level. Experimental findings in an Al-Fe-Si alloy were used to test the accuracy of the models.

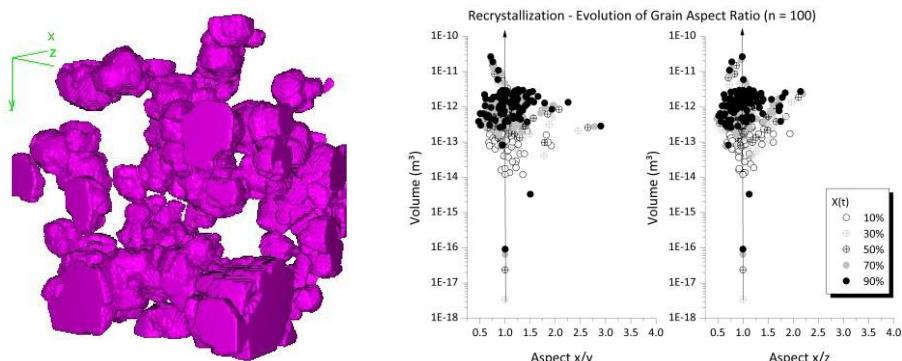


Figure 1: Visualization of the recrystallization front after 20% volume transformation (to the left) and statistics of grain volume and shape at advanced stages of growth (to the right).

The authors gratefully acknowledge the financial support from the Deutsche Forschungsgemeinschaft (DFG) within the Reinhard-Koselleck project GO 335/44-1, in which frame this work is settled.

Validating Phase Field Models using Microstructural Experimental Data

Michael R Tonks¹, Melissa Teague¹, Bradley Fromm²

¹Idah National Laboratory, Idaho Falls, ID 83415

²Washington State University, Pullman, WA 99164

The phase field method has emerged as a powerful tool to model microstructure evolution due to its flexibility. In particular, Idaho National Laboratory's MOOSE framework is making it simpler to conduct 3D multiphysics phase field simulations of the coevolution of microstructure and properties. However, as phase field simulations are more widely used to provide insight on material behavior, it becomes increasingly important to validate these models against experimental data. While some validation can be obtained using homogenized information about the microstructure, such as an average grain size or phase concentration, the most valuable comparisons come from 2D and 3D microstructural characterization across time. New experimental techniques, including nondestructive 3D characterization and in situ microscopy, are providing exciting opportunities for phase field model validation. However, best practices for such validation are still being determined. In this presentation, we will discuss work currently underway at Idaho National Laboratory to directly compare 3D phase field simulation results to data obtained using state-of-the-art experimental techniques. These efforts include attempts to directly reconstruct experimental microstructures as simulation initial conditions and directly compare to the experimental evolution as well as comparisons between similar microstructures.

Understanding deformation mechanisms of a dense hydrous magnesium silicate (Phase A)

K. Gouriet, P. Cordier, A. Mussi

Unité Matériaux et Transformations, UMR 8207 CNRS - Université Lille1, Villeneuve
d'Ascq F-59655, France

Water plays important roles within the upper mantle of the Earth. It promotes partial melting and magma formation, phase transformation kinetics, and affects the mantle dynamics. Dense hydrous magnesium silicates (DHMS), such as Phase A [Mg₇Si₂O₈(OH)₆], are good candidates for water reservoirs in the mantle. Because of Phase A's stability at relatively low pressures and high water contents (>11 wt%), it is the first product of the breakdown of antigorite, which makes it particularly interesting as a possible carrier of water in subduction zones. The importance of these hydrous phases is not restricted to water storage. Indeed, at greater depths, the knowledge of the rheological properties of hydrous phases is also important for a better understanding of the dynamics of subduction.

First, Mussi *et al.* [1] have performed an experimental study of the deformation mechanisms of Phase A at 673°K and 973°K at 11 GPa. They have observed dislocation activity in basal, prismatic and pyramidal planes, with dissociation of dislocations in the basal and pyramidal planes. To complete these studies, we modelled dislocation core structures in this mineral. In this study, we focus on the core structures of dislocations with $\frac{1}{3}[\bar{2}\bar{1}\bar{1}0]$, $\frac{1}{3}[0\bar{1}\bar{1}0]$ and [0001] Burgers vectors. We have first investigated the structural and elastic properties of Phase A at high pressure based on first-principles calculations (or DFT). To understand how the structure of Phase A can be sheared, generalized stacking fault energies (or γ -surfaces) are calculated for the basal and prismatic planes, obtained with accurate DFT calculations. We found several energy minima in the basal plane and in both types of prismatic planes, suggesting possible dislocation dissociations in these planes. The core structures of screw and edge dislocations have been calculated using the Peierls-Nabarro-Galerkin method [2] involving γ -surfaces as an input. These calculations confirm the dissociation of dislocations for all Burgers vectors. Finally, we apply simple shear on our model to obtain the Peierls stress in each plane, in order to determine the easiest slip systems for this mineral.

This work was supported by funding from the European Research Council under the Seventh Framework Program (FP7), ERC grant N°290424 – RheoMan.

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Recent progresses on the characterization of crystal plasticity behavior of nuclear structural materials

Félix Latourte¹, Adrien Guery^{1,3}, Jean-Michel Proix², François Hild³, Stéphane Roux³

¹EDF R&D, MMC Department, Ecuelles, 77818 Moret-sur-Loing Cedex, France

²EDF R&D, AMA Department, 92 Clamart, France

³LMT-Cachan, 94235 Cachan, France

The FP7 PERFORM60 European project [1,2] aims at developing and validating multi-scale models to predict the behavior of reactor pressure vessel steels (tempered bainitic steel) and of in-core materials (made of austenitic steels) for which crystal plasticity laws are to be validated. Crystal plasticity finite element calculations are conducted to reproduce the kinematic fields (displacement and strain) observed at the surface of polycrystalline aggregates during in-situ SEM tensile experiments [3,4]. The observed differences between calculations and experiments are used to optimize crystal plasticity law parameters using a finite element updating procedure, or to compare without parameter optimization different constitutive laws with commonly used parameters validated using only the material effective (macroscopic) behavior. Some recent key results include the introduction of a specific cost function used for the identification of crystal plasticity parameters, a study of the well-posedness of the identification inverse problem depending on the considered set of unknown constitutive parameters, the investigation of strain gradient plasticity effects in the microstructural deformation of austenitic steel aggregates, and the assessment of temperature variation on the reactor pressure vessel steel response in term of crystal plasticity mechanisms and strain distributions.

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Capturing the Response of Polycrystalline Materials at the Mesoscale: Measurements, Modeling and Data Mining

J. V. Bernier¹, S. F. Li¹, J. C. Schuren², T. J. Turner², P. Shade²

¹Computational Engineering Division, Lawrence Livermore National Laboratory,
Livermore, CA 94550, USA

²Materials and Manufacturing Directorate, Air Force Research Laboratory, WPAFB, OH
45433, USA

The development of next-generation engineering materials with transformational properties will rely heavily on the development of predictive models that can link microstructure and its evolution under thermo-mechanical processing with resultant properties/performance. These linkages – and the ability to synthesize “materials on demand” – have long encompassed a significant portion of research within the materials science community. However, without access to experimental data at the relevant length scales, validated models capable of predicting complex phenomena, such as creep, have remained elusive. Both the development of new material systems as well as the adoption of advanced computational methods in engineering design remains dependent on large-scale empirical testing efforts, which are as costly as they are time consuming. Emerging experimental techniques such as High Energy X-ray Diffraction Microscopy (HEDM) address a critical need with respect to validation experiments for multiscale materials models. HEDM measurements provide access to the microstructure and micromechanical state, both inter- and intra- granular, *in situ* for large polycrystalline aggregates. We present results from HEDM measurements as well as complementary finite element simulations of a Titanium specimen subject to uniaxial deformation *in situ*. The evolution of intragranular misorientations and intergranular stresses during continuous deformation are compared. The evolution of intergranular stresses under creep deformation is also presented. We conclude with a discussion on the burgeoning need for application of data mining techniques to these incredibly rich datasets, both in terms of advancing our understanding of emergent properties/responses at the mesoscale as well as in the context of informing the development/validation of multiscale modeling frameworks.

Interaction between toughness anisotropy and loading conditions of a drawn wire

Jean-Hubert Schmitt¹, Aurélie Jamoneau¹, Denis Solas^{2,3}

¹Ecole Centrale Paris, Laboratoire MSSMat – UMR CNRS 8579, Grande voie des Vignes, 92295 Châtenay Malabry Cedex, France

²Univ Paris Sud, ICMMO, 91405 Orsay, France

³CNRS, UMR8182, 91405 Orsay, France

Large drawing deformations of a steel wire induce a strong hardening and an important crystalline and morphological anisotropy (see for instance [1]). This strongly influences the material behavior during subsequent loadings. Usually mechanical properties are studied by tension or torsion of drawn wires. The maximum tensile stress increases with the amount of prestrain, and it results mainly from the internal stresses after wiring (see for instance [1]). It is also shown that specific damage mechanisms develop in torsion after drawing, being linked to the microstructure morphological texture [2].

The present work deals with the understanding of the fracture mechanisms in a thin wire during complex loading paths (tension-torsion-bending). A dedicated experiment has been worked out to twist simultaneously two drawn wires. Finite element calculations allow the various stress components to be calculated within the wire sections. They account for the contact and friction stresses between the two wires, for the internal stresses, and for the wire mechanical behavior after large prestains. The longitudinal stress is in tension from the opposite side of the contact point to the center of each wire. The same is observed for hoop stress. The shear stress is rather high on a large part of the section, except close to the center where it is nearly zero.

The stress state is then related to the different fracture surfaces.

- The surface can be inclined with respect to the wire axis, the cracks following the elongated microstructure, or it can be flat and parallel to the wire section with a dimple character. These observations are explained by an interaction between the complex reloading stress state and the strong toughness anisotropy due to the morphological texture [3]. The shear stress at the wire surface allows the crack propagation along the axis. Then the tensile hoop stress leads to the crack propagation toward the center.
- On another hand, when the internal damage resulting from the wire drawing is large enough, the longitudinal stresses give rise to a ductile fracture of a weakened section, traverse to the wire axis.

These first results and calculations have to be completed accounting for the evolution of the internal stresses. This will lead to quantitative predictions of the rupture mechanisms as a function of the drawing amount and of the mechanical behavior of the wires.

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Virtual X-Ray and Electron Diffraction Characterization of Surfaces and Interfaces in Alumina

Shawn Coleman, Douglas E. Spearot

Department of Mechanical Engineering, University of Arkansas

Structural characterization of metal-oxide surfaces and interfaces poses a unique challenge for atomistic simulation. For example, in the case of alumina (Al_2O_3), typical atomistic simulation characterization techniques, such as common neighbor analysis and the centrosymmetry parameter are incapable of differentiating the subtle structural differences between stable and metastable alumina phases and thus would be similarly unsuccessful in characterizing interfaces in this material system. To address this challenge, a computational technique capable of calculating experimentally comparable x-ray diffraction line profiles and selected area electron diffraction patterns is developed. These virtual x-ray and electron diffraction techniques are employed to study alumina surfaces and both homogenous and heterogeneous alumina interfaces. Virtual selected area electron diffraction patterns and x-ray line profiles show unique features which differentiate between stable and metastable alumina phases, in agreement with experiment. Virtual diffraction characterization of the homogenous and heterogeneous alumina interfaces are used to study the atomic rearrangements that occur at the interface, with the virtual diffraction methods allowing for a direct validation via experimental data.

Theoretical and experimental X-ray spectroscopy of graphene-based supercapacitor electrodes under realistic operating conditions

Brandon Wood¹, Tadashi Ogitsu¹, Michael Bagge-Hansen¹, Juergen Biener¹, Minoru Otani², David Prendergast³, Jonathan Lee¹

¹Lawrence Livermore National Laboratory, Livermore, CA USA

²AIST, Tsukuba, Japan

³Lawrence Berkeley National Laboratory, Berkeley, CA USA

Electric double-layer capacitors, or supercapacitors, store charge via polarization at the electrode-electrolyte interface. Most models of interfacial charging focus almost exclusively on the electrolyte, including the transport, proximity, and arrangement of ions approaching the electrode surface. The electrode is considered fixed, with charge accumulation or depletion as the only response to polarization of the interface. We combine direct ab initio simulation of X-ray absorption spectra under applied voltage bias with corresponding in operando measurements to demonstrate that graphene-based supercapacitor electrodes in fact undergo unanticipated bias-induced electronic structural changes. The data strongly suggest that the origins of these changes arise from phenomena at two different length scales: first, local chemical changes at the nanoscale; and second, broader morphological changes at the mesoscale. Possible scenarios consistent with the observations will be discussed, along with implications for developing more accurate multiscale models of electrochemical operation.

A hierarchical study of grain boundary energy distribution using high-energy x-ray diffraction microscopy

S. F. Li, B. W. Reed, V. V. Bulatov, J. Lind, M. Kumar

Lawrence Livermore National Laboratory, Livermore, California 94550

Studies of grain boundary energy distribution (GBED) have historically been done by measurement of dihedral angles for triple junctions or surface grooving experiments. The number of triple junctions measured typically limits the resulting statistics. Recent advances in 3D x-ray techniques, such as near-field HEDM (nf-HEDM), led to possibilities of probing mm^3 volumes at micron resolution non-destructively. A typical measurement captures ~ 1000 grains and roughly 10^7 sample points along the grain boundaries per volume. When combined with recently published semi-analytical grain boundary energy function, GBEDs can be examined hierarchically for different classes of boundaries. Here, a class of boundaries may define as the set of all low-CSL boundaries, the set of boundaries near triple junctions, or the set of all random high angle boundaries. The result demonstrates the vastly differing nature of boundaries under different local geometrical and topological constraints.

The authors acknowledge useful discussions J. K. Mason. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. This work was supported at LLNL by US DOE Office of Basic Energy Sciences, Division of Materials Science and Engineering.

3D Digital Reconstruction and Numerical Modeling of Microstructurally Small Fatigue Cracks in an Aluminum Alloy from Synchrotron-Based Measurements

A.D. Spear¹, A.R. Cerrone¹, J.D. Hochhalter², S.F. Li³, J.F. Lind³, R.M. Suter⁴, A.R. Ingraffea¹

¹Cornell University, Ithaca, New York 14853, USA

²NASA Langley Research Center, Hampton, Virginia 23681, USA

³Lawrence Livermore National Laboratory, Livermore, California 94550, USA

⁴Carnegie Mellon University, Pittsburgh, Pennsylvania 15213, USA

Advancing the states of materials design and high-fidelity structural prognosis will require a synergistic coupling between multi-scale experimental characterization and numerical modeling approaches. This talk describes recent efforts to couple synchrotron-based measurements of microstructurally small fatigue cracks with multi-scale modeling (mesoscale to macroscale) using three-dimensional finite-element simulations. Ex-situ techniques are employed to characterize three-dimensional fatigue-crack propagation within the microstructure of an aluminum alloy. The experimental characterization involves X-ray tomography along with near-field high-energy X-ray diffraction microscopy (HEDM), which provides a three-dimensional map of the grain morphologies and orientations adjacent to fatigue-crack surfaces. The experimental data is then used to digitally reconstruct and model the measured polycrystalline volume and fatigue-crack morphologies as a way to reproduce the observed crack evolution and thereby compute response fields in the neighborhood of observed crack fronts. Cracks are represented explicitly through the underlying geometry of the finite-element mesh. A concurrent multi-scale modeling technique is employed, whereby a model of the measured polycrystalline volume is embedded within a model of the global fatigue specimen. The mesoscale and macroscale regions are modeled using crystal plasticity and von Mises plasticity, respectively. Such simulation results can be used to inform and validate models that predict three-dimensional crack evolution at the microstructural length scale.

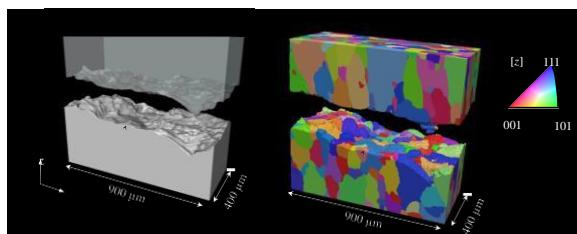


Figure 1. Reconstructions from X-ray tomography (left) and near-field HEDM (right).

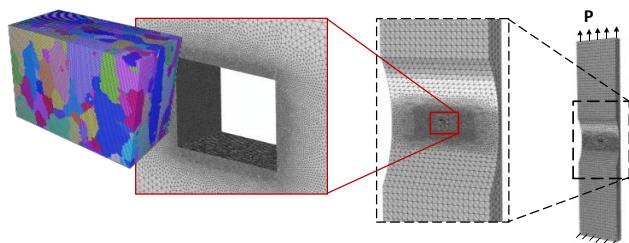


Figure 2. Concurrent multiscale finite element model with polycrystalline region from experiment.

This work is supported by the National Science Foundation Graduate Research Fellowship Program under Grant No. DGE-0707428; under the auspices of the U.S. Department of Energy (DOE) by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344; and by grant DESC0002001 at Carnegie Mellon University. Use of the Advanced Photon Source, an Office of Science User Facility operated for the U.S. DOE Office of Science by Argonne National Laboratory, was supported by the U.S. DOE under Contract No. DE-AC02-06CH11357. HEDM reconstruction was performed using allocation TG-MSS110031 through the Extreme Science and Engineering Discovery Environment (XSEDE), supported by the National Science Foundation grant number OCI-1053575.

Three-dimensional imaging and numerical reconstruction of graphite/epoxy composite microstructure based on ultra-high resolution X-ray computed tomography

Michael W. Czabaj¹, Mark L. Riccio², William W. Whitacre³

¹NASA Langley Research Center, Hampton, VA 23452

²Institute of Biotechnology, Cornell University, Ithaca, NY 14853

³Draper Laboratory, Cambridge, MA 02139

Three-dimensional simulation of constituent-scale deformation, damage, and failure (i.e. virtual testing) in fiber reinforced polymers (FRPs) requires a detailed and accurate numerical representation of the underlying microstructure. Recent advances in high-resolution X-ray computed tomography (CT) have enabled 3D imaging of FRP constituents at a submicron resolution; however, converting X-ray CT-derived data into useful numerical models remains a significant challenge. Specifically, the relatively low contrast between individual constituents (i.e. fibers and resin), small fiber diameter ($\sim 5\text{-}7 \mu\text{m}$), and dense packing (fiber volume fraction $\sim 55\text{-}67\%$) in most FRPs render the available off-the-shelf, image-segmentation-based conversion codes inadequate. The work described here seeks to address the aforementioned challenges through a combined experimental and numerical framework aimed at high-resolution imaging, visualization, and numerical reconstruction of FRP microstructures at the fiber length scale. Three-dimensional imaging of an FRP microstructure is performed using a 3D X-ray microscope. A small "matchstick-type" sample of a unidirectional AS4/3501-6 graphite/epoxy composite is imaged with a voxel size of approximately 460 nm. Collection of the X-ray attenuated data and their conversion into a stack of two dimensional digital images is performed using commercially available software. A template-matching based detection algorithm is implemented to "detect" the centroids of individual fibers in each two-dimensional image. Next, a multi-fiber tracker which uses a Kalman filter and a Kuhn-Munkres assignment algorithm is implemented to track the individual fibers throughout the stack of images. The resulting coordinates of fiber centroids in three-dimensional space from the detection-tracking algorithms are then used to generate a solid-model reconstruction of the imaged volume. Finally, statistical analysis is performed to quantify the spatial variation in the microstructure.

Identification of a crystalline constitutive law using multimodal full-field measurements in grain scale

Wang Chow¹, Guillaume Puel¹, Denis Solas², Thierry Baudin², Véronique Aubin¹

¹ Ecole Centrale Paris, MSSMat, UMR CNRS 8579, F-92296 Chatenay-Malabry, France

² Univ Paris Sud, ICMMO, UMR 8182, F-91405 Orsay, France

The crystalline plasticity constitutive models are remarkable for their mechanical behavior description towards crystalline materials. However, their parameters are generally identified with the data at macroscopic scale without considering the effect of grain scale, which is the origin of the heterogeneities. [1-4]



Figure 1: Assembly of the set up for the in-situ full-field measurements

For this reason, a robust procedure to identify this type of model using the grain scale information is sought. Two aspects are developed respectively: measuring the total ε^t and elastic ε^e strain fields and establishing a crystalline aggregate model to simulate as well as identify the parameters of the behaviour model.

In this study, a sample in Al-alloy with around twenty-five grains is subjected to a simple tensile loading. During this test, the total strain field is observed by digital image

correlation technique while the elastic one is measured by X-ray diffraction simultaneously. The surface fields' information will then be dedicated to identify the parameters of a crystalline constitutive model, using finite element simulation [5].

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Crystal plasticity analysis of scale dependent mechanical properties of ferrite/cementite fine lamellar structure in pearlite steel

Yohei Yasuda¹, Tetsuya Ohashi¹

¹Kitami Institute of Technology, Koencho 165, Kitami, Hokkaido 090-8507, Japan

Pearlite steel is one of the most important metallic materials in industry due to strong yet ductile property. The microstructure has lamellae configuration in which fine layers of ferrite and cementite are piled up alternately in a sub-micron intervals. The major factors for excellent property of pearlite are considered that strengthening of ductile ferrite lamellae by size effect [1] and plastic deformation of brittle cementite lamellae [2]. Recently, we studied these mechanisms and showed that plastic deformation of cementite lamellae was stabilized when yield stress and strain hardening rate of ferrite lamellae were increased [3]. In this conference, we will show the change of mechanical properties of ferrite lamella in pearlite quantitatively by a strain gradient crystal plasticity analysis.

As a simplified pearlite model, we employ three-laminated structures where a ferrite lamella is sandwiched by cementite lamellae. The properties of tensile deformations and shear deformation of the model are studied. Thickness of each lamella is from 100 to 500 nm. Crystal orientations of the ferrite and cementite are defined based on Bagaryatsky model [4]. A crystal plasticity finite element method for body-centered cubic crystal structures is used. We assume the Schmid's law for slip activation and the slip systems of ferrite lamellae are {110}<111> and {112}<111> while plastic deformation of the cementite lamellae is not considered. The critical resolved shear stress of a slip system is given by the lattice friction, contribution from the accumulated dislocations and lamellar wall. Density increment of the statistically stored dislocations is evaluated by Kocks model and density of the geometrically necessary dislocations is evaluated by spatial gradients of plastic shear strain. The mean free path of moving dislocations is given by a function of the accumulated dislocation as well as the layer thickness. Obtained results of macroscopic stress-strain relation of the ferrite phase show increases of yield stress and work hardening rate with the reduction of interlamellar spacing.

This research was supported by Japan Science and Technology Agency (JST) under Collaborative Research Based on Industrial Demand "Heterogeneous Structure Control: Towards Innovative Development of Metallic Structural Materials".

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Grain Growth in Porous Oxides: Diffuse Interface Modeling and Experiments

Karim Ahmed¹, Janne Pakarinen², Lingfeng He², Darryl Butt³,
Brian Jaques³, Anter El-Azab¹

¹School of nuclear engineering, Purdue University, West Lafayette, IN USA

²Department of engineering physics, University of Wisconsin, Madison, WI, USA

³Boise State University, Boise, ID, USA

We present a 3D phase field model for investigating the grain growth process in ceramics. The grain growth process in ceramics is complicated by the interaction between the pores and the grain boundaries. As such, in addition to grain boundary migration, the model takes into consideration pore migration via surface diffusion and hence pore coalescence. Therefore, the model is able to fully capture the microstructure evolution in porous ceramics. All model parameters are obtained from material properties.

Application of the model to uranium dioxide shows that the grain growth in this material is sensitive to the level of porosity. The effects of porosity, temperature, mobilities, and initial microstructure on the grain growth process were investigated. Furthermore, the model captures the pore breakaway phenomenon which takes place due to the difference between the pore mobility and the grain boundary mobility as observed experimentally.

The model results agree well with grain growth experiments. This research was performed as a part of the Energy Frontier Research Center, Center for Materials Science of Nuclear Fuel funded by the U.S. Department of Energy, Office of Basic Energy Sciences.

Through-process Modeling for Alloy Design and Process Optimization for Cold Spray Processing

Danielle Belsito¹, Baillie McNally¹, Luke Bassett¹, Victor Champagne², Diran Apelian¹,
Richard D. Sisson, Jr.¹

¹Worcester Polytechnic Institute

²U.S. Army Research Laboratory

Military aircraft that require high maneuverability, durability, ballistic protection, reparability, and energy efficiency need structural alloys with low density, high toughness, and high strength. The cold spray process, a dynamic powder consolidation technique, produces materials that meet these needs. The primary focus of this effort is to develop a through-process model to be utilized as a predictive tool to design optimum materials and processing parameters for the cold spray process. The four stages in the through-process model are powder production, powder preparation, cold spray processing, and post-processing. Extensive computational thermodynamic and kinetic models are employed for the first two stages to aid in novel material design. Finite element analyses using Johnson-Cook method are used in modeling the third stage. Model predictions are compared with experimental microstructure, microchemistry, and mechanical properties.

Experimental Verification of Through-Process Modeling of Cold Spray Al Alloys

Baillie McNally¹, Danielle Belsito¹, Luke Bassett¹, Victor Champagne², Diran Apelian¹,
Richard Sisson¹

¹Worcester Polytechnic Institute, ²Army Research Lab

The cold spray process is a cost effective process for repairing damaged parts or creating structural bulk materials for military aircraft that require high maneuverability, durability, ballistic protection, and energy efficiency. A high strength, high toughness, light weight alloy is needed for this application. Conventional aluminum powders are currently being used in this process. However, there is a need for a tailored alloy that would optimize the properties of the deposited materials. A through-process model that includes powder production, powder pre-processing, the cold spray process, and post-processing would benefit the current trial and error cold spray process immensely and would aid in the search for an optimal cold sprayable alloy. Thermodynamic and kinetic models are utilized to create the powder production and pre-processing stages. These models can identify the optimum microstructure and microchemistry of the material and any pre-processing steps required. The particle impact model predicts the deformation of powder particles during impact. Current work focuses on the characterization of the microstructural evolution to verify and enhance the powder production and pre-processing models as well as the particle impact model. Particle, grain size and microstructural morphology for powders and corresponding cold sprayed materials are determined through optical and scanning electron microscopy. X-ray diffraction along with scanning and transmission electron microscopy are used to identify the phases present and precipitate morphology. Finally, mechanical property testing will be correlated to the amount of deformation predicted by the particle impact model.

Experimental investigation of the plastic behavior of halite single-crystals at room temperature and 400°C: In-situ approach

David Picard, Alexandre Dimanov,
Jean L. Raphanel

LMS Ecole polytechnique, 91128 Palaiseau,
France

Halite deforms plastically or creeps by several mechanisms: intragranular dislocation glide, grain boundary sliding, pressure solution, ... Among those, the first one, also called crystal plasticity (CP), is a key mechanism at low or moderate strain rates and at room temperature up to high temperatures. Natural rock salt is a crystalline material, consisting of almost pure NaCl which is a ionic crystal, with cubic symmetries. Dislocation glide has been observed to take place on three families of slip planes, respectively dodecahedral {011}, octahedral {111} and cubic {001}, along the same family of glide directions, <011>. The activation of a given system depends on how at a given stage, its critical shear stress compares with the resolved shear stress which may be estimated, given the crystal orientation and the loading mode. The critical shear stress is temperature, history and strain rate dependent. Despite numerous experimental studies, the conditions for the activation of slip systems, i.e. the critical shear stresses and their evolutions (strain hardening) are not well known which has motivated our study of the crystal plasticity of NaCl single crystals deformed in uniaxial compression at different temperatures and strain rates, using several initial crystal orientations. The originality of our approach is to use the Digital Image Correlation (DIC) technique and to observe two faces of our samples which are high purity halite single crystals which are oriented and cut. The DIC method allows to compute the strain field and to evaluate quantitatively the heterogeneity of the local deformation which can be related to local mechanisms such as intracrystalline slip. Compression experiments are performed using both a uniaxial press installed inside a SEM for microscopic tests and a standard uniaxial press equipped with a 10 kN load cell for macroscopic tests. Parallelepiped samples with axes oriented parallel to [001] (sample M00), 45° to [001] in (010) (sample M45) and 30° to [001] in (011) (sample M30) have been prepared. Tests have been performed at room temperature and at 400°C, the strain rate, deduced from the machine constant displacement velocity ranges between 2.4x10-6 s-1 and 2.4x10-5 s-1, the strains of about 5% are reached. At room temperature, the rheological behavior is characterized by an elastic deformation followed by plastic flow with strain hardening. The DIC technique indicates that, for crystals M00 and M45, plasticity is happening by slip on two conjugate dodecahedral systems, whereas for crystals M30 slip occurs on one cubic slip system. The computed critical resolved shear stresses τ_c are ~ 7.5 MPa and 24 MPa for dodecahedral and cubic systems, respectively. The plastic flow is directly dependent on the number of active systems. The strain hardening is linear for the dodecahedral systems and follows a power law for the cubic system. At high temperature a plastic flow takes place with very little hardening. The DIC technique indicates that slip occurs on the systems which present the highest Schmid factor, i.e. dodecahedral, octahedral and cubic systems for crystals M00, M45 and M30, respectively. The critical resolved shear stresses of these 3 different systems have almost the same value.

Results are interpreted and analyzed with the help of CP-FEM simulations.

Solute segregation and dislocation mobility in binary alloys from dynamical variational Gaussian calculations

Evgeniya Dontsova¹, Joerg Rottler², Chad Sinclair¹

¹Dept of Materials Engineering, University of British Columbia, Vancouver, BC V6T 1Z1, Canada

²Dept of Physics and Astronomy, University of British Columbia, Vancouver, BC V6T 1Z1, Canada

Segregation and precipitation of solute atoms at defects and interfaces are common phenomena in alloys, but are difficult to model atomistically as they occur on timescales that far exceed those accessible with standard molecular dynamics. We present a dynamical version of the variational Gaussian method [1] for binary alloys based on the recently proposed Diffusive Molecular Dynamics approach developed to simulate kinetics of vacancy diffusion in crystalline structures at the atomic level [2]. In this approach, a phonon-free description of solids is coupled with statistical averaging over various configurations, from which free energies can be efficiently computed.

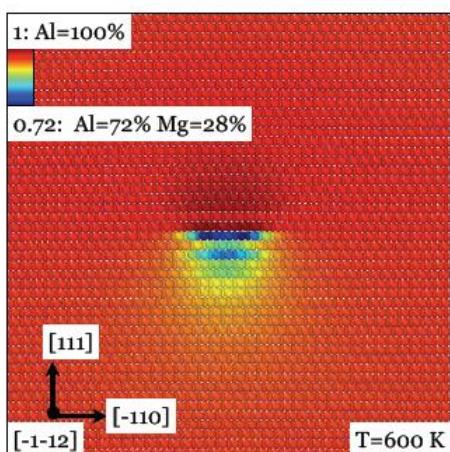


Figure 1: Occupation probability field of Al-Mg crystal (5% Mg) with split partial dislocations.

Atomic positions are represented by Gaussian density fields, whose amplitude is interpreted as an occupation probability that indicates the relative local concentration of each atomic species. Interactions arise from a “thermalized” embedded atom (EAM) potential, and the free energy of the alloy is minimized by optimizing atomic positions and vibrational amplitudes coupled with relaxational dynamics of the concentration fields.

Using this technique, we compute the concentration profile of solute atoms near vacancies, dislocations, and stacking faults for a wide range of solute concentrations and temperatures. Figure 1 shows an example of solute magnesium atoms segregation around a

split edge dislocation in fcc aluminum, where the concentration of magnesium is enhanced in the region under tensile stress. At lower temperatures, ordered intermetallic phases appear, whose symmetry is sensitive to the details of the chosen EAM potential. We then “reverse coarse grain” and construct atomistic realizations of the solute atmosphere around edge dislocations, from which we predict the depinning stress for dislocation glide with molecular statics.

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Stability of a quadruple node in the interfacial network in 3D

Bryan W. Reed¹, Vasily V. Bulatov¹, Shiu Fai Li¹, Jeremy Mason², Mukul Kumar¹

¹Lawrence Livermore National Laboratory, Livermore, California 94550, USA

²Boğaziçi University, Bebek, İstanbul 34342, Turkey

In his 1951 paper Herring presented a concise equation for the mechanical equilibrium of a triple junction (TJ) line formed by three intersecting interfaces [1]. Whereas Herring's original treatment of TJ was confined to two dimensions, here we examine mechanical equilibrium of a quadruple node (QN) in a general three-dimensional interfacial network. The QN is a fundamental unit element of the grain boundary (GB) network in which four grains intersect (see figure). Although topology of a QN is simple, its geometry in a grain boundary network formed by crystal grains is rather complex: even discounting the microscopic variables, it takes 17 macroscopic (geometric) degrees of freedom to uniquely characterize grain mis-orientations and interface plane inclinations associated with a single 4-node [2].

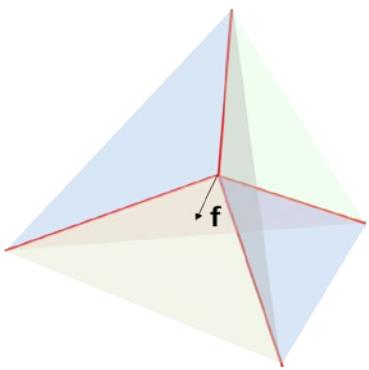


Figure: 4-node is a junction of four grains, six grain boundary interfaces and four triple lines.

High dimensionality of the phase space can give rise to complex anisotropies associated with the QNs. Here we examine the thermodynamic driving force acting on a QN and derive equations defining its mechanical equilibrium in an arbitrary interfacial network. We discuss how the newly derived equilibrium conditions differ from the two-dimensional TJ equilibrium conditions of Herring. Using a selected set of QN geometries as test cases, we demonstrate how interface energy anisotropy can drive GB network evolution to instances where some of the QN become partially or completely locked in space.

Implications of such locking for statistical properties and stability of GB networks and methods for computational modeling of such effects will be discussed.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. This work was supported at LLNL by US DOE Office of Basic Energy Sciences, Division of Materials Science and Engineering. The authors acknowledge useful discussions with J. Lind, T. Lagrange and T. Oppelstrup.

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Phase transitions in metallic grain boundaries

Timofey Frolov¹, Sergei Divinski², Mark Asta¹, Yuri Mishin³

¹University of California, Berkeley

²Institute of Materials Physics, University of Munster

³George Mason University

Recent experimental measurements of Ag impurity diffusion in the S5(310) grain boundary (GB) in Cu revealed an unusual non-Arrhenius behavior suggestive of a possible structural transformation Divinski et al., [Phys. Rev. B 85, 144104 (2012)]. On the other hand, atomistic computer simulations have recently discovered phase transformations in high-angle GBs in metals Frolov et al., [Nat. Commun. 4, 1899 (2013)]. We present atomistic simulations of Ag diffusion and segregation in two different structural phases of the Cu S5(210) GB which transform to each other with temperature. The obtained excellent agreement with the experimental data validates the hypothesis that the unusual diffusion behavior seen in the experiment was caused by a phase transformation. Together, the simulations and experiment provide the first convincing evidence for the existence of structural phase transformations in high-angle metallic GBs and demonstrate the possibility of their detection by GB diffusion measurements and atomistic simulations.

Molecular Origins of the Mechanical Behavior of Hybrid Molecular Materials

Joseph A. Burg, Mark S. Oliver, Yusuke Matsuda, Reinhold H. Dauskardt

Department of Materials Science and Engineering, Stanford University, Stanford, CA

Hybrid organosilicate molecular films processed from small organosilane precursors exhibit unique electro-optical properties while maintaining excellent thermal stability. They can be inexpensively processed using sol-gel or chemical vapor deposition and have application in emerging nanoscience and energy technologies. A fundamental challenge for their integration and application, however, remains their inherently mechanically fragile nature that derives from the oxide component of the hybrid glass network and the presence of terminal hydroxyl and organic groups that reduce network connectivity.

We use molecular dynamics (MD) based simulated annealing to create highly accurate molecular models of hybrid glasses [1,2]. We can create large, distortion-free models with well-controlled network connectivity from any number of existing and potential molecular precursors. Accurate nanoporous models can be generated by employing a strategy that mimics the synthetic porogen burnout approach. Elastic properties are simulated through MD and fracture energy can be accurately simulated using our new minimum-cut fracture model that accurately predicts the 3-D cohesive fracture path at the atomic scale (**Fig. 1**).

A complementary method that we are developing to characterize and model hyper-connectivity is based on a mean-field approach. Characterizing the network connectivity of hybrid glasses is typically very complex because of the absence of long-range order in the glass network and the highly complicated molecular structure consisting of both homo-nuclear (i.e., Si-Si and C-C) and hetero-nuclear bonds (i.e., Si-C, Si-O), and monovalent bonds (i.e., Si-H and C-H). The mean field approach we have been implementing enables us to characterize hyper-connectivity by simply counting the average number of network bonds, $\langle r' \rangle$, in the molecular structure without relying fully on a complex analysis. We have already demonstrated that $\langle r' \rangle$ is correlated very well with both the elastic modulus and cohesive fracture properties of hydrogenated

amorphous SiC hybrid films with stoichiometric compositions ($\text{Si/C} \sim 1$) (**Fig. 2**).

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This work was supported by the US Department of Energy under Contract No. DE-FG02-07ER46391.

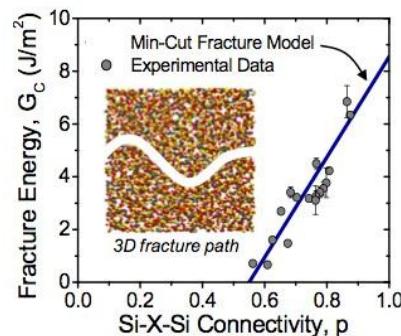


Figure 1: Predicted and experimental scaling of the fracture energy of hybrid organosilicate films as a function of with Si-X-Si network connectivity.

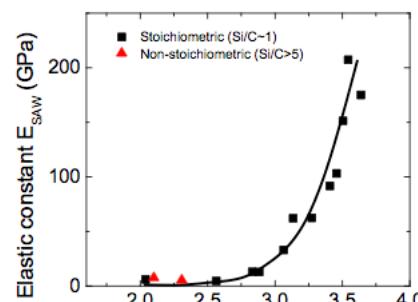


Figure 2: Hybrid elastic constant as a function of the average network bonds $\langle r' \rangle$ calculated using mean field theory

Influence of Interfaces on the Intrinsic Growth Stresses in Nanoscale Metallic Thin Films

Gregory B. Thompson¹, Li Wan¹, Tyler Kaub¹, Bianzhu Fu¹, Xiao-Xiang Yu¹

¹Department of Metallurgical and Materials Engineering, the University of Alabama,
Tuscaloosa, AL 35487

Nanocrystalline thin films are structures with large surface area-to-volume ratios which enable interfacial and grain boundary energies to play a dominate role in the stability and properties of the thin films. Using a laser interferometer technique, the intrinsic growth stresses have been measured for both multilayered and alloy thin films. For the multilayers, which include Ti/Nb and Ti/W, changes in phase have been observed in individual layers for Ti/Nb but not equivalent layer thicknesses for Ti/W. These phase transformations have been correlated to the thermodynamic interfacial energy reduction and stress behavior of the film. For the alloy films, which include Ni-Cu and Fe-Pt, the stress states have been shown to be tunable with which solute element segregates to the grain boundaries, as measured by atom probe tomography. The phase and stress behavior of both classes of films have been rationalized through the use of a hybrid Molecular Dynamics and Monte Carlo simulation that captures the segregation and mixing behavior at the interfaces and/or grain boundaries which are compared to the experimental findings.

Microscale plastic strain distribution in slip dominated deformation of Mg alloys

Guilhem Martin¹, Chad W. Sinclair², R.A. Lebensohn³

¹Laboratoire de Science et Ingénierie des Matériaux et Procédés, Saint Martin d'Hères FRANCE

²Dept. Materials Engineering, The University of British Columbia, Vancouver, BC, Canada

³Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM USA

Though mean-field crystal plasticity models have played an important role in advancing our understanding of the plastic anisotropy of polycrystalline Mg alloys, these mean field predictions can never hope to adequately capture the significant inter- and intragranular plastic strain heterogeneity that has been reported in Mg alloys (see e.g. [1]). While such local strain heterogeneity may be a consequence of twinning, it can also be found in situations where plasticity is slip dominated. In this work the local plastic strain distribution has been evaluated via a micromechanical approach involving coupled EBSD and digital image correlation (DIC) measurements [1-2]. These experiments have been performed on a Mg-RE alloy deformed in tension parallel to the prior rolling direction under conditions favoring slip, rather than twinning. These experiments reveal that the local equivalent strain can be up to 5-6 times the macroscopic tensile strain. This strain localization is seen to not correlate in a simple way to crystallographic orientation. Instead, a strong correlation between strain amplitude and distance to nearest grain boundary is observed, this highlighting the importance of the mechanical interactions between adjacent grains having different orientations. In an attempt to better understand the origins of the observed plastic strain distribution full-field crystal plasticity simulations using a spectral based viscoplastic model have been performed. The simulated strain field exhibits similar features compared to the experimental ones when a sufficiently large anisotropy between the flow stress on basal and non-basal slip systems is adopted.

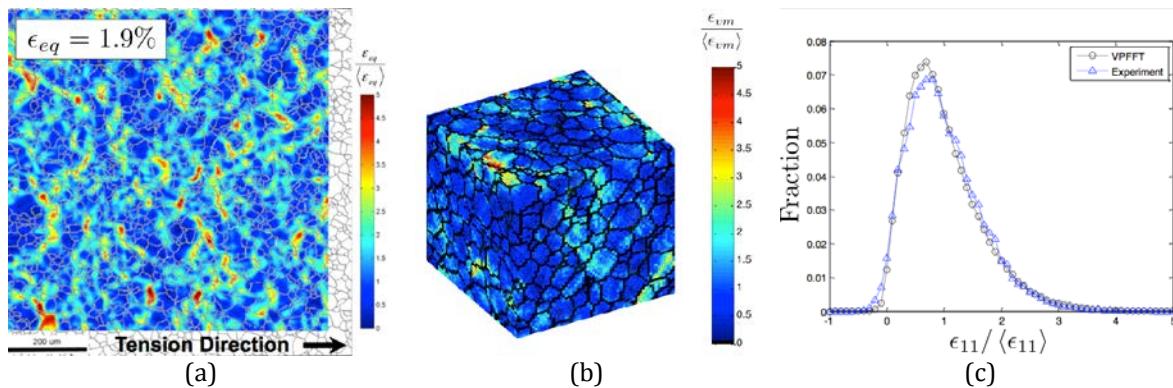


Figure 1: a) Experimental plastic strain distribution b) simulated plastic strain distribution using spectral method crystal plasticity model c) comparison of the histogram of plastic strains from experiment and simulation.

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Formation and structure of first water monolayer on TiO₂ rutile surface

Natalia Skorodumova, Baochang Wang, Mikael Leetmaa

The Royal Institute of Technology (KTH)

Mechanism of first water monolayer formation on TiO₂ (110) rutile surface has been described using a combination of ab initio and kinetic Monte Carlo (KMC) calculations in close collaboration with experiment. The ab initio calculations provided us with reliable information about the energetics of different molecular configurations, diffusion barriers and their dependence on coverage. This information was used in KMC to build a dynamic model of water layer formation. Water is found to partially dissociate on defect free TiO₂(110) at low coverage. Repulsive interaction between dissociated species and clustering of water around them, leading to a creation of hydrogen bonded net, are responsible for the observed dynamics and pattern formation during the layer formation. Interaction with experiment was crucial for this project as it proved theory with necessary knowledge about the composition of water layer at different coverages.

The Origin of Oxygen Strengthening Effect in α -Titanium

Liang Qi¹, Qian Yu¹, Tomohito Tsuru², Andrew Minor¹, Mark Asta¹, Daryl Chrzan¹

¹Department of Materials Science and Engineering, University of California, Berkeley,
CA 94720, USA

²Nuclear Science and Engineering Directorate, Japan Atomic Energy Agency,
Tokaimura, Ibaraki, Japan

Very small concentrations of O interstitials in hexagonal-close-packed (hcp) Ti can induce significant strengthening, but with the detrimental effect of lowering toughness. To provide new insights into this long-studied problem, we performed first-principles calculations to analyze the interactions between interstitial atoms and screw dislocation cores in hcp-Ti. Both indirect studies of generalized stacking fault energy and direct investigation of dislocation cores show that oxygen and other large interstitials are strongly repelled by the screw dislocation core. This repulsion forces these interstitials to move from their original interstitial site during dislocation slip. The origin of this repulsion is the structure of hcp lattice: in the hcp-Ti screw dislocation core, the interstitial volume is largely reduced. The results are shown to be in good agreement with recent experimental observations derived from in-situ small- scale mechanical tests of Ti samples with different oxygen concentrations and scanning transmission electron microscope (STEM) characterizations of their dislocation core structures.

WC-Co microstructure degradation study in rotary-percussive drilling

Dmitry Tkachuk^{1,2}, Vladislav A. Yastrebov², Georges Cailletaud², Alexandre Kane³, Charlie Chunlin Li¹

¹Department of Geology and Mineral Resources Engineering, NO-7465, Trondheim, Norway

²Centre des Matériaux, MINES ParisTech, CNRS UMR 7633, Évry 91003, France

³SINTEF Materials and Chemistry, NO-7465 Trondheim, Norway

Keywords: WC-Co, microstructure, wear, finite-elements, rotary-percussive drilling

This study investigates wear of WC-Co drill bit button during rotary-percussive drilling of hard rock at high pressure and high temperature conditions. Focus of the current study is on micro-mechanisms of WC-Co material degradation. In order to reproduce deformation and failure on such scale 2D finite-element models were generated based on a scanning electron microscopy (SEM) images of a real microstructures. The average size of generated models are 20x20 micro-meters, with 40 to 100 WC grains embedded in the Cobalt matrix (with volume fraction 5 to 20%). Plastic behavior were considered for both WC and Co. Two types of interfaces are modeled by means of cohesive zone elements: WC-WC and Co-WC. The loading is applied by indenter of different sharpness, which represents the rock contact surface micro-asperity.

Degradation mechanisms of a drill bit buttons from real drilling application and from button-rock impact tests have been studied by the use of scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS). Three main typical mechanisms are distinguished: (a) Co binder extrusion, (b) WC grains decohesion, (c) WC grains fracturing. Button-rock interaction conditions (contact morphology, contact temperature, ranges and types of interaction forces) were investigated using non-contact interferometry (rock and drill bit button surface roughnesses) and finite-element simulations (macroscopic button-rock impact, coupled thermo-mechanical microstructure behavior).

Dominating degradation mechanisms at different sets of interaction conditions (mentioned above) accounting for the rock formation response, microstructure composition, grain size and morphology distributions were investigated through series of numerical computations.

Proposed approach could be used to: (a) suggest improvements for material manufacturing process, (b) provide engineers with a numerical tool capable of wear assessment at a macro-scale level, which can be used for optimizing drilling process and drill bit design.

Gas Adsorption in Microporous Materials: Ab Initio Based Grand Canonical Monte Carlo Simulations

Muthuramalingam Prakash¹, Navid Sakhavand¹, Rouzbeh Shahsavari^{1,2}

¹Department of Civil and Environmental Engineering, Rice University, Houston, TX 77005

²Department of Material Science and NanoEngineering, Rice University, Houston, TX 77005

A multiscale approach based on ab initio and grand canonical Monte Carlo (GCMC) simulations is used to report the H₂, N₂, and CH₄ gas uptake behaviors of two microporous materials, i.e. zeolitic imidazolate frameworks (ZIF)-95 and -100, with exceptionally large and complex colossal cages. The force fields describing the weak interactions between the gas molecules and ZIFs in GCMC simulations are based on ab-initio MP2 level of theory aimed at accurately describing the London dispersions. We report the total and excess gas uptakes up to 100 bar at 77 and 300 K. Our results unravel the interplay between the uptake amount, pore volume, guest molecule size, temperature, chlorine functional group, and isosteric heat of adsorption in ZIFs. We found that while the uptake capacity of ZIF-100 outperforms ZIF-95 for small molecules (H₂), ZIF-95 offers a superior adsorption capacity for large molecules (CH₄). Moderately sized molecules (N₂) exhibit a more complex uptake behavior depending on the temperature. Furthermore, we show that the induced dipole interactions, such as those caused by –Cl functional groups, play a vital role on gas adsorption behaviors. This work provides the first report on the N₂ and CH₄ uptake of ZIF-95 and -100 using ab initio based GCMC simulations. Furthermore, it renders a valid path for a reliable computational-driven synthesis and discovery of numerous functionalized ZIFs - via introduction of ligand binding moieties in the pore spaces of ZIFs - to enhance gas adsorption and separation, and potentially enable size- and shape-selective catalysis.

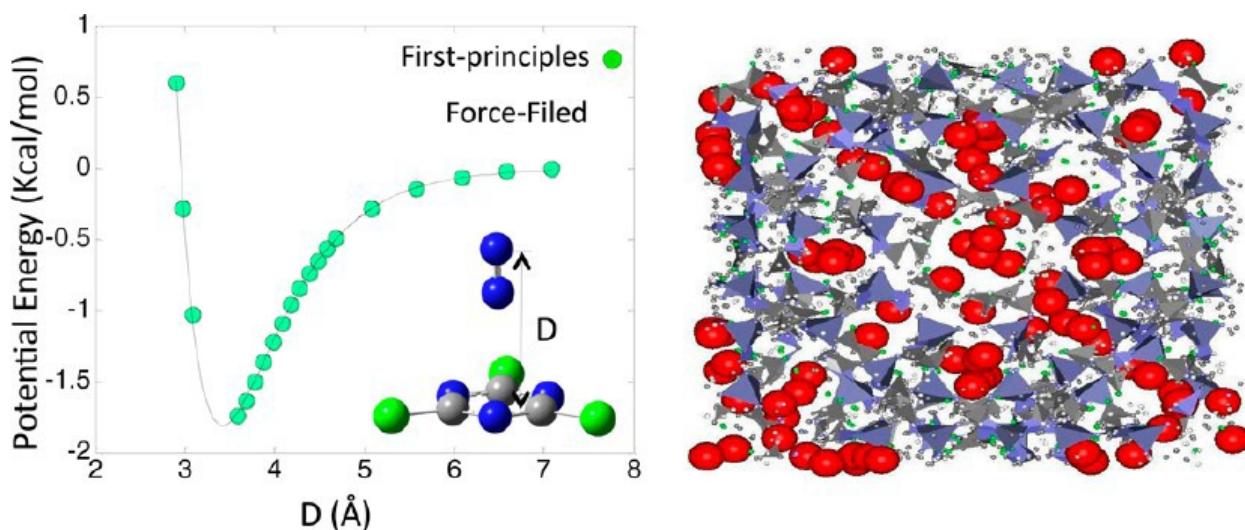


Figure 1. Interaction of N₂ molecules with the ZIF linker (left). A schematic of the porous ZIF structures with adsorbed N₂ molecules in red (right)

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Ultrahigh strength of nanotwinned Ag-Cu dilute alloys by atomistic simulations

Linh Nguyen¹, Enrique Martinez², Y. Morris Wang¹, Jaime Marian¹

¹Lawrence Livermore National Laboratory, Livermore, California 94550, USA

²Los Alamos National Laboratory, Los Alamos, New Mexico, 87545, USA

Nanotwinned (nt) materials with a high density of coherent twin boundaries (CTB) often display a high thermal stability, high yield strength, high ductility, and are more resistant to coarsening than their fine-grained counterparts. However, nt-materials are also known to exhibit a maximum in Hall-Petch strengthening behavior, dictated by dislocation nucleation mechanisms. Continuous strengthening beyond this maximum value has remained impossible experimentally. In this work we perform a systematic atomistic study of nt Ag-1%at Cu bicrystals containing CTB in various densities. First, we perform a thermodynamic relaxation at finite temperature using a variance constrained semi grand canonical Monte Carlo algorithm to place Cu atoms in thermodynamically favorable locations, followed by loading uniaxially along several orientations using molecular dynamics simulations. We study the effect on the overall yield strength of CTB spacing, Cu concentration, and temperature, and point to the causes for such marked yield strength increases observed in the experimental tests.

Comparison of dislocation-based model of recovery and cross-correlation based EBSD measurements in single crystals

Szilvia Kalácska¹, Péter D. Ispánovity¹, István Groma¹

¹Eötvös Loránd University, 1117 Budapest, Pázmány P. stny 1/a, Hungary

Subgrain growth during recovery has been investigated using simulations of two-dimensional discrete dislocation dynamics on a hexagonal lattice having three symmetric slip planes [1]. To account for elevated temperature (i) dislocation climb was allowed and (ii) a Langevin type thermal noise was added to the force acting on the dislocations. The growth exponent and the subgrain structure were examined.

Cross-correlation based analysis of electron backscatter diffraction (EBSD) patterns is often carried out to map plastic strain variations in deformed polycrystalline samples [2]. Firstly, the effects of sample surface preparation methods were investigated including Ar ion polishing and traditional electropolishing treatments. Then the distortion maps of the specimen are computed with the cross-correlation technique. This method is capable of detecting changes of the crystal orientation to higher accuracy, than the commercial software provided for standard EBSD devices that analyze each EBSD pattern individually.

In this work the simulation and experimental results were compared to characterize the evolution of dislocation structures and corresponding distortion fields in highly deformed Cu single crystals during low temperature annealing.

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**Prediction of Microstructural Evolution during Sintering Process using Meso-scale
Simulation and FIB/SEM Tomography**

Shotaro Hara, Akihiro Ohi, Naoki Shikazono

The University of Tokyo

Sintering is one of the critical processes deeply related with a degradation phenomenon in solid oxide fuel cells. However, because of the inherent complexities linking with multiple mechanisms, its quantitative understanding is still lacking. In this study, pure Ni, NiO, 8YSZ, NiO-8YSZ composite were sintered at a wide range of heating rates, and their densification behavior was analyzed by applying a master sintering curve concept. Besides, the microstructural details like porosity, grain size, pore size distributions and curvatures of sintered samples were quantitatively measured utilizing three dimensional reconstruction based on FIB-SEM technique. We also present three-dimensional kinetic Monte Carlo simulations based on Q-state Potts model in order to numerically predict the microstructural evolution of the composite system. To simulate a solid-state sintering process, we have incorporated three kinetic mechanisms into the model: Curvature-driven grain growth, pore migration by surface diffusion and densification mediated by vacancy action. The frequencies of each kinetics are determined to represent our experimental results. We show that our computational tool can successfully track the valid sintering pathway and would be used as a useful tool for designing an anode microstructure in solid oxide fuel cell systems.

Nanoscale superlubricity, peeling and fracture at carbon and silicon interfaces

Naruo Sasaki

Department of Engineering Science, University of Electro-Communications,
Chofu, Tokyo 182-8585, Japan

Control of friction is one of the most practical problems in our daily life, which covers almost all the areas from basic science to applied engineering. In this talk we discuss our recent numerical and experimental studies on nanotribology at nanoscale carbon and Si interfaces.

First we have experimentally developed the fullerene molecular bearings[1,2], measured peeling process of graphene[3], and performed the molecular mechanics simulations of nanoscale friction at the interfaces of the graphene/C₆₀ and graphene/graphene interface[4]. Anisotropy of friction of graphite/C₆₀ interface is found, where the maximum and minimum friction appears for the commensurate and other scan directions, respectively. It is clarified that the small rotation and elastic contact of C₆₀ molecules contribute to the ultralow friction. Similar anisotropy is also found during the peeling process at graphene/graphene interface during surface contact.

Next the nanoscale shear and fracture of the opposing Si tips are studied by molecular dynamics simulation. It is clarified that, under the high loading condition of several GPa, nanocontact region becomes amorphous[5]. During the shear process, the characteristic transition of the dynamics of the amorphous contact region occurs. First amorphous contact region slides at Si/Si interface. [Fig.1a] As the shear proceeds, the amorphous region becomes thinner and longer, and turns into nanowire.[Fig. 1b] The nanowire elongates until it breaks. The simulated contact diameter and angle are in good agreement with experimental one obtained by MEMS in TEM. Thus the dynamics of the amorphous contact region plays a major role in the shear process of opposing Si tips under the high loading condition, which can give us clue to understand one of the dynamics of the single real contact area.

This work was supported by the Grant-in-Aid for Scientific research (B) (No. 23360023) and Specially Promoted research (No. 21000008) from the Japan Society for the Promotion of Science. The author acknowledges collaborations with Prof. K. Miura and Prof. H. Fujita.

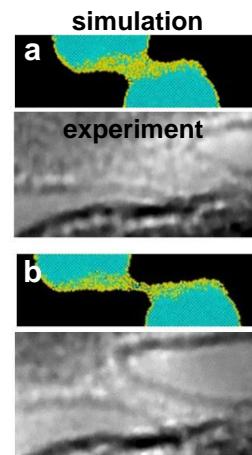


Figure 1: Simulated and measured amorphous contact regions of Si/Si interface.

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Atomistic modeling friction on graphene: effects of hydrogenation, substrate roughness and electron-phonon coupling

Yalin Dong¹, Xiawa Wu², Ashlie Martini³

¹Department of Mechanical Engineering, the University of Akron, Akron, OH 44325

²Department of Mechanical Engineering, Purdue University, West Lafayette, IN 47907

³School of Engineering, University of California Merced, Merced, CA 95343

Thanks to the development of atomic force microscopy, many interesting tribological properties have been discovered on graphene from superlubricity and thickness dependence, to friction enhancement resulting from fluorination or hydrogenation. Due to the extreme difficulty to “see” what really occurs in the buried interface using experimental techniques, some of the underlying mechanisms remain unknown or controversial. We carry out molecular dynamics simulation to model single asperity friction to address these issues, and provide atomic level information to interpret related experimental observations obtained by atomic force microscopy. First, we perform simulations to model the friction on hydrogenated graphene, and reveal that the roughness induced by hydrogenation is the most likely origin of friction enhancement. Second, we study the effects of substrate roughness and electron-phonon coupling on thickness-dependent friction, and clarify their contributions to friction in general. Lastly, we briefly discuss how to use these principles we learned from our simulation to predict tribological properties of other materials.

Kinetic nanofriction: effect of temperature on the frictional mechanism of mobile molecules on a surface

Mehdi Jafary-Zadeh, Chilla Damodara Reddy, Yong-Wei Zhang

Institute of High Performance Computing (IHPC), A*STAR, Singapore 138632

To develop high-performance nano-electro-mechanical systems (NEMS) using bottom-up approaches, understanding frictional mechanisms of nanoscale building blocks is essential.¹ Such understanding allows us to quantify the frictional forces at single-atomic/molecular level, offering possibilities to precisely manipulate these building blocks by controlling their driving forces. Although nanoscale imaging and testing techniques, *e.g.* atomic force microscopy (AFM), are recently employed to measure *static nanofriction* of atomic/molecular adsorbates,² they are too slow to measure the *kinetic nanofriction* of the mobile adsorbates.³ On the other hand, Brownian motion of a single nanoparticle on a surface, which was recently found far below room temperature, poses an opportunity to study the kinetic nanofriction.³⁻⁶ Here, using prototype C₆₀/graphene system and employing large-scale molecular dynamics (MD) simulations, we study the variation of kinetic nanofriction coefficient with temperature. We show that the kinetic nanofriction coefficient decreases by increasing the temperature, and its temperature dependence follows an Arrhenius-form with two distinct regimes that have a crossover merely by changing the temperature. Moreover, we explain the mechanisms of interaction between the admolecule and the substrate at these regimes. The C₆₀/graphene is a prototypical physisorbed system fascinating for fundamental studies of mass transfer and frictional phenomena at the nanoscale. Moreover, it is a promising system for various important applications such as nano-bearing, molecular spintronics and quantum computing. Our findings illustrate the important role of temperature in the performance of nanosystems and shed lights on the development of NEMS.

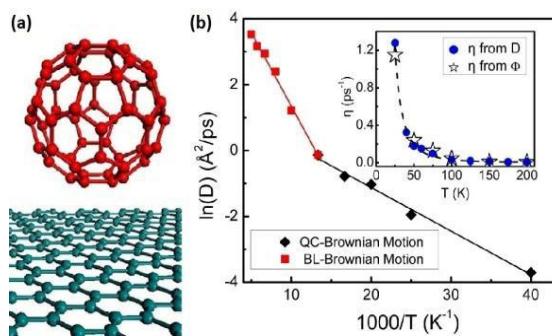


Figure 1| (a) Our computational model consists of a single C₆₀ molecule on top of a graphene sheet, *i.e.* C₆₀/graphene system. (b) The Arrhenius analysis of surface diffusion coefficient, D , indicates that in the temperature range of 25 K to 200 K, the C₆₀ admolecule exhibits two distinct regimes of Brownian motion with a crossover at about 75 K. The inset of (b) shows the kinetic nanofriction coefficient, η , calculated from D as well as velocity

autocorrelation function, Φ , at different temperatures.

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Simulation of a Dental Tribological System at a Microscopic Scale

Christian Nutto¹, Sandra Sarmbe², Matthias Scherge¹, Claas Bierwisch¹

¹Fraunhofer IWM, 79108 Freiburg, Germany

²Fraunhofer IWM, 06120 Halle, Germany

For the investigation of abrasive processes in the field of oral hygiene, the complex interactions of dental care products with biological materials have to be considered. In the case of tooth-cleaning, toothpastes need an optimized cleaning efficiency to remove stains and biofilms from the teeth, which can be influenced by adding abrasives of various sizes, shapes and mechanical properties. In contrast, the concentration and material selection of the abrasives should be carefully chosen to avoid abrasion effects on the teeth. In order to understand the process of tooth cleaning and possible tooth wear, there is a need to investigate in detail how the abrasive particles interact with the toothbrush filaments in a cleaning contact. Up-to-now, due to the variability of the parameters, these data are hardly achievable.

The objective of this study was to investigate the interactions between toothbrush, toothpaste - including the abrasive grains - and human enamel during dental care. Therefore, the process of tooth cleaning is reduced to a tribological system of a single toothbrush filament, human enamel and different particle suspensions representing a mixture of toothpaste and water.

We have developed Smoothed Particle Hydrodynamic (SPH) simulations at a microscopic scale for the investigation of abrasive processes between a toothbrush filament, abrasive grains, and enamel. We focused on the induced stresses onto the enamel by varying process parameters, i.e., suspension viscosity, tilt-angle of filament and size of abrasive grains. The determined stresses are an indicator for the cleaning effectiveness of the abrasives but also for the wear risk on the enamel.

We can demonstrate how the variation of each of the parameters affects the interaction between all involved components. The results from our simulations at a grain-size scale support the interpretation of accompanying experiments.

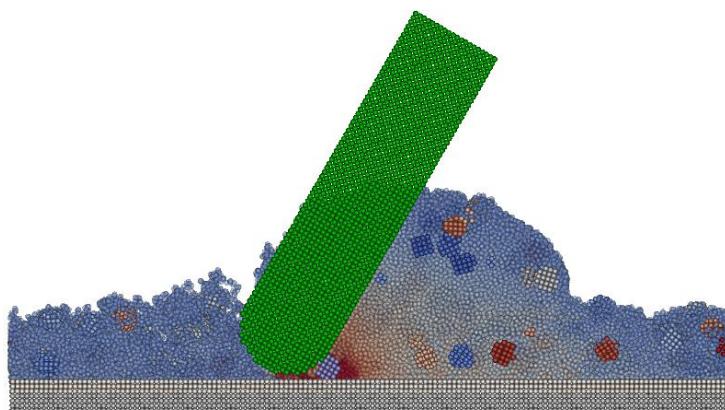


Figure 1 Numerical model of a toothbrush filament, enamel, and a toothpaste containing abrasive particles. The color scale shows the pressure distribution within the toothpaste at an instant of the abrasive process.

Nano scale contribution to features occurring at the macro scale in lubricated contacts

Philippe Vergne¹, Daniele Savio^{1,2}, Nicolas Fillot¹

¹ Université de Lyon, INSA-Lyon, CNRS, LaMCoS, UMR5259, F-69621, France

² SKF Aeroengine France, Valenciennes F-59309, France

Nowadays the thickness of the film separating two lubricated surfaces can decrease down to a few nanometers, thus becoming comparable with the size of the fluid molecules. Under such severe confinement, the continuum hypothesis upon which the traditional lubrication models are based may not be valid anymore. Understanding the properties of nanometer-thin lubricant films has thus been a major concern in the past 20 years, leading to the development of experimental and numerical methods capable of accessing quantities at the molecular scale. The current challenge consists to take into account the results in real-size contacts.

The integration of nano scale effects into the lubrication theory would allow unraveling the influence played by molecularly thin films on the global contact behavior. The main difficulty arises from the significant difference in scale between the atomistic simulation methods (for instance Molecular Dynamics) which are limited to some nanometers, and the existing continuous models for lubricated contacts of the order of one millimeter in size. A promising way to overcome this issue involves deriving the results of nano scale simulations through representative expressions, which can then be straightforwardly coupled to the equations of the classical lubrication theory in which a Navier-type boundary condition is imposed.

This multi-scale coupling strategy was successfully applied [1] to reflect the influence of wall-slip (quantified from MD simulations as a function of macro scale parameters like pressure, sliding velocity and thickness) onto a macro scale contact lubricated by a simple hydrocarbon fluid. The continuous problem was solved on the basis of a FE method solver [2]. This approach is now extended to more realistic situations in which firstly the wall-slip characterization was more extensively studied [3] and parameterized using atomistic simulations, and secondly the composition and thus the wettability of the bounding surfaces were considered as input parameters. According the different cases investigated, significant modifications of the film thickness profiles, fluid mass flow and friction were observed in the resulting thin films.

All in all we propose a way to bridge the gap between nano and macro scale simulations for lubricated contacts.

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Molecular dynamics study of automotive lubricants: linking molecular structure and friction

Michael Doig¹, Philip J. Camp¹, Chris P. Warrens²

¹School of Chemistry, Joseph Black Building, University of Edinburgh, West Mains Rd, Edinburgh, EH9 3JJ, UK

²BP Technology Centre, Pangbourne, RG8 7QR, UK

Lubricant oils are used to reduce friction and wear in a wide range of industrial and mechanical processes. Lubricant additives play a vital role in the oils' overall performance, particularly surface-active additives which can significantly affect the tribological properties of solid surfaces. However, there is insufficient understanding of the link between the atomic-level structure of tribofilms and the macroscopic properties such as friction, to direct the development of new lubricant formulations.

Using large-scale molecular dynamics simulations, we investigate a range of lubricated systems, studying the structural properties of surface-adsorbed tribofilms on metal-oxide surfaces, and how they vary with temperature, pressure, surface coverage and shear rate. Several important trends are identified linking molecular isomerism and architecture with the structure and stability of the adsorbed films. In addition, the simulation results are used to gain insight on recent experimental measurements of film structure [1]. Some examples of the systems studied include oleic acid and stearic acid films lubricated by squalane (see figure 1) [2], and hexadecylamine films lubricated by dodecane [3], both adsorbed on iron oxide surfaces.

The friction coefficients in these systems are computed and analysed with reference to the structure of the adsorbed films, to yield new insights on the intimate link between the molecular properties of lubricants and the macroscopic frictional properties of lubricated systems.

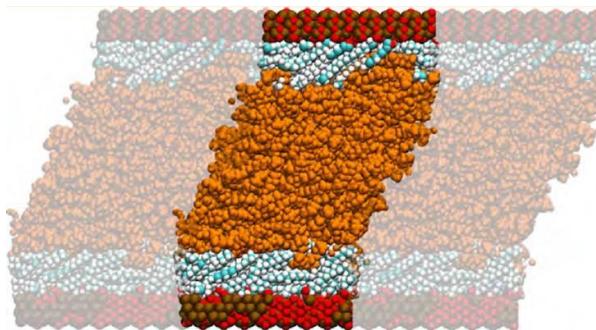


Figure 1: Lubricated system of oleic acid adsorbed on iron oxide lubricated by squalane base oil, under applied shear.

This work was supported through a CASE studentship by BP International Ltd and EPSRC(UK).

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Shear-induced amorphization of silicon crystals

Gianpietro Moras¹, Andreas Klemenz¹, Hiroshi Uetsuka²,
Michael Moseler¹, Lars Pastewka^{1,3}

¹Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

²Asahi Diamond Industrial Co., Ltd., Ichihara, Japan

³Institute of Applied Materials - Reliability of Components and Systems IAM-ZBS,
Karlsruhe Institute of Technology, Karlsruhe, Germany

Phase transformations, and in particular amorphization, of crystalline silicon occur under contact loading [1]. The formation of amorphous silicon has been reported to occur during machining, indentation and scratching processes. However, little is known about the mechanisms leading to silicon amorphization under these loading conditions, where shear stress is present. Recently, thanks to the development of accurate reactive potentials for classical molecular dynamics simulations [2, 3], the atomic-scale mechanisms that lead to shear-induced amorphization of diamond, and the crucial role they play in the wear of diamond during mechanical polishing were unveiled [4]. Here, we report the results of reactive molecular dynamics simulations of silicon crystals upon sliding load and compare them to analogous results obtained for diamond crystals.

At temperatures higher than the melting temperature, a melting process starts at the silicon/silicon sliding interface. The thickness of the melted region grows rapidly and linearly in time, with a rate that depends on the difference between the actual temperature and the melting temperature for any applied normal pressure. For temperatures lower than the melting temperature, two different processes are observed for applied pressures ranging from 1 to 15 GPa. When the pressure is lower than the beta-tin transition pressure, and therefore the cubic diamond crystalline structure is stable, a thin (< 1 nm) amorphous region abruptly forms at the sliding interface. During the sliding process, the thickness of such region does not grow due to competing amorphization and recrystallization processes, and the sliding proceeds in a stick-slip-fashion. When the applied pressure exceeds the beta-tin transition limit, the thickness of the amorphous region grows in time and its growth rate increases at increasing applied loads, at odds with the apparently similar amorphization process observed for diamond crystals.

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Friction Process of Silicon Carbide under Water Lubrication: Quantum Chemical Molecular Dynamics Approach

Yoshihiko Kobayashi¹, Hiroki Murabayashi¹, Seiichiro Sato¹, Shandan Bai¹,
Yuji Higuchi¹, Nobuki Ozawa¹, Koshi Adachi², Jean Michel Martin³, Momoji Kubo¹

¹Fracture and Reliability Research Institute Graduate School of Engineering,
Tohoku University, Sendai, Japan

²Division of Mechanical Engineering, Tohoku University, Sendai, Japan

³Laboratoire de Tribologie et Dynamique des Systemes,
Ecole Centrale de Lyon, Lyon, France

Water lubrication has the characteristic of low environmental burden. When silicon carbide (SiC) slides in water, low friction coefficient is obtained experimentally. It is thought by experiments that chemical reactions during friction are important to gain low friction surface. Understanding of the mechanism is essential to improve friction characteristic. However, it is difficult to directly obtain atomic-scale dynamics during chemical reactions by experiments. In this study, our purpose is to reveal the chemical reactions of the SiC surface under water lubrication by our tight-binding quantum chemical molecular dynamics (TB-QCMD) method.

To reveal friction phenomena of SiC sliding in water environment, we performed friction simulation of SiC under water lubrication by our TB-QCMD method (Figure 1).

Chemical reaction processes at frictional interface are shown in Figure 2. After 5 ps of the sliding under a pressure of 3 GPa, an OH⁻ ion was adsorbed on a Si atom of the SiC surface (Figure 2(a)). Moreover, after the O atom in the OH group also interacted with another Si atom of the SiC surface, a Si-O-Si bond was generated (Figure 2(b)). In addition, many Si-O-Si bonds were formed as friction time passed. Then, the growth of Si-O-Si bond chains was observed (Figure 2(c), and (d)). In experiment, SiO₂·n H₂O film is formed on the low friction surface of SiC under water lubrication. The generation of Si-O-Si bonds is initial process of the film formation. Therefore, we suggest that this growth relates to low friction property of SiC surface.

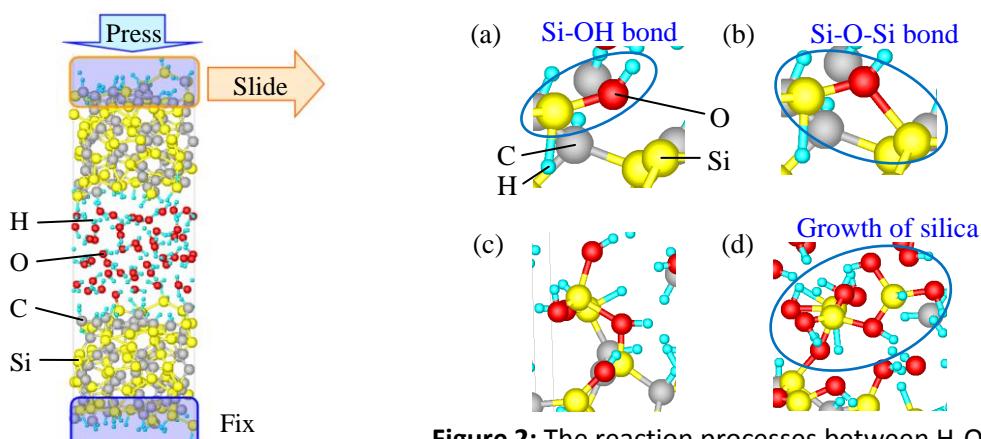


Figure 1: Friction simulation model of SiC films in water environment by TB-QCMD method.

Figure 2: The reaction processes between H₂O and SiC films during friction under a pressure of 3 GPa with 50 water molecules at (a) 5.185 ps, (b) 5.190 ps, (c) 30.535 ps, and (d) 43.070 ps.

Polishing of Gallium Nitride: Quantum Chemical Molecular Dynamics Simulations

Kentaro Kawaguchi, Takehiro Aizawa, Yuji Higuchi, Nobuki Ozawa, Momoji Kubo

Fracture and Reliability Research Institute, Tohoku University, Sendai, 980-8579, Japan

Gallium nitride (GaN) is a next-generation semiconductor material with a wide band gap and high electron mobility. Although the atomic-level planar polished surface is essential for practical GaN devices, it is difficult to polish efficiently the GaN substrate because of its high hardness and chemical stability. The chemical mechanical polishing (CMP) is promising for efficient polishing of the GaN substrate. However, the detailed CMP mechanisms are unclear, and designing of the processes is difficult. In this study, in order to design the efficient and precise GaN CMP processes, we investigate the GaN CMP via our tight-binding quantum chemical molecular dynamics (TB-QCMD) method.

We use our TB-QCMD code “Colors” to investigate the CMP process of GaN(0001) surface by a SiO₂ abrasive grain in chemical solutions. We apply a pressure of 1.0 GPa on the SiO₂ abrasive grain and forcibly slid it with 50 m/s. All simulations are performed at a temperature of 300 K.

We perform CMP simulations of a GaN surface by a SiO₂ abrasive grain in aqueous H₂O₂ solution and aqueous NaOH solution to clarify the chemical reactions of each solution. We reveal that OH radicals and OH- ions are adsorbed on the GaN surface in aqueous H₂O₂ solution and aqueous NaOH solution, respectively.

Moreover, we elucidate that Ga-N bonds of the GaN substrate in aqueous H₂O₂ solution are weaker than that in aqueous NaOH solution. Therefore, we suggest that the OH radicals are effective for efficient GaN CMP. To confirm the effectivity of OH radicals, we add one OH radical into the solution every 4.0 ps until 64.0 ps during polishing simulation under pure water environment. Fig. 1a shows a snapshot after 8 OH radicals are added.

The 8 added OH radicals are adsorbed on the GaN surface. Fig. 1b shows a snapshot after

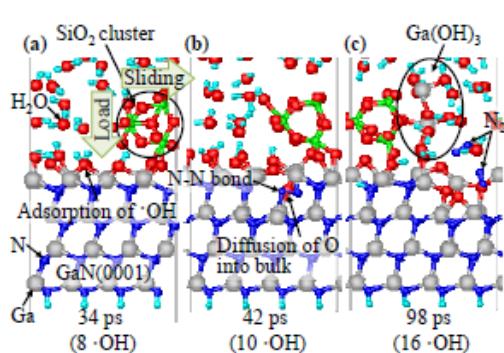


Figure 1: Snapshots of the GaN CMP simulation by a SiO₂ abrasive grain with 16 OH radicals

10 OH radicals are added. We observe the following oxidation reaction: the added OH radicals abstract H atoms from the adsorbed OH radicals, surface-adsorbed O atoms are generated, the surface-adsorbed O atom diffuses into the GaN bulk, and Ga-O bonds are generated. The N-N bond in the GaN substrate is generated due to the dissociation of Ga-N bonds by the oxidation reaction (Fig. 1b). Fig. 1c shows a snapshot after 16 OH radicals are added. The Ga atom of the first layer binds with 3 OH radicals and Ga(OH)₃ is desorbed

from the surface. The N₂ molecules are generated and desorbed from the surface due to the dissociation of Ga-N bonds by the generation of Ga-O bonds. We reveal that the GaN CMP process efficiently proceeds due to the oxidation reactions by the OH radicals.

On the importance of timescales in the atomistic modelling of friction

Danny Perez¹, Yalin Dong², Ashlie Martini³

¹Los Alamos National Laboratory, Los Alamos, New Mexico, 87545, USA

²The University of Akron, Akron, Ohio, 44325, USA

³University of California at Merced, Merced, California, 95343, USA

Friction is an inherently multiscale phenomenon where both characteristic length- and time-scales span many orders of magnitude. This fact makes the direct investigation of friction through atomistic simulation methodologies, such as molecular dynamics (MD), very challenging, especially as far as timescales as concerned. Indeed, conventional MD on leadership class computers can simulate trillion of atoms. While this is still short of completely embracing the mesoscale, it is probably sufficient to simulate the regions where atomic resolution is necessary. In contrast, conventional MD can only generate individual trajectories for times of the order of microseconds, even for small systems containing only thousands atoms.

Over the last few years, we demonstrated that the physics of friction at scanning velocities constrained by MD timescales could differ considerably from that prevailing at experimentally relevant FFM velocities [1], severely limiting the direct correspondence to experiments. We demonstrated two strategies that can be used to bridge that gap: first, using Accelerated Molecular Dynamics (AMD) techniques [2] that aim at directly extending the timescales amenable to MD simulations, and second, by parameterizing rate theory models directly from atomistic simulations [3]. I will introduce and discuss these two approaches and demonstrate their ability to address the timescale issue. I will conclude by highlighting the remaining challenges that needs to be addressed in order to simultaneously tackle both the length- and time-scale issues in their full generality.

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Atomic scale modelling of third body formation and wear in hard carbon materials

Michael Moseler

Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstr. 11, 79108 Freiburg Germany
 Physics Department, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

Despite the fact that diamond and diamond-like carbon (DLC) [1] coatings are used in an increasing number of applications, not much is known about the atomic scale processes that cause the wear of these films. For instance, the microscopic mechanisms that occur in DLC films in tribological applications [2,3] or the polishing of diamonds are still poorly understood [4]. Molecular dynamics is ideally suited to gain a deeper understanding of the underlying wear processes. In this talk a variety of atomistic simulations employing a novel Brenner bond order potential [5,6] that has been corrected for a faithful description of bond breaking processes are reported. For diamond polishing, the occurrence of soft polishing direction can be related to the generation of thick amorphous soft layers [7] that are not stable with respect to mechanical plowing or oxidative etching by ambient air [8]. The velocity of the diamond/amorphous-carbon interface depends crucially on the diamond surface orientation with the highest speed found for (110) surfaces that are rubbed in the (001) direction, while the lowest interface speed was observed for the diamond (111) surface. These finding are in perfect agreement with a 600 years old experimental knowledge of diamond polishers. The anisotropy of the wear is rationalized within a rate model based on a yield criterion for single bonds at the crystalline/amorphous interface [7]. Wear in hydrogen-free DLC films follows a similar route [9]. Both theory and experiment demonstrate the formation of a soft amorphous carbon (a-C) layer with increased sp^2 content, which grows faster than an a-C tribolayer found on selfmated diamond sliding under similar conditions. The faster $sp^3 \rightarrow sp^2$ transition in ta-C is explained by easy breaking of prestressed bonds in a finite, nanoscale ta-C region, whereas diamond amorphization occurs at an atomically sharp interface. A detailed analysis of the underlying rehybridization mechanism reveals that the $sp^3 \rightarrow sp^2$ transition is triggered by plasticity in the adjacent a-C. Rehybridization therefore occurs in a region that has not yet experienced plastic yield. The resulting soft a-C tribolayer is interpreted as a precursor to the experimentally observed wear that proceeds by removing the a-C from the sliding interfaces by plowing or etching [8]. The talk will close with new results on wear of lubricated rough ta-C surfaces and wear of diamond in contact with iron surfaces.

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Tight-Binding Quantum Chemical Molecular Dynamics Study on Tribo-Chemical Reaction of Diamond-Like Carbon under Water Lubrication

Shandan Bai¹, Yasunori Niiyama², Yoshihiko Kobayashi¹, Seiichiro Sato¹, Yuji Higuchi¹, Nobuki Ozawa¹, Koshi Adachi¹, Shigeyuki Mori², Kazue Kurihara^{3, 4}, Jean Michel Martin⁵, Momoji Kubo¹

¹ Graduate School of Engineering, Tohoku University, Sendai 980-8579, Japan

² New Industry Creation Hatchery Center, Tohoku University, Sendai 980-8579, Japan

³ Advanced Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

⁴ Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan

⁵ Laboratoire de Tribologie et Dynamique des Systemes, Ecole Centrale de Lyon, 69134 Ecully Cedex, France

[Introduction] Much attention has been paid to Diamond-Like Carbon (DLC) coatings, which have low friction and anti-wear tribological performances. The friction coefficient of the DLC films drastically changes under the water lubrication, since some tribo-chemical reactions occur during sliding. The details of the chemical reaction are difficult to be revealed only by chemical analyses. In this study, we use the computational method to reveal the chemical reaction at an atomic scale.

[Method] In order to understand tribo-chemical reactions of DLC films under water lubrication, we apply our tight-binding quantum chemical molecular dynamics method [1]. Figure 1 shows the model of DLC film under water lubrication.

[Results and Discussion] Figure 2 shows the snapshots of dynamic behaviors of upper DLC substrate. Figure 2 (a) shows the initial state of upper DLC substrate. At 0.235 ps, the C-H bond is formed between the water molecule and upper substrate of DLC, and then the H atom is terminated at the surface as shown in Figure 2 (c). We also observe the C-OH bond formation between the water molecule and upper DLC substrate at 0.015 and 0.840 ps, as shown in Figure 2 (b) and (d). Then, the DLC surface becomes progressively terminated by H/OH. These results show that the water molecule dissociates into H and OH, which terminated the surface of DLC during friction.

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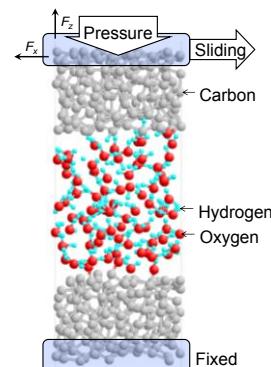


Figure 1: Model of DLC under water lubrication.

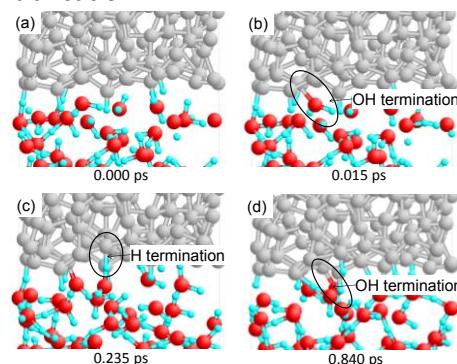


Figure 2: Snapshots of dynamic behaviors (a) initial state, (b) OH termination at 0.015 ps, (c) H termination at 0.235 ps, and (d) OH termination at 0.840 ps.

Tribochemical interactions between DLC coatings and hydrocarbon gases

Komlavi Dzidula KOSHIGAN¹, Julien FONTAINE¹,
Christophe HEAU², Christophe DONNET³, Florence GARRELIE³

¹Laboratoire de Tribologie et Dynamique des Systèmes, UMR5513 CNRS / Ecole
Centrale de Lyon, 69134 Ecully cedex, France

²IREIS, HEF Group, 42162 Andrézieux-Bouthéon, France

³Laboratoire Hubert Curien, UMR 5516 CNRS / Université Jean Monnet, Saint-Etienne,
France

Diamond-Like Carbon coatings are increasingly popular in tribological applications, not only as solid lubricants, but also in combination with lubricant additives for boundary-lubricated conditions. Modern automotive engines are indeed relying on these materials both for wear protection and for friction reduction of severe contacts. Nevertheless, the solid lubrication processes of Diamond-Like Carbon coatings are not fully elucidated: these coatings are usually as hard or harder than most metallic substrates and counterfaces, and yet provide low friction coefficient as soft solid lubricants do. Clearly, surface phenomena are paramount in these peculiar solid lubrication processes, especially tribochemical interactions. Furthermore, wear rates of different DLC coatings in base oil – without lubricant additives – are not necessarily related to the coating hardness, emphasizing the critical role of tribochemistry.

In this study, 3 different DLC have been compared: a hydrogen-free DLC obtained by Pulsed Laser Deposition, and two hydrogenated DLC obtained by Plasma-Enhanced Chemical Vapor Deposition, with respectively 20 at.% and 36 at.% of hydrogen. It is noteworthy that sp^2 content in all these films is expected to be larger than 50%. The effect of hydrocarbon molecules has been evaluated with an environmentally controlled tribometer, allowing to perform experiments from ultra-high vacuum to atmospheric pressure. Linear reciprocating sliding experiments have been conducted with both pin and flat coated with the same DLC coating. Three hydrocarbon gases have been considered, at the same pressure of 10 kPa: C_2H_6 , C_2H_4 and C_2H_2 .

These experiments reveal that the friction coefficient is significantly affected not only by the hydrogen content of the DLC coating, but also by the nature of the hydrocarbon molecule. Furthermore, both wear and triofilm build-up could be observed on the pin wear scars, but in amounts that strongly rely on both coating and hydrocarbon gas nature. The role of tribochemical interactions, and especially the contributions of both hydrogen and sp^2 carbon, will thus be discussed in light of these experiments.

Smoothed Particle Hydrodynamics Simulations of Abrasive Flow Machining

Claas Bierwisch, Christian Nutto, Hanna Lagger, Michael Moseler

MikroTribologie Centrum µTC, Fraunhofer IWM, Wöhlerstr. 11, 79108 Freiburg, Germany

Manufacturing techniques of complex geometries often rely on the precise finishing of surfaces in order to achieve their designated performance. Obtaining the necessary surface roughness and a sufficiently high material removal rate in finishing processes of hard-to-access surfaces remains a great challenge. An example process is abrasive flow machining (AFM), where abrasive suspensions are forced to flow along internal geometries resulting in an abrasive wear on the work piece. In spite of the huge range of applications for this process, the difficulties to adjust the parameters correctly for each work piece geometry prevents its utilization in a greater variety of industrial applications.

We numerically study the process of abrasive flow machining at the scale where the actual interaction between the abrasive grains of the applied suspension and the work piece occurs. We present the development of smoothed particle hydrodynamics (SPH) models for this purpose. Rheological properties of the carrier fluid are included by using the viscoelastic model of Phan-Thien and Tanner [1]. Abrasive grains are modeled as perfectly rigid bodies. Material removal from the ductile work piece is described by the Johnson-Cook flow stress model in combination with a strain-based failure model [2]. The predictive power of the numerical simulations is demonstrated by comparison with experimental studies.

We study the influence of various parameters such as grain shape, fluid viscoelasticity, and work piece temperature on the material removal (Fig. 1). Based on these analyses design rules for abrasive suspensions are discussed.

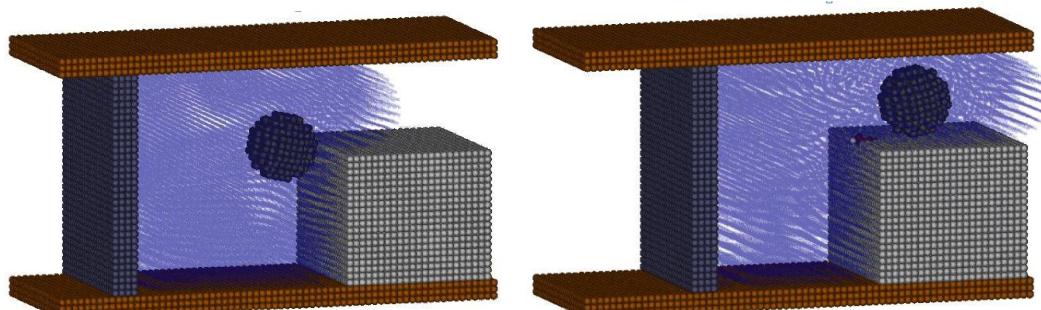


Figure 1: Simulation snapshots of an abrasive grain (dark grey) in a viscoelastic carrier fluid (blue) which removes material from a ductile work piece (light grey).

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Multiscale-Multiphysics Approach to Polyelectrolyte Brush Friction

Hitoshi Washizu^{1,2}, Tomoyuki Kinjo^{1,2}, Hiroaki Yoshida^{1,2}

¹ Toyota Central R&D Labs., Inc., Nagakute, Aichi 480-1192, Japan

²Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, Katsura, Kyoto 615-8520, Japan

The final goal of controlling frictions in automotive tribology may be dependent on the control of forces in the ion atmosphere that surrounds the charged particles or polymers in solution [1]. Not only the static but also the dynamic behavior of the ions in the ion environment is different [2]. Synovial joints are a typical biomimetic system of tribology, which is governed by this force, and the tribological properties of polyelectrolyte brushes have been widely examined as model systems [3].

The Monte Carlo Brownian Dynamics method [4] was used to simulate the nature of polyelectrolyte brushes. For the basic understanding, the effect of linear charge density

on the polyions, added salt, and surface charge on the structure of polyelectrolyte brushes was studied [5]. In order to discuss the friction behaviors in these systems, improvements in the simulator were then needed to include the effect of the solvent in multiscale environments (Fig. 1). First, the solvent model was made to include the solvation effect of polymers and counter- and co-ions. In the framework of dissipative particle dynamics, the polarizability of a set of solvent molecules was described as oscillators [6]. The solvent flow was then included by calculating the Brownian particles by Langevin dynamics and the solvent flows by the Lattice

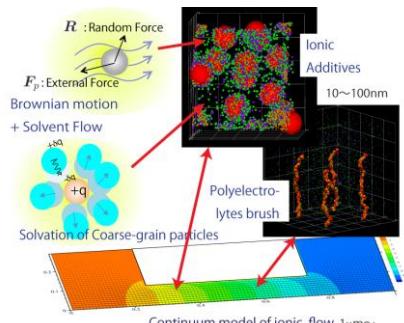


Figure 1: Molecular simulations for ionic systems..

Boltzmann method [7]. In this method, the dynamics of a huge amount of small ions were enabled by treating each Brownian particle as a point described by a Stokes-source.

These methods essentially treat ions as particles. In order to treat macroscopic phenomena, a multiphysical simulator based on continuum equations of ion solvent flow and electric fields was created. The distributions of small ions are treated by the Nernst-Planck equations to determine transitional and nonbulk ion distribution [8]. Whereas these methods are under investigation, the friction of a very complicated tribo-system, which is governed by long-range Coulomb interactions, should be considered before long.

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Instabilities at Frictional Interfaces: Creep Patches, Nucleation and Rupture Fronts

Yohai Bar-Sinai¹, Robert Spatschek², Efim A. Brener^{1,3}, Eran Bouchbinder¹

¹Chemical Physics Department, Weizmann Institute of Science, Rehovot 76100, Israel

²Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

³Peter Grünberg Institut, Forschungszentrum Jülich, D-52425 Jülich, Germany

The strength and stability of frictional interfaces, ranging from tribological systems to earthquake faults, are intimately related to the underlying spatially-extended dynamics. Recent experimental discoveries have revealed rich spatio-temporal dynamics that precede the onset of sliding motion, and occur well below the nominal static friction coefficient. In this talk we will highlight novel features of frictional constitutive laws – most notably a transition from velocity-weakening friction at small slip velocities to velocity-strengthening friction at higher velocities – and theoretically explore their implications on the stability and failure of spatially-extended frictional interfaces. We provide a comprehensive theoretical account, both analytic and numeric, of spatio-temporal interfacial dynamics in a realistic rate-and-state friction model. Slowly extending, loading-rate dependent, creep patches undergo a linear instability at a critical nucleation size, which is nearly independent of interfacial history, initial stress conditions and the frictional behavior at high velocities. Nonlinear propagating rupture fronts – the outcome of instability – depend sensitively on the stress state and velocity-strengthening friction. The rupture fronts are related to steady state fronts solutions and span a wide range of propagation velocities, in some cases much smaller than elastic wave speeds, possibly related to the recently much-debated phenomenon of “slow rupture”. This work provides theoretical tools to aid the understanding of the onset of frictional motion and precursory dynamics within a general continuum-mechanics framework.

Effects of atomic-scale geometry on rough contact

Tristan Sharp, Lars Pastewka, Mark O. Robbins

Johns Hopkins University

Continuum models show that surface roughness can control the contact area, friction, and wear between two contacting solids. Intriguingly, the smallest resolved surface features in the continuum model can play the largest role, but continuum descriptions break down at small scales. Here, we use molecular dynamics simulations to illuminate how atomic scale features on surfaces affect contact properties. Beginning from the established case of continuum linear elasticity that gives a linear relationship between real contact area and load, we systematically introduce atomic-scale physics to determine the affects on normal contact. Replacing an ideal linear isotropic elastic medium with a harmonic atomic lattice produces only small changes in the mechanical response. For more realistic interactions, plasticity increases the contact area when the surface is sufficiently rough. The atomic steps present on crystal surfaces lead to increased plasticity and change the small scale structure of contacts. Depending on the tendency for the material to yield, the presence of steps can increase or decrease the area of very high pressure, but steps always decrease the area of very low pressures. The large scale structure of the contact is the same for all cases.

Rate-dependent contact mechanics of polymer composites

Sam Krop, Han. E.H. Meijer, Lambert C.A. van Breemen

Eindhoven University of Technology, Mechanical Engineering, Polymer Technology,
5600MB Eindhoven, The Netherlands

Polymers play an increasingly important role in tribological applications. This is a challenging subject because of the complex contact conditions involving many variables. Therefore, simplification to a well-defined contact situation is needed: the single-asperity sliding friction test. With this test, a wide range of surface mechanical properties is analysed in a controlled manner. In a previous study a hybrid experimental-numerical approach was employed which revealed the subtle interplay between the constant polymer-indenter adhesion and the velocity/rate-dependent deformation of the polymer during a single-asperity sliding friction test [1]. Understanding and quantifying the polymers' intrinsic mechanical response [2] proved to be key.

In practice, however, most polymers are filled. These fillers are added for many different reasons: e.g. to improve mechanical properties, to change the appearance through colorants, or even to reduce costs by adding a cheaper material in the polymer matrix. These additives have an effect on both the intrinsic mechanical response, and the adhesive interaction with the indenter tip. Consequently, the frictional response of the polymer changes completely.

To characterize the effect of filler particles experimentally, our model materials, i.e. polycarbonate and epoxy, are filled with either hard (TiO_2) or soft (MBS) particles. An identical experimental-numerical approach is used to investigate the response of these model systems. The effect of adding fillers to the polymer matrix is revealed by scratch tests; finite-element simulations reveal the interplay between composite-indenter adhesion and the composites' response to deformation. Adding either soft or hard fillers only results in a change in magnitude of intrinsic mechanical properties like modulus and yield stress. A similar effect is seen for the response in friction; the dependence on scratch velocity does not change, whereas the penetration into the composite changes with filler type and amount.

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Coupled Experiments and Simulations of Atomic Stick-Slip Friction: Effects of Sample Dimensionality and Sliding Speed

R.W. Carpick¹, X.-Z. Liu¹, P. Egberts¹, Z. Ye², Y. Dong³, A. Martini², Q. Li¹, S. Li⁴, J. Li⁵, S.-P. Kim⁶, V. Shenoy¹, J.T. Robinson⁷, P. E. Sheehan⁷

¹Mechanical Engineering and Applied Mechanics, U. Pennsylvania, Philadelphia PA 19104, USA

²School of Engineering, U. California Merced, Merced CA 95343, USA

³School of Mechanical Engineering, Purdue U., West Lafayette IN 47907, USA

⁴Karlsruhe Institut für Technologie, Karlsruhe, Germany

⁵Department of Nuclear Science and Engineering and Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge MA, 02139

⁶Department of Materials Science and Engineering, Brown U., Providence, Rhode Island 02912, USA

⁷Naval Research Laboratory, Washington, D.C. 20375, United States

A gap in our current fundamental understanding of the mechanisms governing nanoscale friction exists, resulting in an ongoing challenge as technologically-relevant mechanical devices are miniaturized, and as the demands for energy-efficient, sustainable technologies increases. Studies combining atomistic simulations and experiments are yielding new insights into the origins of friction, particularly into mechanisms governing atomic-scale stick-slip behavior. As a first example, the behavior of atomic-scale stick-slip friction for truly 2-dimensional materials will be discussed. For nanoscale contacts to graphene, we find that the friction force exhibits a significant dependence on the number of 2-D layers[1,2]. Surprisingly, adhesion (the pull-off force) does not[3]. Our further studies have revealed further complexities that arise from the combined effects of high flexibility and variable substrate interactions that occur at the limit of atomically-thin sheets. Specifically, the pull-off force is determined by a competition between interactions between the tip and the top-most graphene layer, and the graphene- substrate interaction, and also exhibits a sliding history dependence. An even stronger increase in friction occurs when graphene is fluorinated, where experiments and simulations both show that friction between nanoscale tips and fluorinated graphene (FGr) monolayers exceeds that for pristine graphene by an order of magnitude[4]. We attribute this to an entirely different effect: the enhanced corrugation of the interfacial potential due to the highly localized charge at fluorinated sites. The results are consistent with the Prandtl- Tomlinson (PT) model of stick-slip friction. We have also explored the speed dependence of atomic friction between AFM tips and graphene-coated substrates and gold, as there is both experimental and simulation evidence indicating that friction can be significantly affected by the sliding speed in accordance with the thermally-activated (PT) model[5]. However, conclusive evidence linking the variation of friction with sliding speed and thermal activation have not yet been fully developed, largely because experiments have not yet been able to achieve sliding speeds comparable to those attainable in atomistic simulations. We explore the fundamental mechanisms of sliding by conducting matched ultra-high vacuum AFM experiments and molecular dynamics (MD) simulations. All controllable parameters, including tip shape, tip material, sample material, applied load, and mechanical stiffnesses, are matched between experiment and simulation. High experimental sliding speeds are enabled by fast data acquisition coupled with an adapting scanning apparatus. Slower sliding speed simulations are attained using accelerated MD. We will show the first results where scanning speeds in both experiments and simulations are matched, with results compared against the predictions of the thermally-activated PT model.

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Shear-induced Effects in Boundary Film Formation on Copper

Heather Adams, Wilfred T. Tysoe

Department of Chemistry and Laboratory for Surface Studies, University of
Wisconsin Milwaukee, Milwaukee, WI 53211, USA

The formation of a boundary film by reaction with a gas-phase lubricant or lubricant additive formally occurs in several steps that involve the initial adsorption and reaction of the lubricant molecule on the surface, followed by shear-induced decomposition and formation of the boundary film. Fully understanding this sequence of reaction steps will enable the structure of the additive molecule to be related to the nature of the resulting boundary lubricating film. This reaction sequence is explored by examining the surface chemistry of the reactant in ultrahigh vacuum to identify the adsorbed species that form from the molecular precursor. The effect of shear is investigated by carrying out friction measurements using an ultrahigh vacuum tribometer, by analyzing the elemental composition in the wear track region using Auger spectroscopy and by detecting gas-phase products evolved during sliding.

The approach is illustrated using several examples. The first is gas-phase lubrication of copper by dialkyl disulfides and trisulfides. They initially react to form thiolate species on the surface and shear at the interface causes sulfur and some carbon to penetrate the substrate to form a boundary film that reduces friction. The variation in the amount of methane desorbing from the surface per pass during sliding allows the shear-induced rate of thiolate reaction to be measured. This enables models for the shear-induced decomposition to be tested experimentally.

In a second example, the tribological chemistry of borate esters on copper is explored using isopropoxy tetramethyl dioxaborolane (ITDB), and tetramethyl dioxaborolane (TDB) as gas-phase lubricants. TDB decomposes to deposit BO_x species on the surface and produces an initial decrease in friction coefficient that is not sustained. ITDB, which reacts at room temperature to form a surface tetramethyl dioxaborolide species, results in an immediate and sustained decrease in friction coefficient when used as a gas-phase lubricant for copper. Thus, the surface chemistry of the borate esters can be correlated with their tribological properties and illustrates that replacing a hydrogen atom in TDB with a 2-propoxy group in ITDB has a profound influence on both the surface and tribological chemistry.

Friction and wear of nanocrystalline copper

Ao Li¹, Izabela Szlufarska^{1,2}

¹Materials Science Program, University of Wisconsin, Madison, WI

²Department of Materials Science and Engineering,
University of Wisconsin, Madison, WI

Identifying fundamental mechanisms that govern mechanical properties of nanocrystalline materials, such as friction coefficient and wear rate, is critical for rational design of wear-resistant materials. We performed large-scale molecular dynamics (MD) simulations of plowing friction on fcc crystalline Cu surface (25~30 millions atoms) with a rigid SiC tip. We investigated how friction depends on the average grain size (which varied from 5nm to 30nm), on concentration of impurities (Ag), and on plowing depths. Our results show that the friction coefficient becomes larger as the average grain sizes decreases. Interestingly, the friction coefficient first decreases and then increases with increasing Ag concentration. The plowed volume in front of the tip is larger for nanocrystalline Cu than that of a single crystal copper. Deformation mechanisms and microstructural evolution have also been elucidated. Cracks are formed and grow along grain boundaries in the plowed-out material in front of the sliding tip, which might be one of the factors influencing the friction coefficient in addition the grain boundaries sliding and dislocation activity. Pronounced grain growth is observed in the deformed region.

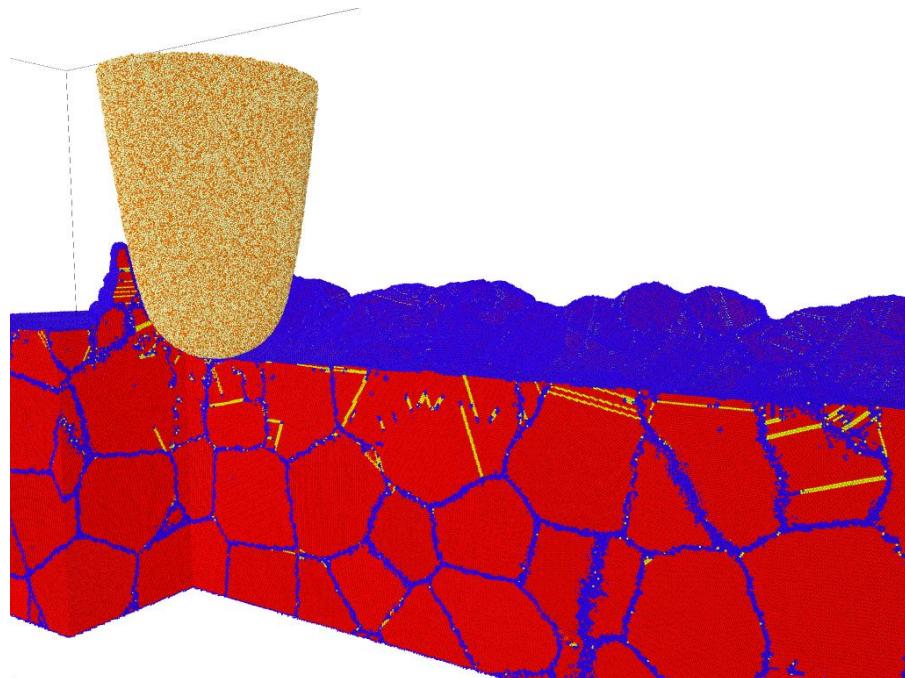


Figure 1 MD simulations of plowing friction on nanocrystalline Cu surface using a rigid SiC tip. The average grain diameter of this sample is 15nm.

Tribological behaviors of C18 fatty acids blended in PAO 4: coupling experimental and computational studies

Sophie Loehle¹, Christine Matta², Clotilde Minfray², Jean-Michel Martin²,
Raphael Iovine¹, Akira Miyamoto³

¹TOTAL, Solaize Research Center, BP22 – 69360 Solaize Cedex, France

²Laboratory of Tribology and System Dynamics, Ecole Centrale de Lyon, 36 Avenue, Guy de Collongue 69134, Ecully Cedex, France

³New Industry Creation Hatchery Center Industry, Tohoku University, 6-6 Aoba, Aramaki, Aobaku, Sendai 980-8579, Japan

In the automotive industry, the control of friction and wear by the lubricant in thermal engines is one of the most important issues for fuel economy. Therefore, it is needed to better understand the nature of tribochemical reactions and competition of additives in the formulated lubricant in order to design and develop better lubricants that also address environmental requirements.

Therefore, the lubrication mechanism of fatty acids is revisited with a new approach combining experimental and computational chemistry studies. The lubricating properties of single and mixtures of stearic, oleic and linoleic acids in a synthetic Poly-Alpha-Olefin base oil (PAO4) on iron oxide surface are investigated under mixed boundary regime with temperatures from 50°C up to 150°C.

Experimentally, low friction coefficient (about 0.055) with no visible wear is reported in presence of single stearic acid at high temperature. This lubricating behavior is inhibited in presence of unsaturated fatty acids highlighting an anti-synergic effect of a saturated/unsaturated mixture, especially at 150 °C as shown in figure 1 [1].

To understand the anti-synergic effect and the adsorption mechanism of these molecules, Molecular Dynamic (MD), Quantum Chemistry (QC) and Ultra-Accelerated QCMD [2] simulations are performed to evaluate their diffusion coefficient in PAO4 and their adsorption mechanism on iron oxide surface at different temperatures. MD simulation results show a faster diffusion towards the surface for unsaturated fatty acids than for saturated fatty acid at all the studied temperatures. This means that unsaturated molecules arrive and mainly adsorb before stearic acid on the surface leading to a tribological behavior of the mixture characteristic of the unsaturated molecule. Computational chemistry suggests that all fatty acids (saturated and unsaturated) adsorption mechanism is due to the chemisorption of the carboxylic group on iron oxide surface with no desorption up to 150°C [1].

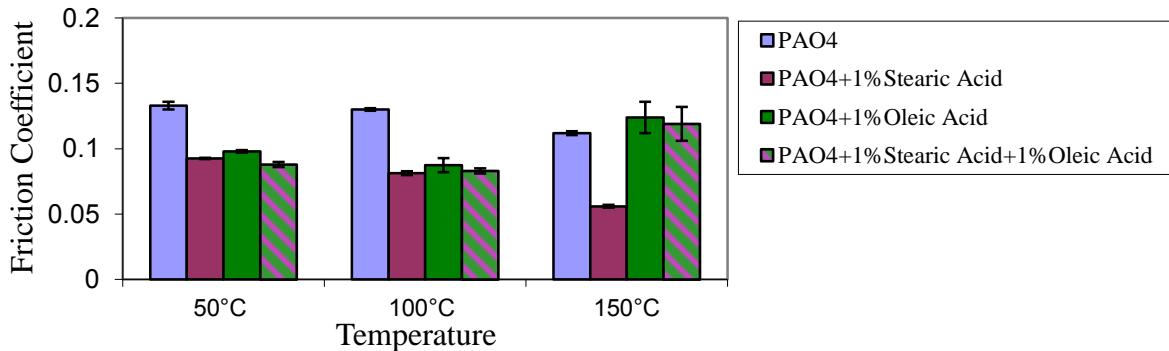


Figure 1: Steady-state friction coefficient versus lubricant mixtures on an AISI 52100 steel surface at 50, 100 and 150 °C

[1] Loehlé S et al. *Tribology Letters* 53 (2014) 319-328

[2] Md. Korshed Alam et al. *Catalysis Today* 164 (2011) 9–15

Shear accommodating third body layers between metallic nano-asperity contacts

Pedro A. Romero^{1,2}, Tommi T. Järvi^{1,2}, Nils Beckmann^{1,2}, Michael Moseler^{1,3,4}

¹Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstraße 11,
79108 Freiburg, Germany

²Karlsruhe Institute of Technology, Institute for Applied Materials IAM, Kaiserstraße 12,
76131 Karlsruhe, Germany

³K Freiburg Materials Research Center, Stefan-Meier-Straße 21,
79104 Freiburg, Germany

⁴University of Freiburg, Physics Department, Hermann-Herder-Straße 3,
79104 Freiburg, Germany

Tribological shearing of polycrystalline metallic surfaces typically leads to grain refinement and amorphization near the sliding interface. Therefore, one might expect this behavior to persist as the grain size is reduced to a few nanometers until an amorphous phase is established. Using atomistic nanotribology models [1], we show that for system with sufficiently large initial grains (> 100 nm), grain refinement is indeed observed. Similar for alloy like system with large degrees of impurities, amorphous third body layers are formed. Here, however, we demonstrate that for highly pure nanocrystalline counter bodies with grain level surface roughness; grain growth and cold welding is the preferred atomic structure evolution at the sliding interface as this leads to more deformable third body layers (see figure 1). Through large scale (spatial and temporal) atomistic simulations, we show that in the case of nanocrystalline iron (with grain size ~ 25 nm), the contacting surfaces employ the shear energy introduced by the sliding motion to move grain boundaries and to reorient, rotate and elongate grains in order to create a coarsened third body layer with the $\langle 111 \rangle$ bcc packed direction aligned with the shearing direction. The enlarged reoriented interface grains are then capable of accommodating the sliding motion and deformation through dislocation and twin boundary nucleation and propagation. Shear bands and dynamic twin boundaries, oriented along the sliding direction and traveling perpendicular to the sliding motion within the coarsened grain region, enable the creation of shear planes which accommodate the sliding motion.

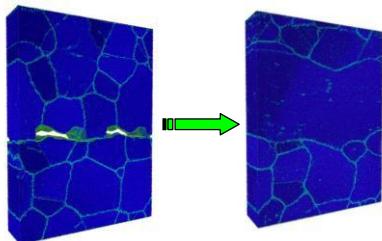


Figure 1: Coarsened third body layer formation between iron nanocrystalline asperity contacts.

Much of the simulation work was performed at the Jülich Super Computing Center. The authors acknowledge useful discussions with Matous Mrovec.

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Atomistic Modeling and Simulation of Mechanical and Sliding Properties of Cu-S and Cu-Fe-S Crystal Systems

Ken-ichi Saitoh¹, Tomohiro Sato², Yoshimasa Hirai², Masanori Takuma¹, Kengo Otsu¹

¹Department of Mechanical Engineering, Kansai University, 3-3-35 Yamate-cho, Suita, Osaka 564-8680, Japan

²Kurimoto Ltd., 2-8-45 Shabatani, Suminoe-ku, Osaka 559-0021, Japan

Today, from consideration of environment, the use of lead is strictly disabled in industrial materials for sliding equipments, and so copper (Cu) alloy material including sulfur (S) is known to be a prospective replacement especially for a heavy-load bearing and so on. It is experimentally confirmed that a microstructural precipitation of copper-sulfide (Cu_2S) is one of causes for good lubrication[1]. However, the atomistic structure and mechanism which will provide good lubrication is yet to be clarified. We construct an atomistic simulation model of Cu_2S crystal where the materials are contacting and sliding each other with a large compressive load, for the purpose of obtaining the knowledge about the atomic behavior. First, we perform a structural optimization using DFT (Density Functional Theory) calculation-software (Wien2K) to determine the lattice constants and bond angles in hexagonal unit of periodic Cu_2S crystal. These quantum-mechanics-based parameters are applied to the construction of an interatomic potential of Cu-S system including pairwise and angular terms[2]. Then, we conduct classical molecular dynamics

(MD) simulations of shearing of Cu_2S hexagonal crystal on its basal plane in several different temperatures and pressures. Consequently, it is recognized that, in sliding condition, Cu_2S crystal exhibits not a simple crystal slip, but a complicated bond-switching mechanism or crystalline disordering (amorphization). Besides, the higher the sliding velocity is, the larger the shear stress becomes, which is understood as a typical behavior in flowing liquid.

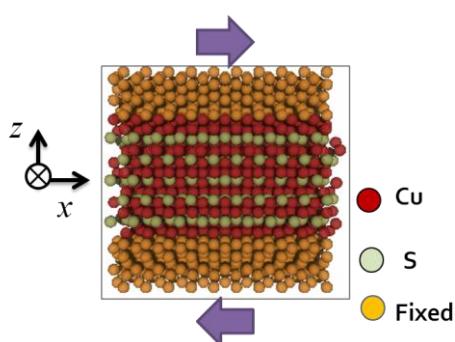


Figure 1: Molecular dynamics simulation of hexagonal Cu_2S crystal structure in shearing and sliding, using a DFT-based interatomic potential.

We study also on the Cu-Fe-S system, where the “bornite” crystal appears as one of actual precipitates. The crystalline structure and mechanical properties of the bornite are investigated here. The DFT results show a clear difference in chemical bond state owing to inclusion of iron atoms.

This work was supported by the New Energy and Industrial Technology Development Organization (NEDO) of Japan.

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Multiscale Modeling of Surface Texture Effect on Hybrid Bearing

Shiyuan Pei, Yu Xing, Wei Chang, Xu Hua

School of Mechanical Engineering, Xi'an Jiaotong University,
Xi'an, Shaanxi 710049, China

It is difficult to determine how the multiscale texture influences the performance of hybrid bearing. On the one hand, because of the journal eccentricity, the height profile of the texture becomes non-periodic in circumferential direction, which makes a number of multiscale methods incapable of solving the problem; On the other hand, hybrid bearing has complex boundary conditions, such as shallow/deep recess, resistor, cavitation, which makes the corresponding equation even more difficult to solve. To the best of author's knowledge, none of multiscale methods has successfully solved the texture-hybrid-bearing lubrication problem.

In this study, we advance a deterministic multi-scale computation method, proposed in ref. [1], to calculate the hybrid-bearing performance with non-periodic textures profile under complex boundary condition. A novel reduction method based on substructure and a two-step condensation technique are employed to handle the nonperiodicity, which simplifies the problem size from 2D to one column. The proposed method has been implemented for a hybrid bearing, which has 4 resistors and 4 grooves. The eccentricity ratio is 0.3, as shown in Fig. 1. Furthermore, the cavitation effect has taken in to account by the implement of Swift-Stieber boundary condition. The total number of textures is 352 textures (32 columns in circumferential direction whereas 11 rows in axis direction, both uniformly distributed, as shown in Fig. 2). Each texture was meshed by 60×60 elements, so the total system nodes number are 1.3×10^6 . The calculation was conducted using MATLAB with 2.8 GHz CPU and 4 GB RAM, and the pressure distribution is shown in Fig 3. It takes less than 1 minute to solve this multiscale problem, which indicates that the proposed method is a high efficient way to solve the non-periodic problems under complex boundary conditions.

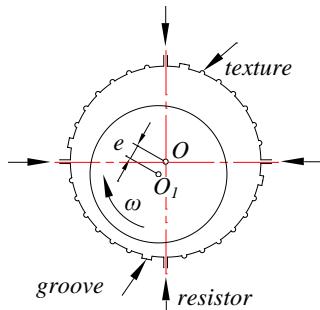


Fig.1: Schematic of the textured hybrid bearing

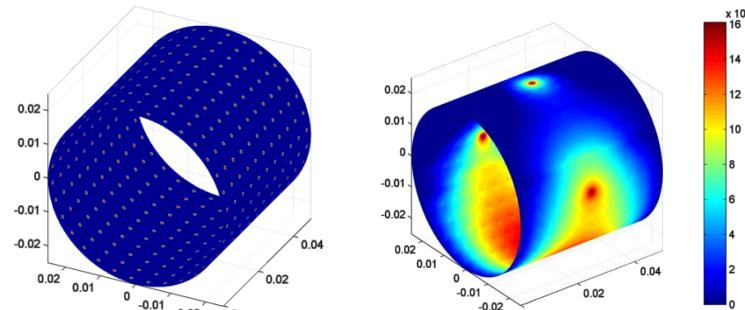


Fig.2: Schematic of the texture distribution

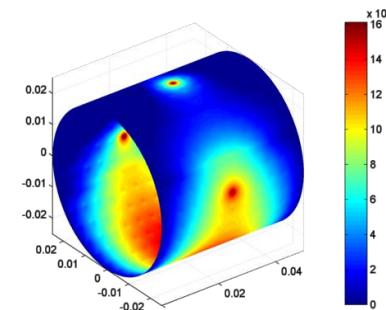


Fig.3: Pressure Distribution of the textured Hybrid Bearing

We gratefully acknowledge the National Basic Research Program of China (2009CB724404) and (No. 2011CB706601) of their financial support on this research.

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Multi-physical contact between elastic and elasto-plastic solids with fractal surfaces

Vladislav A. Yastrebov¹, Guillaume Anciaux², Frederick S. Mballa Mballa^{1,3}, Georges Cailletaud¹, Jean-François Molinari², Henry Proudhon¹, Frédéric Houzé³, Sophie Noël³, Philippe Teste³

¹Centre des Matériaux, MINES ParisTech, CNRS UMR 7633, Evry 91003, France

²Computational Solid Mechanics Laboratory (LSMS, IIC-ENAC, IMX-STI), Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne 1015, Switzerland

³Laboratoire de Génie Electrique de Paris (LGEP), UMR 8507 CNRS-Supelec, UPMC and Paris-Sud Universities, Gif sur Yvette 91192, France

We study the mechanical and physical properties of the normal contact between solids with fractal surfaces. Both experimental and synthetic surface topographies are investigated. To solve the mechanical boundary value problem with contact constraints we use the finite and boundary element methods as well as a simple asperity based model with interactions [1].

Properties of rough surfaces (spectrum breadth [2,4] and Gaussianity [3]) and their effect on mechanics of contact are discussed. We study the evolution of the true contact area [3,4], probability density of contact pressure at the interface, topography of the free volume and topology of contact clusters. We also carry out an extensive comparison with analytical models and numerical results of other groups. We consider both elastic and elasto-plastic material models (the later within a large deformation formalism); a special focus is put on the transition between these two deformation regimes.

Next this work is extended to take into account multi-physical phenomena, namely (i) the fluid flow through the free volume in the contact interface, and (ii) the electric and heat transfer through contact clusters. These extensions are done within the finite element framework.

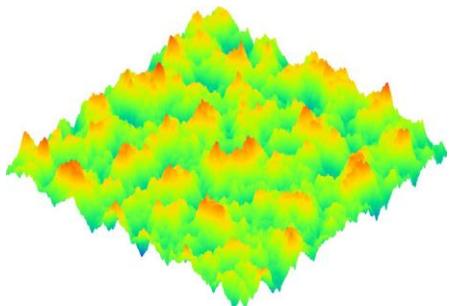


Fig. 1: Synthetic rough surface

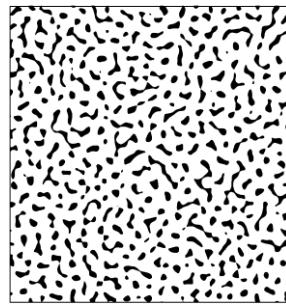


Fig. 2: Contact clusters for a surface with small spectrum breadth

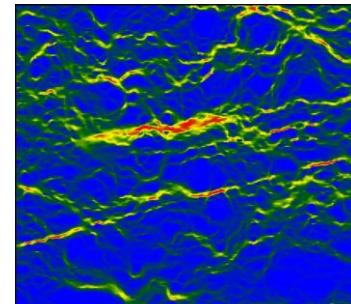


Fig. 3: Fluid flow through the contact interface between elasto-plastic solids

GA and JFM greatly acknowledge the financial support from the European Research Council (ERCStg UFO-240332). VY, FSMM, HP, GC, FH, SN and PT acknowledge the financial support of the Labex LaSIPS.

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Wear, plasticity, and rehybridization in tetrahedral amorphous carbon

T. Kunze¹, M. Posselt², S. Gemming², G. Seifert¹, A. R. Konicek³, R. W. Carpick³, L. Pastewka⁴, M. Moseler⁴

¹Theoretical Chemistry, University of Technology Dresden, D-01662 Dresden, Germany

²Helmholtz-Zentrum Dresden-Rossendorf, P. O. Box 510119, D-01314 Dresden, Germany

³Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, PA 19104, USA

⁴Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstrasse 11, D-79108 Freiburg, Germany

Wear and friction in self-mated tetrahedral amorphous carbon (ta-C) films is studied by molecular dynamics and compared to results of near-edge X-ray absorption fine structure spectroscopy. The simulations demonstrate the formation of a soft amorphous carbon (a-C) transfer layer with increased sp^2 content, which grows faster than the a-C tribolayer found on self-mated diamond sliding under similar conditions. The faster $sp^3 \rightarrow sp^2$ transition in ta-C is explained by easy breaking of prestressed bonds in a finite, nanoscale ta-C region, whereas diamond amorphization occurs at an atomically sharp interface. A detailed analysis of the underlying rehybridization mechanism reveals that the $sp^3 \rightarrow sp^2$ transition is triggered by plasticity in the adjacent a-C. Rehybridization therefore occurs in a region that has not yet experienced plastic yield. A detailed characterization of the a-C transfer layer reveals the absence of well-ordered graphitic structures. The resulting soft a-C tribolayer is interpreted as a precursor to the experimentally observed wear.

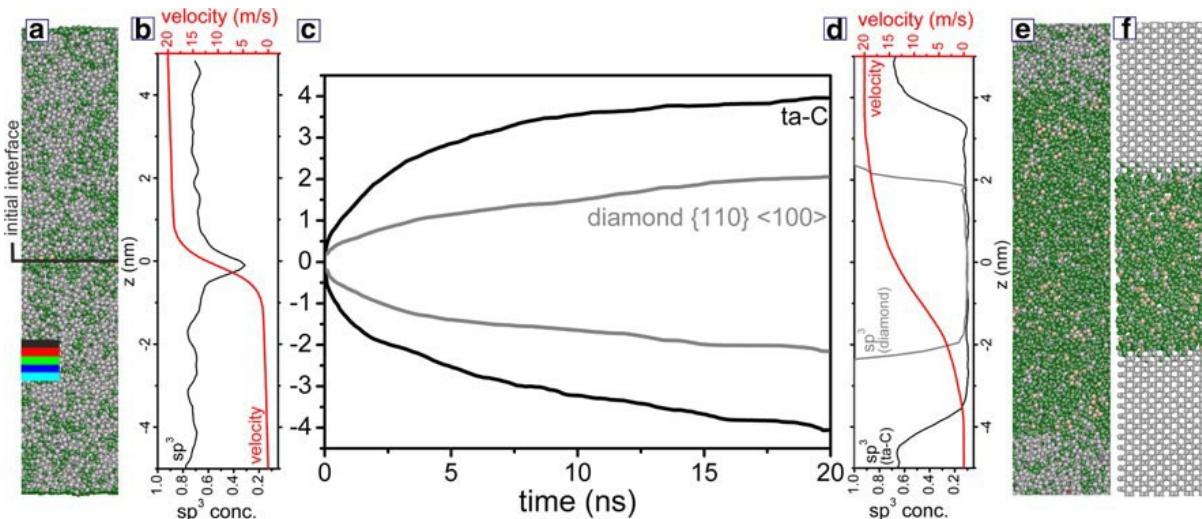


Figure 1: (a) side-view snapshot of the ta-C/ta-C tribosystem after 0.1 ns of sliding. Atoms are color-coded according to their atomic coordination: white – sp^3 , green – sp^2 , yellow – sp^1 , (b) sp^3 concentration (black curve) and velocity profile (red curve) across the ta-C/ta-C tribocouple, (c) evolution of the upper and lower boundary of the a-C tribofilm formed between two ta-C surfaces (black curve) compared to a corresponding film formed between two diamond {110} surfaces rubbed in $<100>$ direction (gray curve), (d) sp^3 concentration (black curve for ta-C and gray curve for diamond) and velocity profile of the ta-C system (red curve) after 20 ns of sliding, (e) and (f) are side-view snapshots of the ta-C/ta-C and diamond/diamond tribosystems after 20 ns sliding.

Quantifying touch-feel perception: Tribological Aspects on a new artificial finger design

Hui Niu¹, Xianping Liu¹, Hin Kwan Wong²

¹School of Engineering, University of Warwick, Coventry CV4 7AL, UK

²Warwick Manufacturing Group, University of Warwick, Coventry CV4 7AL, UK

The human skin tribology is a research topic that has continuously attracted scientific studies over the past years. It has applications in enabling the sense of touch in robotics and enhancing touch-feel ergonomics in products [1]. Artificial fingers are able to characterise surface roughness by emulating the ability of human fingertip to sense friction.

To mimic human finger doing so by stroking on the object this, an artificial finger is combined with a linear flexure mechanism and a reciprocal stage to form a friction measurement device. By measuring the contact force and friction force simultaneously, the friction coefficient can be calculated and therefore the surface roughness characterised. This paper continues on earlier work [2] on the friction measurement device and presents a new design capable of measurement profiles closely matching that obtained from a human finger. In the original setup in [2], the friction coefficient was measured manually by applying pressure on the test material with a finger.

However, this friction measurement rig was extremely sensitive to the humidity of the human fingertip and may become inconsistent if the test were not performed in one sitting. The original design was later improved by addition of a roller-on-block structure in order to replace the human finger and therefore reduce the variance of the applied contact force [2]. The rollers were made of steel, brass and silicone rubber materials whose Young's moduli were close to that of a human fingertip.

The current artificial fingertip design used in this paper (Fig. 1) has a multi-layered construction comprising of the cover layer and the filler layer, both made of silicone rubber with different hardness, and an internal bone support structure made of aluminium. Instead of having a roller mechanism, the artificial finger is fixed on a linear stage that enables a reciprocating back-and-forth motion more representative of human touch movement. Experimentation was carried out to measure surface frictions of aluminium and steel plates with different roughness, under different contact forces and different stroking speeds. High correlations ($R=0.85\sim0.98$) between artificial finger friction measurements and those obtained by human finger were observed for the steel samples and the milled aluminium samples.

The results show that the artificial finger can be very close to the human finger in terms of the friction sensing characteristics. The results also indicate that in the low roughness range, the friction coefficient decreases as the contact force increase, but the difference is slight in the high roughness range. Finally, the measured friction coefficient increases with the linear stage sliding speed.

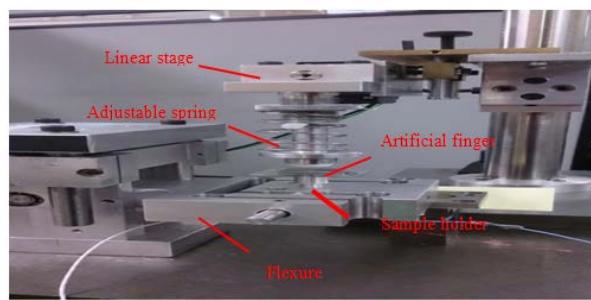


Fig.1 The artificial finger set up with the linear stage

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Multiscale estimating technique of rubber friction on surface asperities depending on sliding velocity

Hiro Tanaka¹, Kimiyasu Yoshimura¹, Junpei Aramaki¹, Satoshi Izumi¹, Shinsuke Sakai¹, Hiroshi Kadowaki²

¹University of Tokyo, 7-3-1, Hongo, Bunkyo-Ku, Tokyo, Japan

²Bridgeston Corporation, 3-1-1, Ogawahigashi-Cho, Kodaira-Shi, Tokyo, Japan

According to Persson's statement [1][2], the friction coefficient of a rubber is mainly determined by both the rubber's viscoelasticity and the surface property on multiscale asperities which can be represented by surface roughness power spectrum (SRPS). In this study, we conduct friction testing for a carbon filled rubber sliding on dry surface asperities. Based on the experiment results, we estimate the net friction coefficient related to energy dissipation resulting from cyclic deformations of the rubber, which derived from the Persson's mathematical model.

The friction coefficient developed by Persson [1] reads

$$\mu_{\text{Persson}} = \frac{1}{4\pi} (q_0 h_0)^2 H \int_1^{q_1/q_0} d\zeta \zeta^{-2H+1} P(\zeta) \int_0^{2\pi} d\phi \cos \phi \operatorname{Im} \frac{E(\zeta q_0 v \cos \phi)}{(1-v^2)\sigma_0} \quad (1)$$

In our procedure, the Hurst exponent H and roll-off wavelength q_0 were obtained by the measured SRPS (see Fig. 1), and the complex elastic modulus E was represented by the generalized Maxwell model identified by the viscoelasticity measurement of a rubber specimen. In Eq. (1), the cut-off wavelength q_1 is known as a free parameter. Hence we determined q_1 so that the velocity dependency of μ_{Persson} agreed well with that of μ_{exp} measured by the friction test. Figure 2 shows the μ - v curves: the solid line indicates the experiment value and the dashed line does the value of μ_{Persson} estimated from the relationship of $\mu_{\text{Persson}} \approx \mu_{\text{exp}} - \mu_{\text{offset}}$, assumed that μ_{offset} doesn't depend on sliding velocity.

The part of this work was supported by the Japan Society for the Promotion of Science under the grand-in-aid for scientific research (B) (JSPS KAKENHI Grand No. 24360044).

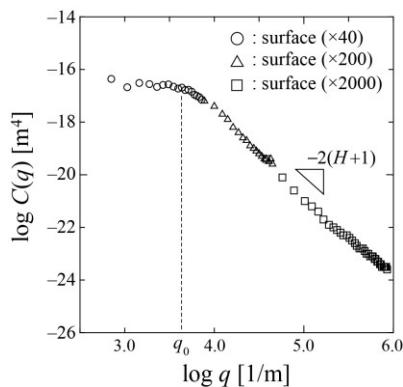


Figure 1: Surface roughness power spectrum measured by a laser microscope.

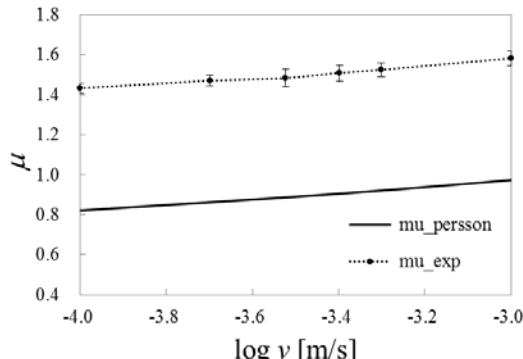


Figure 2: μ - v curves: the experiment value and the net value estimated using Eq. (1).

[1] B.N.J. Persson, J. Chem. Phys. **115**, (2001), pp. 3840–3861.

[2] B.N.J. Persson et al., J. Phys.: Condens. Matter. **17**, (2005), R1–R62.

Nanoindentation and wear of graphene-covered surfaces

Andreas Klemenz¹, Lars Pastewka¹, Michael Moseler^{1,2}

¹Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstr. 11, 79108 Freiburg, Germany

²University of Freiburg, Physics Department, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

Graphene has the highest stiffness and the highest breaking strength that have ever been measured in an experiment [1]. If these properties could be transferred to the surface of a soft material, graphene could be used as the thinnest possible protective coating. Usage of graphene for this purpose requires a deep understanding of its influence on wear and tribological processes. Since all relevant processes take place on an atomic length scale, atomic force microscopy is usually used for experimental investigations. Such studies can give basic insight into the system behavior, but detailed analyses are often difficult.

Details of the setup like the surface roughness of the indenter cannot be controlled but can have a strong influence on experimental results. Roughness has a considerable influence on the stress distribution under the tip [2] and can modify the result of a work of adhesion measurement by more than an order of magnitude [3]. Apart from this, it is often not possible to perform an indentation and simultaneously observe the surface. In the special case of a graphene-covered surface, it is therefore difficult to tell, if the graphene has ruptured at a certain point and which signature in a force penetration curve indicates graphene rupture.

In atomistic simulations, the setups can be controlled exactly and every interesting property of the material can be monitored simultaneously. In this work, we therefore use quasistatic simulations of indentation processes. We use platinum as a model for soft surfaces and investigate the behavior of Pt (111) surfaces coated with single layers of graphene when indented with rigid tips. Since the relevant processes can be rather slow, we use a quasistatic approach as a model for infinitely slow indentations. We vary the size and shape of the indenter and discuss the influence of graphene coatings on the hardness of the surface. Finally we compare our results with those of an experimental study.

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Seamless elastic boundaries for atomistic calculations

Lars Pastewka¹, Tristan A. Sharp², Mark O. Robbins²

¹Fraunhofer IWM, ²Johns Hopkins University

The elastic response of an infinite bulk crystalline solid with a free surface can be renormalized into a linear operator, the surface Green's function that acts on the surface's degrees of freedom only [1]. We here present general transfer matrix and renormalization group formulations that allow the computation of the elastic surface Green's function from the knowledge of the interatomic interaction [2]. Our approach naturally allows a treatment of multi-atom unit cells that are necessary to couple a renormalized substrate to a full atomistic system that interacts via long-ranged forces. The substrate interaction is treated exactly up to harmonic order and the full system comprising atomistic and elastic boundary regions is described by a single Hamiltonian. This concurrent multi-scale coupling enables simple, seamless semi-infinite elastic boundary conditions for atomistic simulations where near-surface deformations occur, such as nanoindentation, contact, friction, or fracture. We demonstrate this method on problems from contact mechanics and tribology.

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Improving Estimates of Fretting Wear Rates through Microscale Simulations

Areg V. Hayrapetian¹, Michael J. Demkowicz²

¹Department of Mechanical Engineering, Massachusetts Institute of Technology,
Cambridge, Massachusetts 02139, USA

²Department of Materials Science and Engineering, Massachusetts Institute of
Technology, Cambridge, Massachusetts 02139, USA

Fretting wear is a problem that comes up in many engineering applications. Work-rate models, such as Archard's law [1], with constant empirical wear coefficients are commonly used to estimate wear rates for most wear applications. Their shortcoming is that they cannot describe wear under conditions that may change the wear coefficient. To improve on the work-rate model, a model of fretting wear is needed that can simulate wear mechanisms at the micron length scale. This goal necessitates simulation methods capable of modeling elasticity, fracture, contact, generation of wear debris, and tracking and contact interaction of the third-body wear debris particles.

We present work in progress on a new modeling framework with these capabilities. This modeling framework allows for simulations of the fretting wear mechanics at the micron length-scale such as the fracture of asperities on two sliding brittle surfaces. A snapshot of a preliminary simulation of this type completed on a small-sized system can be seen in Figure 1. Similar simulations on larger systems will allow us to better understand the behavior of fretting wear as a function of parameters such as the normal contact load, slip amplitude of the oscillatory sliding, surface roughness, and type of fretting motion. The results of these simulations will be used to construct a wear mechanism map for fretting

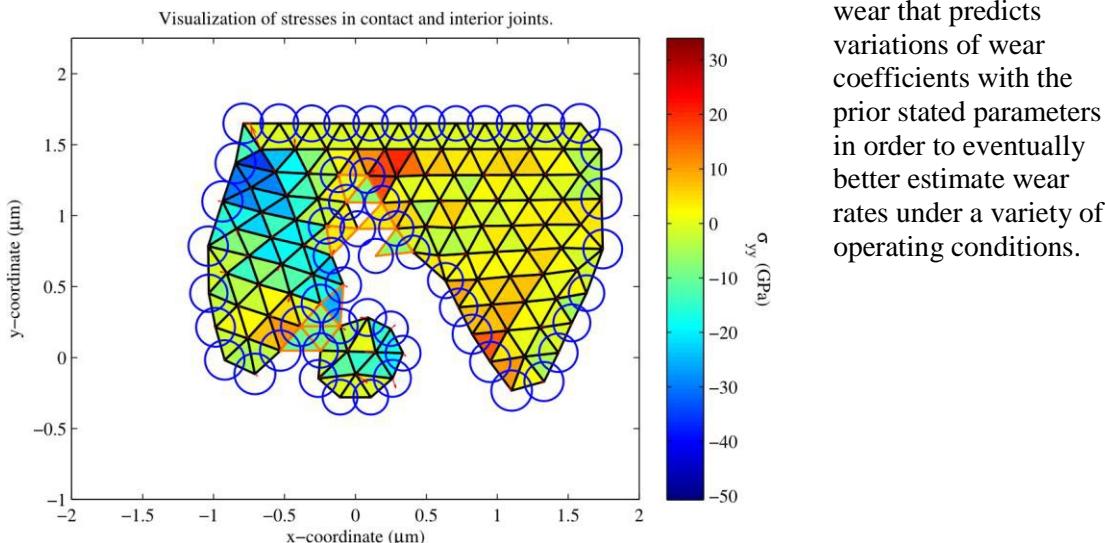


Figure 1: Snapshot of asperity fracture simulation.

This project was supported by the Consortium for Advanced Simulation of Light Water Reactors (CASL): a Department of Energy (DOE) Energy Innovation Hub.

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Theoretical modeling and molecular dynamics simulation of atomic scale wear: A combined study

Yuchong Shao, Michael L Falk

Johns Hopkins University

Frictional running-in and material transfer in wear take place at the micro- and nano-scale but the fundamental physics remains unclear. In recent years, various mechanisms including cluster-detachment process and atom-by-atom attrition have been reported in simulation and experimental work.

Here we propose a multi-bond dynamics model based on Filippov et al [Phys. Rev. Lett. 92, 135503 (2003)] that qualitatively captures those two distinct behaviors under a unified theoretical framework. In the model, the interfacial bond formation, rupture and wear are depicted as three competing thermally activated processes. We demonstrate that depending upon the external normal stress and sliding rate, different regimes of wear behavior exhibited in such a model.

To test this theory we perform molecular dynamics simulation of a silicon-based AFM and quantified the rate of material transfer as a function of the coverage of non-bridging oxygen atoms, which has a pronounced change of the system's tribological and wear behaviors. Results show that adhesive wear takes place across the interface in an atom-by-atom fashion which remodels the tip. Comparisons to experimental data and other wear simulations are also discussed.

Multiscale Modelling for Atomic Force Microscopy

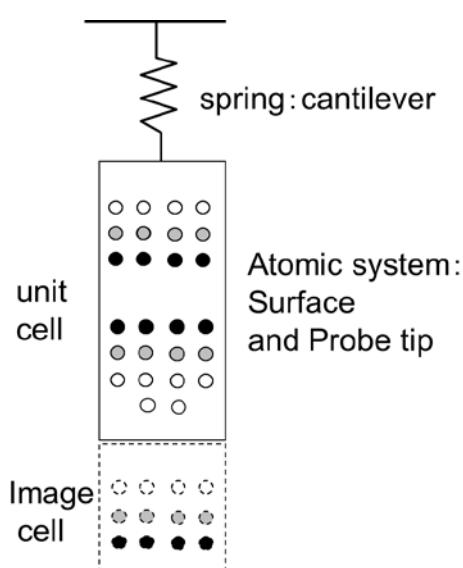
Yasuhiro Senda¹, Shuji Shimamura¹, Janne Blomqvist², Risto Nieminen²

¹Department of Applied Science, Yamaguchi University, Yamaguchi, 755-8611, Japan

²COMP Centre of Excellence, Department of Applied Physics,
Aalto University, P.O. Box 11100, 00076 Aalto, Finland

Atomic Force Microscopy (AFM) is promising tool capable to providing atomic resolution images for a variety of materials. The macroscale cantilever of the AFM is oscillated in macroscale time on the surface and its resonance frequency is changed by the atomic interaction between the tip of the cantilever and the surface. The multiscale behavior of the macroscopic motion of the cantilever and the atomic interaction between the tip and the surface provides the atomic resolution image of the AFM experiment. In addition to the change of resonance frequency, the oscillation of the cantilever is damped and this energy dissipation also offers a structural atomic image. The origin of the energy dissipation, however, has been the subject of debate over the past decade.

We propose a multiscale model of the AFM using a coupling method of molecular dynamics (MD) and continuum in order to investigate mechanism of the observed energy dissipation of the AFM experiment. The motion of cantilever is described by a spring, and the atomic interaction between the tip attached on cantilever and surface is calculated by MD method as shown in the below Figure. The motions of the spring and atoms are concurrently coupled by the MD/continuum hybrid method [1,2]. The Lennard Jones potential is used as the inter-atomic interaction.



The energy dissipation of the spring (cantilever) is calculated using the above multiscale model, and the calculated dissipation on each atomic site of the surface for Lennard Jones crystal can provide the atomic image of the surface. The mechanism of the energy dissipation in the present AFM model will be explained and discussed.

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Figure: Schematic view of the multiscale model for AFM. Lennard Jones atoms are drawn by circles. Atoms drawn by solid circles are fixed.

**Density Functional Study of Gold-Coated Iron Nanoparticles
(Potential for Medical Applications)**

Eyachew Misganew

Debre Tabor University, Ethiopia

In this paper, the first principle studies on the ground state structure, binding energy, and magnetic moment of gold-coated Fe_n , bare Fe_n , and their oxides, Fe_nO_2 have been carried out within a density functional formalism. The first systematic theoretical study of gold-coated iron nanoclusters, aiming at understanding the magnetic properties of this core-shell structure used in biomedical applications. The calculations based on density-functional theory focus on the effect of gold coating on the magnetic and structural properties of iron clusters of various sizes, and the reaction of the bare iron clusters with oxygen. My results show that the magnetic moment of iron nanocore with gold coating is still significantly higher than that in bulk Fe; the coupling between Fe atoms remained ferromagnetic. The improved chemical stability by gold coating prevents the iron core from oxidation as well as the coalescence and formation of thromboses in the body. Thus, it is shown that gold coating is very promising for the magnetic particles to be functionalized for targeted drug delivery. The ground states of Fe_n clusters have a magnetic moment of around $2.94 \mu\text{B}$ per atom. The O_2 molecule is found to be dissociatively absorbed and its most significant effect on spin occurs in Fe , Fe_2 , Fe_5 and Fe_6 , where FeO_2 , Fe_2O_2 , Fe_5O_2 , and Fe_6O_2 show antiferromagnetic spin arrangements, respectively.

Computational Chemistry Study on Resin/Metal Interface: Triboochemical Reaction and Its Effect on Friction

Tasuku Onodera¹, Kenji Kawasaki¹, Takayuki Nakakawaji¹, Yuji Higuchi², Nobuki Ozawa², Kazue Kurihara³, Momoji Kubo²

¹Hitachi, Ltd., Hitachi Research Laboratory, 7-1-1 Omika-cho, Hitachi 319-1292, Japan

²Fracture and Reliability Research Institute, Graduate School of Engineering, Tohoku University, 6-6-11 Aoba, Aramaki, Aoba-ku, Sendai 980-8579, Japan

³WPI-Advanced Institute for Materials Research & Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan

Polytetrafluoroethylene (PTFE) is a useful bearing material because it shows a low friction when rubbed against metallic surfaces. However, the tribological performance of PTFE is strongly influenced by its working environments such as humidity; wear amount is increased under low humid condition. Therefore, it is necessary to develop a novel PTFE composite material for use as bearing under dry condition. For this purpose, the mechanism of chemical interaction on PTFE/metal interface should be worked out. In this study, a computer chemistry approach was adopted for revealing the chemical phenomena at PTFE/metal interface. A tight-binding quantum chemical molecular dynamics method was used to observe the triboochemical reaction between PTFE and metallic surface. The model is shown in Figure 1(a) and is consisted of crystalline PTFE and aluminum oxide terminated partially by some hydroxyl (OH) groups. Figure 1(b) shows the final structures of this system, and a bond dissociation reaction between carbon and fluorine atoms was observed. Moreover, the bond formation reaction was found in which the dissociated fluorine atom bonded to a bare aluminum atom. The results indicate that PTFE triboochemically reacts with a aluminum surface to form aluminum fluoride as a product. The subsequent chemical reaction with environmental gaseous molecule and the effect of the unveiled reactions to the tribological property will be presented in our presentation.

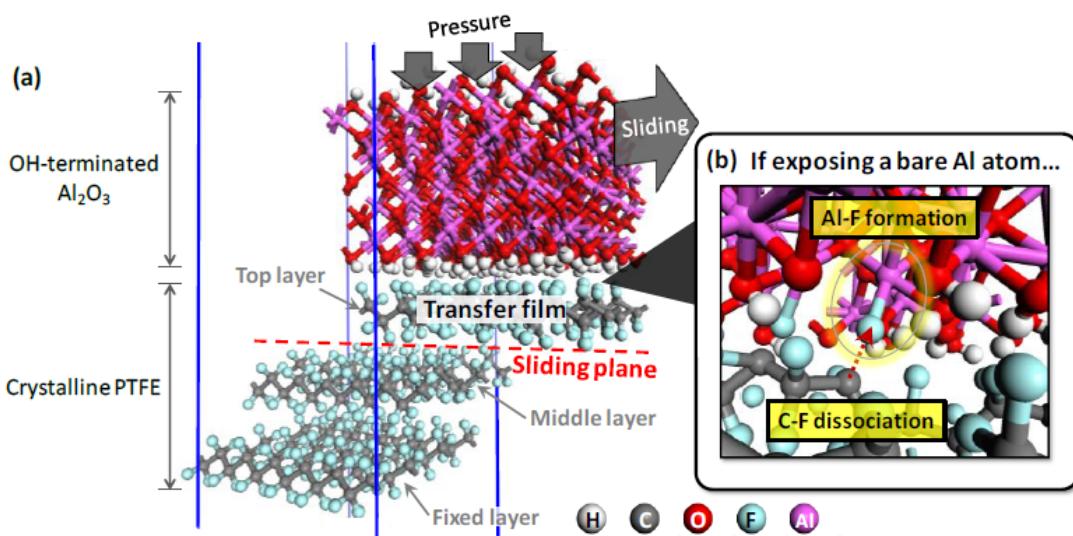


Figure 1: (a) Model structure during friction process, and (b) the triboochemical reaction.

Piston pin lubrication

Hannes Allmaier¹

¹Virtual Vehicle Research Center, Graz, Austria

Of all moving parts in the internal combustion engine (ICE) that can be investigated in terms of friction and lubrication, the piston pin represents a unique challenge [1]. Due to its floating movement, extreme temperatures and oil mist lubrication, this part works not only under extreme operating conditions, but is also very difficult to describe numerically. Being not fixed on any end, the piston pin is free to move, only driven by the lubricant film, which, however, is also unknown at the beginning.

A simulation method is developed that considers the thermal deformation of the piston and the piston pin and incorporates an extensive rheological model for the lubricant [2]. With this model it is possible to describe the lubricant film and with it the friction and movement of piston pin accurately as direct comparisons to experimental data show. In the following it can be used to develop measures to ensure a better lubrication of this critical part.

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Roughness induced hysteretic behavior of adhesive contacts

Giuseppina Recchia¹, Elena Pierro², Giuseppe Carbone¹

¹Dipartimento di Ingegneria Meccanica e Gestionale, Politecnico di Bari, v.le Japigia 182, 70126 Bari - Italy

²Scuola di Ingegneria (SI - UniBas), Università degli Studi della Basilicata, Campus di Macchia Romana - Via dell'Ateneo Lucano 10, 85100 Potenza – Italy

In this paper we investigate the adhesive contact between a rubber block and rigid randomly rough profiles (Figure 1), in loading and unloading conditions. The roughness is assumed to be described by a self-affine fractal on a limited range of wave-vectors.

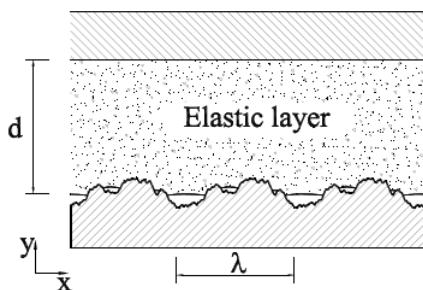


Figure 1: An elastic layer of thickness d in adhesive contact with a rough rigid substrate.

We employ a spectral method to generate such randomly rough surfaces with different root mean square roughness values and fractal dimensions. Calculations are performed for each profiles by means of an ad hoc numerical code previously developed by the authors [1-2]. The calculated data are then statistically averaged, and the contact area, the applied load are shown as a function of the penetration, both for loading and un-loading conditions. It is found that the combination of adhesion forces and roughness leads to a hysteresis loading-unloading loop, which might be unexpected for perfectly elastic materials. This result is very interesting as it shows that energy can be lost simply as a consequence of roughness

vand der Waals forces. Our calculations enable us to numerically quantify such an energy loss and, in particular, to assess the influence of the fractal dimension D_f and of the Duprè energy of adhesion this hysteresis process.

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Molecular dynamics study of automotive lubricants: linking molecular structure and friction

Michael Doig¹, Philip J. Camp¹, Chris P. Warrens²

¹School of Chemistry, Joseph Black Building, University of Edinburgh, West Mains Rd, Edinburgh, EH9 3JJ, UK

²BP Technology Centre, Pangbourne, RG8 7QR, UK

Lubricant oils are used to reduce friction and wear in a wide range of industrial and mechanical processes. Lubricant additives play a vital role in the oils' overall performance, particularly surface-active additives which can significantly affect the tribological properties of solid surfaces. However, there is insufficient understanding of the link between the atomic-level structure of tribofilms and the macroscopic properties such as friction, to direct the development of new lubricant formulations.

Using large-scale molecular dynamics simulations, we investigate a range of lubricated systems, studying the structural properties of surface-adsorbed tribofilms on metal-oxide surfaces, and how they vary with temperature, pressure, surface coverage and shear rate. Several important trends are identified linking molecular isomerism and architecture with the structure and stability of the adsorbed films. In addition, the simulation results are used to gain insight on recent experimental measurements of film structure [1]. Some examples of the systems studied include oleic acid and stearic acid films lubricated by squalane (see figure 1) [2], and hexadecylamine films lubricated by dodecane [3], both adsorbed on iron oxide surfaces.

The friction coefficients in these systems are computed and analysed with reference to the structure of the adsorbed films, to yield new insights on the intimate link between the molecular properties of lubricants and the macroscopic frictional properties of lubricated systems.

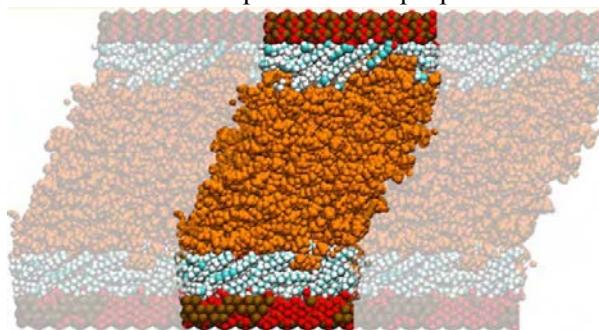


Figure 1: Lubricated system of oleic acid adsorbed on iron oxide lubricated by squalane base oil, under applied shear.

This work was supported through a CASE studentship by BP International Ltd and EPSRC(UK).

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Materials Aging at Mesoscale: Activated Kinetics and Self-Organized Criticality

Sidney Yip

Nuclear Science & Engineering and Materials Science & Engineering
Massachusetts Institute of Technology
Cambridge, MA 02139 USA

There exists a class of materials durability problems where understanding of the microstructure evolution on spatial-temporal scales of micrometers-seconds is lacking. Fundamental phenomena such as creep, corrosion, and fatigue cracking have in common the processes of deformation and flow of inhomogeneous matter out of equilibrium. The challenge of resolving the governing mechanisms currently constitutes a frontier of materials modeling at the mesoscale [1]. In this perspective we describe a time-dependent transition-state theory approach to address two problems, strain-rate dependence of yielding [2], and the transition from logarithmic (primary) to tertiary (damage) creep [3]. In the former we point out an analogy between crystal plasticity and glass rheology, in the latter we suggest an example of self-organized criticality in the form of strain localization. Additionally, we propose a phase diagram in strain-rate and temperature as a mechanism map where thermal and stress activated processes compete [4].

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Low cycle fatigue modeling of dislocation patterning in FCC metals in single and multiple slip by crystal plasticity finite element method

Nicolò Grilli^{1, 3}, Koenraad G. F. Janssens¹, Helena Van Swygenhoven^{2, 3}

¹Laboratory for Nuclear Materials, Nuclear Energy and Safety Department,
Paul Scherrer Institut, Switzerland

²Material Science and Simulations, NUM/ASQ, Paul Scherrer Institut, Switzerland

³NXMM Laboratory, IMX, École Polytechnique Fédérale de Lausanne, Switzerland

Modeling low cycle fatigue in FCC metals is a long-standing problem which has been a topic of research in the past analyzed with different computational methods. The ultimate goal of computational modeling is the prediction of the mechanical behavior and the lifetime of components. The Crystal Plasticity Finite Element (CPFE) method [1] has been used successfully for studying plasticity in metals and is highly compatible with dislocation-based theories. However it has only been applied sporadically to cyclic plasticity because the computational resources needed to solve many cycles are substantial. CPFE can simulate geometries with arbitrary boundary conditions. Current constitutive equations for low cycle fatigue do not fully capture the dislocation structures emerging during cyclic deformation, e.g. the vein-channel structures for single slip cyclic deformation, or cell and labyrinth structures for multiple slip conditions. Modified constitutive laws are proposed that describe the material at a length scale smaller than previous models [2]. Representative volumes with an element size of approximately 200 nm, which is smaller than the periodicity that is typically observed in these dislocation structures, are used in the simulations. The small size of the elements is necessary if one wants to be able to predict the patterning in dislocation structures, which in turn leads to the cyclic mechanical properties. We will present simulations for cyclic shear deformation of single crystals in single and multiple slip orientations up to 100 cycles. The time evolution of the volume fraction of dislocation structures, the strain distribution in low and high dislocation density areas, and local crystal lattice misorientation will be discussed. These quantities will be validated by using various electron microscopy techniques [3] and in-situ synchrotron Laue micro-diffraction [4].

This research is performed using the DAMASK Crystal Plasticity Finite Element open source code of the Max-Planck-Institute for Iron Research.

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**Modeling dislocation climb at the atomic scale
in MgSiO₃ perovskite in the conditions of Earth's lower mantle**

Pierre Hirel, Philippe Carrez, Patrick Cordier

Unité Matériaux et Transformations, CNRS UMR 8207
Université des Sciences et Technologies de Lille 1, 59655 Villeneuve d'Ascq

Convection and plastic deformation in the Earth's lower mantle occur in extreme conditions of pressure and temperature, and at geological times that are reflected in the very low strain rates (10^{-12} to 10^{-16} s $^{-1}$). Although the composition of the Earth's lower mantle is dominated by the MgSiO₃ perovskite, the mechanical properties of this phase, its microstructure and the mechanisms responsible for its plastic deformation are still a matter of debate. Given the thermodynamic conditions, both dislocation glide and climb are expected to contribute significantly to the plastic flow, however the activation energies and rates of these mechanisms are still to be determined.

In this study we utilize atomic-scale calculations to investigate the interaction of vacancies with edge dislocations, an elementary process of dislocation climb. The interaction energies are explicitly computed, and it is shown that contrary to metals where the interaction is almost purely elastic, in MgSiO₃ the vacancy-dislocation interaction is dominated by electrostatic effects due to the ionic character of this material. As a result, ions with different charges have different behaviours: anions (oxygen) are attracted to the dislocation, while cations are repelled. The consequences for dislocation climb are discussed. These results give insight into the importance of dislocation activity in the rheology of the mantle.

This work was supported by funding from the European Research Council under the Seventh Framework Program (FP7), ERC grant N.290424 – RheoMan.

Free energy of dislocations: Collective equilibrium behavior and driving forces for dynamics

Marleen Kooiman, Markus Hütter, Marc Geers

Eindhoven University of Technology, Materials Technology Institute,
PO Box 513, 5600 MB Eindhoven, The Netherlands

Dislocations are an important underlying mechanism for crystal plasticity at small scales. As metals usually contain many dislocations, it is crucial to examine the collective behavior of all dislocations and to obtain the emergent mechanical response of the system. To bridge the micro and mesoscale, we focus on the free energy of dislocation densities. Once calculated, the free energy yields the equilibrium behavior of the system through minimization. Moreover, driving forces for the dynamics of dislocations can be determined from free energy derivatives. Numerous frameworks have been developed that use free energy derivatives in the dynamical equations [1-2]. However, the explicit energy expressions used are still mainly phenomenological in nature.

Here, we present a free energy expression derived by systematic coarse-graining [3]. We have averaged over a grand-canonical ensemble of discrete dislocations, where we restrict ourselves to straight and parallel dislocations. From the obtained grand-canonical partition function, the free energy as a functional of dislocation density profiles is derived by means of a Legendre transform.

The obtained free energy expression consists of the elastic energy in the system, both due to the presence of dislocations and due to applied boundary loading. Moreover, the free energy entails an ideal gas contribution of the dislocations, and a many-body contribution that accounts for screening. The latter is a truly collective term that is not present for a system of discrete dislocations. We show that this many-body contribution can be approximated by a local density approximation.

From the explicit free energy expression, we derive pair correlation functions and the equilibrium pile-up profiles of dislocations on a single slip system. Moreover, we discuss the role of temperature for dislocation systems.

The focus of future research is on the implementation of the current free energy expression in a dynamical framework.

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Thermally-activated dislocation glide from the atomic scale

Laurent Proville¹, David Rodney²

¹CEA, DEN, Service de Recherches de Métallurgie Physique,
Gif-sur-Yvette 91191, France

²Institut Lumière Matière, University of Lyon, Villeurbanne 69622, France

Atomic-scale simulations of the slow and thermally-activated glide of high Peierls stress dislocations remains a challenge but is of fundamental importance to understand plasticity for instance in body-centered cubic (bcc) and hexagonal (hcp) metals and alloys. First, developing realistic interatomic potentials, which reproduce satisfactorily ab initio predictions about dislocation cores and glide processes, is difficult. Second, the average timescale of the glide process, which involves crossing the Peierls barrier by the thermally activated nucleation of kink-pairs, becomes rapidly too slow when the temperature is lowered, to be accessible to direct Molecular Dynamics (MD) simulations. As a consequence, there is still much to be understood and in particular, the well-known discrepancy between atomic-scale simulations and experiments about the Peierls stresses of screw dislocation in bcc metals.

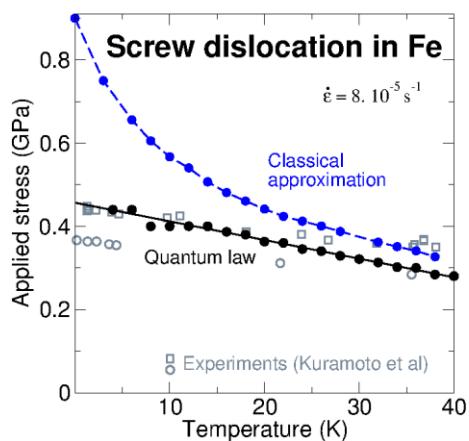


Figure 1: Critical shear stress versus temperature in α -Fe: experimental data from [1], and computed data from classical Orowan law and quantum Orowan law [2].

when comparing the experimental data [1] with our computations [2]. We will tentatively extend our results to other materials., including Si and Mg.

We present recent advances in modeling the glide of high Peierls stress dislocations. We employ saddle-point search methods (Nudged Elastic Band method) in conjunction with the transition state theory, to predict the pathways and kinetics of dislocation glide. The data computed at the atomic scale allow us to determine the input parameters for transition state theories derived within either classical or quantum statistics. We show in α -iron how the Peierls stress of bcc screw dislocations may be decreased by quantum effects, namely the crystal zero-point vibrations, giving rise at temperatures below 20 K to a large vibrational entropy of kink-pair formation, thus lowering the Peierls barrier. A remarkable agreement is found

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A phase field model for dislocation climb

Pierre-Antoine Geslin, Benoît Appolaire, Alphonse Finel

LEM, Onera/CNRS, 29 avenue de la division Leclerc, 92320 Châtillon

Dislocations are linear defects responsible for plastic deformation in crystalline solids. These defects change glide plane by absorbing point defects (climb). Whereas this climb mechanism is inhibited at low temperature, it becomes an essential part of plastic activity at high-temperature (creep). Therefore the analysis of climb dynamics is mandatory to have a better understanding of the creep behavior of metals and alloys. Most of the current modeling techniques for dislocation climb are based on an analytical solution valid under given assumptions [1,2]. First, the dislocation line is generally assumed to be at equilibrium with the surrounding vacancies (local equilibrium assumption). This might be a crude approximation in the case of fcc metals where jogs are high energy defects and can present low concentrations along the dislocation. Second, dislocations are supposed to be far enough from each other such that diffusion is assumed to take place in a hollow cylinder around each dislocation.

To go beyond these assumptions and measure their influence, we first propose an analytical solution for the climb of a isolated dislocation presenting a periodic distribution of jogs. This solution shows that, below a given jog concentration, the local equilibrium assumption can not be valid and the climb rate drops significantly. Second, we propose a phase-field model for dislocation climb to investigate the climb behavior of complex dislocation microstrctures. This model incorporates all the necessary features of dislocation climb, including a dynamic coefficient which controls the kinetics of vacancy absorption/emission at the dislocation core. We show how this parameter can be chosen to reproduce the climb behavior of a weakly jogged dislocation using the analytical solution mentioned before. We use this phase-field model to study the climb behavior of random dislocation distributions and compare it with the simple solution assuming vacancies diffuse in a hollow cylinder around each dislocation.

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Atomistic study of dislocation mobility and obstacle hardening in bcc-Fe: versatility of embedded atom method potentials

S.M. Hafez Haghigiat¹, R. Schäublin², J. von Pezold¹, C.P. Race^{1,3}, F. Körmann¹, M. Friák^{1,4}, J. Neugebauer¹, D. Raabe¹

¹ Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany

² Ecole Polytechnique Fédérale de Lausanne (EPFL), Centre de Recherches en Physique des Plasmas, Association Euratom-Confédération Suisse, CH 5232 Villigen PSI, Switzerland

³ School of Materials, University of Manchester, Manchester, M13 9PL, United Kingdom

⁴ Institute of Physics of Materials, Academy of Sciences of the Czech Republic, v.v.i., Žižkova 22, 616 62, Brno, Czech Republic

In crystalline materials the mobility of dislocations and their interactions with obstacles determine the material strength due to dislocation plasticity. Atomistic simulation using the embedded atom method (EAM) is the method of choice to study the kinetics and mechanisms of dislocations. In this study four commonly used EAM potentials for bcc-Fe, namely Ackland et al. (1997), Mendelev et al. (2003), Chiesa et al. (2009) and Malerba et al. (2010), are critically evaluated with respect to their description of the dynamic behavior of $\frac{1}{2} a_0 <111>$ edge and screw dislocations [1]. In the specific case of edge dislocation we find that there is a strong correlation between the dislocation core structure and its glide stress. Analysis of the dislocation migration reveals that the dominant migration mechanism is via progressing straight line segments of the dislocation. This is further confirmed by the excellent qualitative agreement of nudged elastic band calculations of the Peierls barrier with the dynamically determined critical shear stresses. In the second part, the interaction of a $\frac{1}{2} a_0 <111>\{110\}$ edge dislocation with different microstructural defects such as nano-sized obstacles [2,3], second phase precipitates [4] and other dislocations [5] will be discussed. We detail the formation and unzipping process, and the strength of the $<100>$ binary junction through interaction between two $\frac{1}{2} a_0 <111>$ dislocations of edge and screw character. Effects of temperature and strain rate on the unzipping of the junction are quantified. The critical stress, at which the edge dislocation is detached from the screw dislocation, decreases when the temperature increases from 10 to 300 K, whereas it increases with increasing applied strain rate, or dislocation speed. The interaction mechanism and strength of the $a_0 <100>$ binary junction as an obstacle to the edge dislocation are compared to that of other types of defect, namely nano-sized voids, Cu and Cr precipitates and dislocation loops in Fe. The binary junction strength is in the lowest range, comparable to that of a coherent Cr precipitate. However, it appears that the sensitivity of results to the selected empirical potential can be significant and shouldn't be overlooked.

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A 3D dislocation dynamics analysis of the development of size effects at high temperature during micropillar compression of LiF [111] single crystals

H.-J. Chang¹, J. Segurado^{1,2}, R. Soler¹, J. M. Molina-Aldareguía¹, Javier Llorca^{1,2}

¹IMDEA Materials Institute, 28906 Getafe, Madrid, Spain

²Department of Materials Science, Polytechnic University of Madrid, 28040 Madrid, Spain

Compression tests of [111] LiF micropillars with a diameter in the range 1 to 5 μm did not show any size effect on the flow stress [1]. However, more recent experimental data have shown that a strong size effect (“smaller is stronger”) develops progressively as the test temperature increases. At 250°C, the micropillars of 1 μm in diameter were twice stronger than those with 5 μm in diameter [2]. 3D discrete dislocation dynamics (3DDD) of the micropillar compression tests were carried out in order to understand the emergence of a size effect in the flow stress as a function of temperature. Micropillars of diameters in the range 1 to 4 μm and an aspect ratio of 2 (in agreement with the experiments) were studied. The top and bottom surfaces of the circular micropillar were impenetrable to dislocations while the dislocations could leave the micropillar through the lateral surfaces and image stresses on the Peach-Koehler forces were taken into account. The three hard slip systems, [-10-1] (0-10), [0-1-1] (100) and [110] (001), that are activated during compression of LiF along the [111] direction were included in the 3DDD model, as well as the anisotropy in the mobility between edge and screw dislocations, typical of LiF. The evolution of the lattice resistance and of the dislocation mobility with temperature were obtained from theoretical considerations based on experimental results of LiF single crystals [2]. Frank-Read sources were randomly distributed in the three slip systems and the initial dislocation density was equivalent to the experimental one ($\approx 2.5 \cdot 10^{13} \text{ m}^{-2}$).

The results of the 3DDD simulations were able to capture the emergence of the size effect on the flow stress of the [111] LiF micropillars with temperature. This was due to the reduction of the lattice resistance, which become comparable to the size-dependent contribution to the flow stress at 250°C. The changes in the dislocation mobility with temperature only played a secondary role in this respect. Finally, the influence of temperature on the dislocation structures was ascertained from the 3DDD simulations.

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Dislocation Interactions in a Continuum Dislocation Dynamics Formulation

Katrin Schulz¹, Severin Schmitt¹, Doyl Dickel¹, Peter Gumbsch^{1,2}

¹ Institute for Applied Materials (IAM), Karlsruhe Institute of Technology, Kaiserstr.12,
76133 Karlsruhe, Germany

² Fraunhofer Institute for Mechanics of Materials (IWM), Wöhlerstr.11, 79108 Freiburg,
Germany

The strive for advanced materials with well-defined microstructures has also led to an increasing effort towards a physically based description of the motion of dislocations as the cause of plastic deformation and the origin of materials failure. Several dislocation based continuum theories have been introduced, but only recently have rigorous techniques been developed for performing meaningful averages over systems of moving, curved dislocations, yielding evolution equations for a higher order dislocation density tensor, see [1].

In order to reduce the computational complexity of the theory, a simplified theory has been developed [2], which more readily allows for numerical implementation. In order to construct a self-consistent coarsening, several issues have to be resolved including calculation of the stress field of a system of dislocations, correlation functions, and boundary conditions.

Accurate solutions have been found for one dimensional systems [3]. Fully two- and three-dimensional systems will be compared to ensemble averages over discrete dislocation distributions. A continuous field approach including stress interactions perpendicular to the slip planes is introduced and an overview of results for a distribution of one-dimensional glide planes in two-dimensional elastic media is presented. Several aspects of numerical homogenization are analyzed and discussed. Using comparisons with Discrete Dislocation Dynamics (DDD) in a few simple systems, the multi-component stress field which must be considered for dislocation density motion is discussed and enhanced by a statistical model for the representation of dipole interactions in the continuum formulation.

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Atomistically informed discrete dislocation dynamics simulations and the origin of anomalous slip in tungsten

K. Srivastava¹, D. Weygand¹, C. Marichal^{2,3} H. Van Swygenhoven^{2,3}, P. Gumbsch^{1,4}

¹Karlsruhe Institut of Technology KIT, Institute for Applied Materials, Kaiserstr. 12,
76131 Karlsruhe, Germany

²Materials Science and Simulation, NUM/ASQ, Paul Scherrer Institut, CH-5232 Villigen
PSI, Switzerland

³Neutrons and X-rays for Mechanics of Materials, IMX, École Polytechnique Fédérale de
Lausanne, CH-1012 Lausanne, Switzerland

⁴Fraunhofer IWM, Wöhlerstr. 11, 79108 Freiburg, Germany

A computational framework for the discrete dislocation dynamics (DDD) simulation of body-centered cubic (bcc) metals which incorporates atomistic simulation results [1] is developed here on the examples of iron and tungsten. Atomistic simulations suggest kink-pair nucleation on {110} planes only. Mobility rules for the screw dislocations in the DDD simulations are based on the kink-pair mechanism which is controlled by a stress-dependent activation enthalpy. This activation enthalpy not only depends on the resolved shear stresses but also incorporates so called non-Schmid stresses. It is demonstrated that this description of the dislocation mobility provides a physical basis to naturally explain many experimentally observed phenomena in bcc metals like the tension–compression asymmetry, the orientation dependence of loading, and the temperature dependence of the yield stress. We demonstrate the power of such atomistically informed DDD techniques by analysis of anomalous slip behaviour in tungsten.

Several bcc metals exhibit significant plastic flow on planes with low stresses, a phenomenon which is not generally understood and termed anomalous slip. Here and in [2] we report on experimental observations of the occurrence of anomalous slip during compression of tungsten micropillars within an in-situ Laue microdiffraction setup. DDD simulations of the compression of micrometer sized tungsten single crystals in exactly the same geometry as in the in-situ experiments also show the occurrence of a significant amount of anomalous slip. A detailed analysis of the evolving dislocation microstructure reveals the underlying mechanism. Anomalous slip mainly occurs as a consequence of so called cross-kinks, topological configurations generated by prior dislocation interactions.

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Screw Dislocation Cross-slip at Cross-slip Plane Jogs and Screw Dipole Annihilation in FCC Cu, Ni Investigated via Atomistic Simulations

S.I. Rao¹, D.M. Dimiduk¹, J.A. El-Awady²,
T.A. Parthasarathy³, M.D. Uchic³, C. Woodward³

¹Air Force Research Laboratory, Materials and Manufacturing Directorate, AFRL/MLLM
Wright-Patterson AFB, OH 45433-7817

²Johns Hopkins University, Baltimore, MD

³UES, Inc., 4401 Dayton-Xenia Rd, Dayton, OH 45432-1894

Using atomistic (molecular statics and molecular dynamics) simulations and embedded-atom-method potentials, cross-slip of screw dislocations at cross-slip plane jogs and screw dipole annihilation at cross-slip plane jogs were examined for FCC Cu, Ni. After conjugate gradient energy minimization, two different core structures were obtained for the screw dislocation having a cross-slip plane jog: a) a configuration where most of the screw dislocation was dissociated on the (111) glide plane, having an extended jog spread on the (11-1) cross-slip plane, and b) most of the screw dislocation was dissociated on the (111) glide plane having a sharp jog on the (11-1) cross-slip plane. The sharp jog configuration had an energy approximately 0.4 eV lower than the extended configuration in FCC Cu. Nudged-elastic-band-method calculations of the energy pathway between the sharp and extended jog configurations showed that the energy hump near the extended configuration is shallow and, that the activation energy required to transform the screw dislocation from the sharp to the extended configuration (activation energy for cross-slip) is close to 0.4 eV in FCC Cu (a factor of 4-5 lower than the activation energy for cross-slip in the absence of a jog). Similar results were obtained for FCC Ni.

Molecular dynamics simulations were used to study the annihilation of a jog-containing screw dipole. The dipole was separated approximately by 14 and 45 nm along the (111) direction in each of two simulations and, under application of Escaig stresses acting to constrict the screw dislocation on the (111) glide plane. The simulations showed that the critical Escaig stress for dipole annihilation significantly drops from the 0K value (~400 MPa) and, dipole annihilation is nearly athermal at room temperature. At 5K, Escaig stresses on the cross-slip plane are a factor of 1.5 less effective than the Escaig stresses on the glide plane and, glide stresses on the cross-slip plane are a factor of 3 less effective for dipole annihilation by cross-slip. However, it was found that if the screw dislocations are initially positioned away from each other by 14nm along the y direction on the (111) glide plane, in addition to their separation perpendicular to the glide plane, the screw dislocations move toward each other with the jog acting as a pinning point and extending an edge dipole due to their movement. This process makes cross-slip at the jog on the screw dislocation almost prohibitive. Application of glide stresses on the (111) glide plane accentuated this effect.

Based on these atomistic simulation results, dislocation dynamics simulations accounting for Shockley partials were also used to investigate the dipole annihilation process in FCC Cu, and Ni. These atomistic simulation results are expected to be useful in physics-based modelling of bulk cross-slip in higher length scale 3-D dislocation dynamics simulations investigating dislocation pattern formation and fatigue structures in FCC crystals.

From atomic to mesoscale diffusion equations for alloys

M. Nastar

CEA, DEN, Service de Recherches de Métallurgie Physique, F-91191 Gif-sur-Yvette,
France

Up to now there is no satisfying atomic theory of diffusion. Although diffusion at the atomic scale is strongly involved in aging phenomena of nanoscale devices and bulk materials with nanoscale microstructures. Bulk diffusion experiments are conducted at a micrometric spatial scale which is too large to highlight the atomic scale features of diffusion phenomena. Instead, interdiffusion experiments performed on nanoscale composition-modulated foils are perfect for the characterization of atomic diffusion. Since the 70s, a complex variation of the interdiffusion coefficient D with respect to the wavevector of a sinusoidal concentration modulation has been evidenced: while at small wavevector, a linear variation of D with respect to the square of the wavevector is observed; at wavelengths smaller than a few lattice parameters a deviation from linearity is observed. The implementation of Atomic Kinetic Monte Carlo simulations and new developments of the Self-Consistent Mean Field (SCMF) theory demonstrate that in alloys with short range interactions, a non-linear deviation of D is due to wavevector dependent kinetic correlations produced by the vacancy diffusion mechanism. A measure of this deviation can be used to determine the off-diagonal phenomenological coefficient of the Onsager matrix which is extremely difficult to extract from classical diffusion experiments, although it is an essential parameter for the prediction of microstructures induced by irradiation. To conclude, a new atomic diffusion equation for non-homogeneous alloys has been established. As wavevector gets small, it tends to a general diffusion equation different from the Cahn-Hilliard equation, showing that the latter currently used in phase field methods to describe vacancy diffusion controlled phenomena should include the interface-dependent kinetic correlations in addition to the interface-dependent driving forces.

Thermal properties of point defects and their clusters in bcc Fe

D. Murali¹, M. Posselt¹, M. Schiwarth^{1,2}, J. Kortus²

¹Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research,
P.O.Box 510119, D-01314 Dresden, Germany

²TU Bergakademie Freiberg, Institute of Theoretical Physics, Leipziger Str. 23, D-09596
Freiberg, Germany

Ferritic Fe and Fe-Cr alloys are basic structural materials of present and future nuclear fission and fusion reactors. The formation of the micro- and nanostructure of these alloys and the structural evolution under irradiation is essentially influenced by the interaction between solutes, vacancies and self-interstitials. These processes take place in different alloys such as reactor-pressure-vessel and oxide-dispersion-strengthened steels. The understanding of the nanostructure of those materials and of its radiation-induced evolution is indispensable for nuclear reactor safety. First-principle calculations based on the Density Functional Theory (DFT) are a very useful method to get atomistic insights into the interactions between solutes, vacancies and self-interstitials in bcc Fe. Traditionally, formation and binding energies of these species are investigated at T=0 and these data are further used in calculations on larger length and time scales such as in kinetic Monte Carlo simulations and Rate Theory.

The main objective of present work is the determination of the temperature-dependent free formation and binding energy of selected point defects and their clusters in bcc Fe. For this purpose DFT is used to obtain the corresponding vibrational free energies within the framework of the harmonic approximation. The substitutional solutes Cu, Y and Ti, the interstitial solute atom O, the vacancy as well as small clusters consisting of solute atoms and vacancies are considered. The results are compared with theoretical data obtained by other authors and discussed in relation to experimental solubility data. Fig. 1 (a) shows the temperature dependence of the free formation energy of substitutional Cu in comparison with recent DFT data of Reith et al. [1], whereas Fig. 1 (b) depicts the data for interstitial O. In both cases a significant dependence on temperature is found. This must be taken into account in multiscale simulations that use DFT input data.

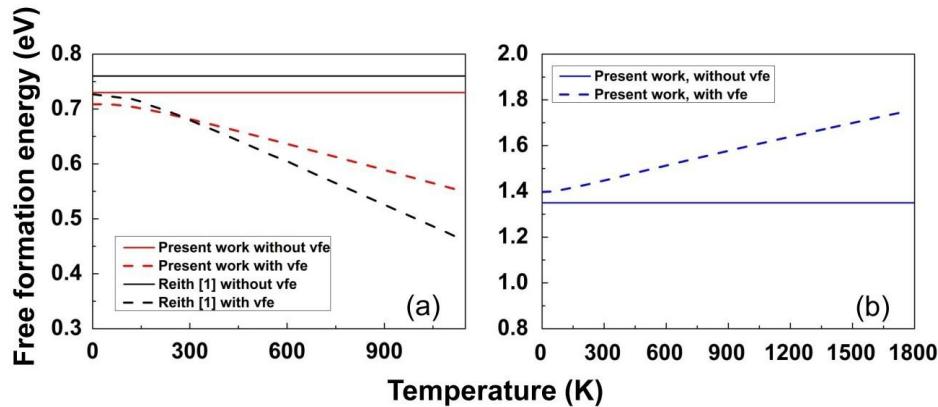


Figure 1: Total free formation energies of Cu (a) and O (b) in bcc Fe determined with and without considering the contribution of the vibrational free energy (vfe).

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Theory of Solid Solution Strengthening in High Entropy Alloys

Céline Varvenne¹, Aitor Luque Gomez¹, Satish I. Rao^{1,2}, William A. Curtin¹

¹Laboratory for Multiscale Materials Modeling, EPFL, Lausanne CH-1015, Switzerland

²UES Inc., 4401 Dayton-Xenia Road, Dayton, OH 45432 USA

High-entropy alloys represent a new class of advanced materials with unique properties that cannot be achieved by microalloying processes. In particular, mechanical strength and toughness are usually seen to be improved by increasing the number N of alloy components [1]. The origins of strengthening in these alloys remain uncertain, and there have been no theories that predict the observed trends. We present a new theory which generalizes the predictive dilute-solute strengthening model of Leyson *et al.* [2] to the case of N components with high concentration of all elements. The theory predicts that energy barriers for dislocation motion and zero temperature yield stresses do not scale with N, but are mainly driven by the effective misfit volumes of the alloy components. Together, these quantities provide predictions for the finite-T, finite-strain-rate strengthening and show that increasing the number of components N leads to higher strengths, provided that their volume misfits follow some rules. Application of the model to recent experiments shows that the theory predicts the same trends as found in experiments, as well as some deviations from the general trends including that some binary alloys are as strong as ternaries and that some ternaries as strong as quaternaries. Extensions of the model to include the effects of stacking fault energy, solute-solute interactions, and chemical short-range-order are discussed.

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The Evolution Process of Transformation Crystallography in Cu-Cr System

-----A Hybrid Monte Carlo and Molecular Statics Method Simulation

Fu-Zhi Dai, Wen-Zheng Zhang

School of Materials Science and Engineering, Tsinghua University, Beijing 100084, China

Morphology of precipitates in various alloys is an essential microstructure feature that affects the properties of the alloys. Precise measurements of precipitate morphologies in metallic systems often reveal reproducible habit plane (HP) in irrational orientations together with irrational orientation relationship (OR). It is now clear that the HP of a well-developed precipitate usually contains a singular interfacial structure of a single set of dislocations (O-line criterion), which is possible only in interface(s) of discrete irrational orientations and with irrational ORs. An unsolved problem is why a particular HP is preferred among numerous interfaces that can meet the O-line criterion. While it would be desirable to investigate the process of precipitate evolution from beginning of the growth, the experimental study is extremely difficult with the available techniques. Atomistic simulation serve as an alternatively approach to solve this problem. In this work, a hybrid method which combines Monte Carlo and Molecular Statics is adopted to study the evolution process of crystallographic features. A Cu-Cr alloy is chosen as a model system, since reliable experimental crystallographic data of Cr-rich precipitates in this system is available for testing the simulation results [1, 2].

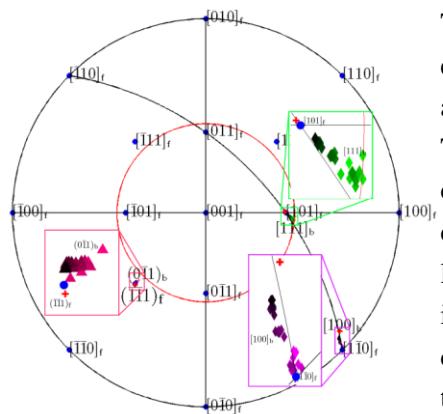


Figure 1. Stereographic projection of the simulated OR evolution. Δ represents the projection of $(0-11)_b$ plane, while \diamond shows the projection of $[100]_b$ (purple) and $[111]_b$ (green). $+$ is the projection of values corresponding to the ideal O-line criterion. The darkness of the marker indicates the size of the precipitates, i.e., the darker is the marker, the bigger is the size.

The evolution of the OR is demonstrated in Figure 1. At the early stage, the OR between a small coherent precipitate and the matrix is close to the N-W OR ($[100]_b$ near $[1-10]_f$). The OR changes towards the K-S OR ($[111]_b$ near $[101]_f$) discontinuously with generation of each dislocation loop during the growth of the precipitate. Simultaneously, the long axis of the precipitate changes from $[101]_f$ towards the invariant line direction that lies on $(-1-11)_f$ and the HP changes from $(-1-11)_f$ towards the orientation which meets the O-line criterion. This result agrees with the observation by Fujii et al. [2], in that the near N-W OR disappears and the near K-S OR prevails as the precipitates grow. In addition, by extrapolating the results with the same dislocation loops to meet the O-line criterion, we found that the simulated crystallographic features agreed consistently with the measurements by Luo et al. [1]. This HP was proved to be the O-line interface with the lowest energy in a recent calculation [3].

This work is supported by National Nature Science Foundation of China (No. 51171088).

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Creep modeling in Olivine by 2.5D dislocation dynamics simulations

Francesca Boioli¹, Benoit Devincre², Philippe Carrez¹, Patrick Cordier¹

¹ UMET, University of Lille1, Villeneuve d'Ascq, France

² LEM, CNRS-ONERA, Chatillon, France

Large scale flow in the Earth's mantle involve plastic deformations of rocks and their constitutive minerals. Due to the extremely slow strain rate conditions in the Earth's mantle, it is very challenging to identify the fundamental mechanisms controlling such process. Thus, the development of a multi-scale approach linking the atomic scale properties and the microscopic elementary mechanisms to the macroscopic behavior is needed [1]. Within this framework, we present a model to investigate the creep of olivine, one of the main constituent of the Earth's mantle, at the mesoscopic scale. In the past years, it has been demonstrated that dislocations play an important role in the creep flow of rocks and minerals. However, the influence of the climb mechanism, which is expected to be dominant in high temperature plasticity, and extent of the glide versus climb process have not yet been clarified. To this aim, we performed 2.5D Dislocation Dynamics (DD) simulations coupling the climb with the glide dislocation motion. Within this approach, dislocations are approximated by straight segments and their dynamics is modeled in a reference plane, as sketched in Fig. 1a,b). Moreover, local rules are implemented to reproduce the relevant three-dimensional dislocation mechanisms, as originally proposed to model fcc metal plasticity [2]. Finally, the transport of matter through vacancy diffusion is taken into account and directly related to the climb dislocation velocity, similarly to Ref. [3]. In this work, we discuss the interplay between thermally activated glide and climb motion and we study the effect of climb on the creep strain rate. As shown in Fig. 1c), at high temperature and low applied stress, climb plays a key role in the creep behavior.

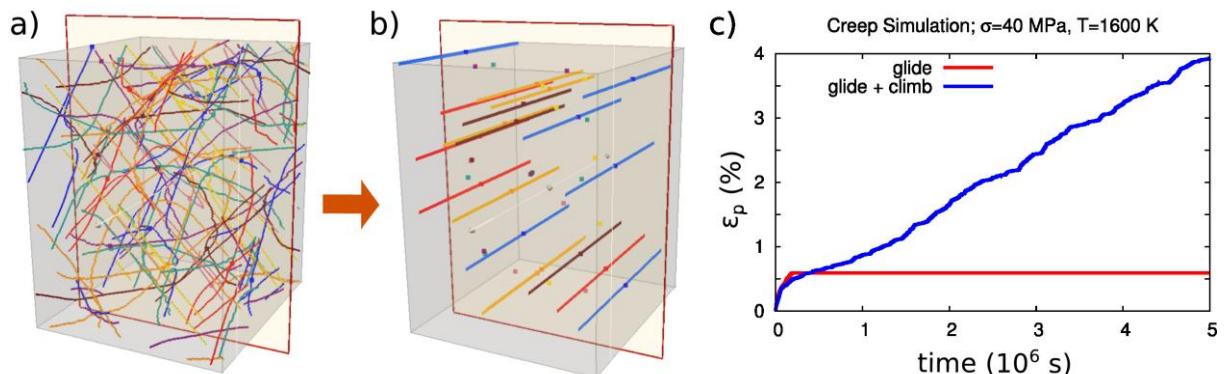


Figure 1: Sketch of full 3D- a) and 2.5D-DD simulation volume. c) Plastic deformation ϵ_p vs. time, as obtained by 2.5D-DD simulations in creep conditions, assuming glide only (red curve) and glide coupled with climb (blue curve) dislocation motion.

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Deformation and failure of curved nanocrystalline shells

M. Carmen Miguel

Departament de Física Fonamental, Facultat de Física, Universitat de Barcelona Diagonal
645, E-08028 Barcelona, Spain

We study the mechanical response of curved crystalline shells subject to load. These structures, mainly conceived for encapsulation purposes at small scales, show peculiar behavior due to their topological properties, i.e., the minimum energy configuration of any curved crystalline surface contains geometrically necessary topological defects in agreement with its Euler characteristic. The microstructure evolution is therefore influenced by the dynamics of those topological defects on the curved interface and exhibits a rather rich and non-trivial phenomenology. The quasi-static deformation of these structures is characterized by intermittent dynamics with collective particle reorganizations mediated by the proliferation of dislocation pairs and the dynamic delocalization of disclinations in the form of grain boundary scars. At large deformations, depending on bending rigidity, sample size, and geometry, one may observe buckling instabilities and structural failure phenomena such as the cavitation of the crystal shells.

Theory, Modeling and Experiments of Nano-structured Surfaces by Plasma Ions

N.M. Ghoniem¹, Daniel Walgraef², Christopher Matthes²

¹Mechanical & Aerospace Engineering Department, UCLA, Los Angeles, CA 91344

²Instituto de Fisica Interdisciplinar y Sistemas Complejos (CSIC-UIB),
E-07122 Palma de Mallorca, Spain

A theoretical framework for the evolution of solid surfaces bombarded with plasma ions is presented. The continuum model is based on the original developments of Sigmund[1], Bradley and Harper (BH)[2], and Makeev[3]. Recognizing that near surface energy deposition can produce sputtering events downstream rather than at the point of ion impact, the theory takes into account the interplay between the curvature-dependent sputtering and additional surface relaxation processes, for example as a result of surface diffusion. Taking Sigmund's conclusions that the surface height evolution rate is proportional to its curvature normal to the ion beam, κ , BH balance the roughening rate by surface relaxation rate that is proportional to the second spatial derivative of κ . Thus, the evolution equation for the surface height is [4]: $h_{,t} = Sk + B\kappa_{,ss}$, where the subscripts denote time (t) derivative and arc length (s) derivatives. The BH equation is usually replaced by a small slope approximation, $\kappa \approx \Delta h$, where Δ is the Euclidian Laplacian. The coefficients S and B are for the rate of roughening by sputtering (includes angular dependence of the sputtering coefficient), and the surface diffusion smoothing rate (includes surface diffusion coefficient), respectively. We present linear, non-linear and numerical simulations of the equations governing surface patterning under ion or plasma bombardment. We also show experimental results on the influence of pre-existing surface texture on pattern-forming instabilities. Experiments show that low-energy (150 eV) Ar ion energy deposition in the near surface layer result in the amorphization of W at room temperature to a depth of 5-10 nm. The surfaces of nano rods become rippled as a result of an ion-induced roughening instability, with an observed wave-length of 300 nm. Because of the low sample temperature and incident ion energy, the origin of surface ripples does not appear to be related to thermal surface diffusion nor near surface collision cascades.

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Predicting interface dislocation structure and energy using anisotropic elasticity theory

N. Abdolrahim¹, A. J. Vattré², K. Kolluri¹, M. J. Demkowicz¹

¹Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge MA, 02139

²CEA, DAM, DIF, F-91297 Arpajon, France

Frank-Bilby theory generates multiple candidate misfit dislocation structures for an interface with given crystallography. Additional conditions are required to determine which of these structures is the unique structure exhibited by a real interface. We compute the strain energies of all candidate structures generated by Frank-Bilby theory and predict that the one with lowest energy is the correct solution. Our calculation is based on anisotropic linear elasticity theory and uses Burgers vectors consistent with prescribed far-field displacement gradients. We compare our predictions with MD simulations of several fcc/bcc interfaces using disregistry analysis and discuss the potential impact of our findings on engineering of designer interfaces.

Thin film buckling on substrate: effect of pressure and plasticity

Jérôme Colin, A. Ruffini, Christophe Coupeau, Alain Cimetière, Jean Grilhé

Institut P', Université de Poitiers, ENSMA, SP2MI-Téléport 2, F86962 Futuroscope-Chasseneuil cedex, France

The thin film buckling on substrate has been theoretically investigated at the mesoscopic scale in the framework of the Foppl-von Karman (FvK) theory of thin plates and, at the microscopic scale, through atomistic simulations.

The first problem to be considered is the buckling of a stressed thin film when an overpressure is considered onto the upper free surface of the film. It is found from an analytical description using the FvK formalism that an overpressure may be responsible for the partial re-deposition of the buckle or its complete re-deposition through the snap through phenomenon. A shape diagram of the film is finally displayed in the stress-applied pressure plane.

In a second part, atomistic simulations of the thin film buckling are presented and the formation of dislocations in the film/substrate interface after the film has buckled is discussed. The formation of the buckle and the dislocation emergence at the buckle edges has been then analytical described using the linear elasticity theory. A stability diagram for the film is provided with respect to the buckling and dislocation emission phenomena.

A microstructural phase field approach to shock-induced martensitic transitions in iron

Aurélien Vattré, Christophe Denoual

CEA, DAM, DIF, F91297 Arpajon, France

A thermodynamically consistent phase field approach for multivariant transformations for shock wave propagation is developed at large strains. Thermodynamic potential includes the description of complex energy landscapes based on reaction pathways and the second law of thermodynamics is used to determine the driving force for change in transformational strain gradients. Kinetic relations lead to the time-dependent Ginzburg-Landau equations with nonlinear, anisotropic and different elastic properties of phases. The morphological features of the bcc–hcp–bcc transformations in iron are investigated and the importance of the plastic deformations in the shock- induced structural transitions is discussed in details.

Phase Field Modeling of Widmanstätten structures

Maeva Cottura, Benoît Appolaire, Yann Le Bouar, Alphonse Finel

ONERA-CNRS, Laboratoire d'Etude des Microstructures, 29 avenue de la division
Leclerc, 92320 Chatillon, France

Widmanstätten microstructures have long been studied in physical metallurgy. Numerous experimental observations have evidenced the growth of colonies composed of parallel lamellae, sharing a same crystalline orientation, starting most often from grain boundaries of the mother phase to the grain interior. Such microstructures, resulting from a diffusion-controlled process at high temperatures, have been observed in many metallic alloys such as steels, Cu-Zn or Ti-based alloys. Despite a large number of studies devoted to this microstructure, the understanding of Widmanstätten structures remains incomplete, in particular their growth kinetics featuring a stationary rate under isothermal conditions, as opposed to the usual kinetics observed in diffusion-controlled phase transformations.

Following the first calculations performed by [*M. Fleck, C. Hüter, D. Pilipenko, R. Spatschek, E.A. Brener, Phil. Mag. 90 (2010) 265*], a phase field model has been developed to investigate the role of anisotropic elasticity on the diffusion-controlled growth of acicular precipitates featuring stationary growth rates.

In a first step, the consequences of the elastic driving forces on the microstructure evolution will be discussed for different anisotropies, corresponding to different materials where Widmanstätten structures are observed. In a second step, the model extended to account for a viscoplastic activity will be used to study in what respect plasticity may change the conclusions drawn previously.

2D phase-field simulation of grain size distribution in ceramics

Diego Gómez-García, Bibi Malmal Moshtaghioun, Francisco Luis Cembrera Hernández,
Arturo Domínguez Rodríguez

Department of Condensed Matter Physics, University of Seville, P. O. Box 1065, 41080
Seville, SPAIN

Grain size distribution is a landmark for the analysis of mechanical response of sintered ceramics. It is particularly remarkable to determine the parameters controlling the stationary grain size distribution of a collective of grain powders during sintering. This research work describes a phase-field simulation of the evolution of grain size distribution under external fields (mechanical or electrical forces). A model for the stationary grain size distribution is proposed and it is assessed from the simulation runs. A comparison with different ceramic systems is outlined and discussed in detail.

This research work is funded by the Spanish Ministry of Economy through the project MAT2012-38205-C02-01.

A Phase-field model for Displacive Phase Transformations in Elastically Anisotropic and Inhomogeneous Polycrystals

Tae Wook Heo¹, Long-Qing Chen²

¹Condensed Matter and Materials Division, Lawrence Livermore National Laboratory, Livermore, California 94550, USA

²Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania 16802, USA

Displacive phase transformations are common in a wide spectrum of materials ranging from metals to ceramics when a material is subject to temperature variation and/or mechanical deformation. In this presentation, we present a phase-field model for displacive phase transformations in polycrystalline materials incorporating inhomogeneous elasticity. The relaxation of misfit strain between parent and transformed product phases or among different structural variants of transformed product phases near grain boundaries is taken into account. It is applied to the *fcc* to *bcc* martensitic transformation described by a Bain strain in a polycrystalline Fe-31at.%Ni metallic alloy. The focus is on the effect of grain boundaries on the displacive transformation behavior and microstructure evolution. Employing simple bicrystals, the effects of grain boundary characteristics such as the degree and range of the misfit strain relaxation at the grain boundary and grain boundary curvature on the phase behaviors near a grain boundary are examined for both a flat or a curved grain boundary. The model is then applied to polycrystals containing multiple grains. The effects of misfit strain relaxation at grain boundaries, elastic anisotropy, grain texture, and applied stress on the kinetics and the microstructures of displacive transformations are discussed. The predicted microstructures near grain boundaries are compared to the experimental observations in literature.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. This work was funded by the Laboratory Directed Research and Development Program at LLNL under project tracking code 12-ERD-053.

Multi-scale Modeling of Irradiation-Induced Morphology Evolution

Dr. Scott A. Norris

Southern Methodist University

Ion beam irradiation is an essential basic tool in many industries, used widely for chemical doping and surface processing. For over 50 years, spontaneously-forming ripple-like structures have been occasionally observed during this process, but the observation in 1999 of highly-ordered, hexagonal arrays of nanoscale dots on irradiated GaSb has sparked an intense renewed interest in ion-induced surface modification. It has been hoped that this process could form the basis of a "bottom-up" process to cheaply and rapidly manufacture arrays of nanostructures, or induce surface coatings with tunable opto-electronic properties. However, despite many years of accumulated study of ion irradiation, and thorough knowledge of the generic ingredients for ordered structures, a definitive explanation for their origin in this system has remained elusive.

In this talk I will describe a multi-scale approach to this problem: a means by which statistical information extracted from an ensemble of single-ion impact simulations – lasting only picoseconds – can be incorporated into a continuum-level partial differential equation on the surface evolution that occurs over seconds. The result is a generic framework relating surface normal velocity to the moments of the function describing the single-ion impacts (the "crater function"). After describing the general result, and application to a simple system with reasonable success, we will discuss extensions underway:

- * to rapidly explore a large parametric space of materials and conditions
- * to also inform a continuum description of the significant stress imparted into the film
- * to describe multi-component materials, which exhibit a greater variety of patterns
- * to describe the related regime of Ion-Beam Assisted Deposition (IBAD)

The latter extension is of particular future interest, as the fundamental nature of the phase-separation instability is modified by the IBAD process, which additionally provides a means of transferring compositional patters from the thin film into the bulk, as the patterned surface is continually covered up by new material.

Probing Deformation on the Mesoscale Using Submicron-Resolution 3D X-Ray Microscopy and Dislocation Dynamics Simulations

Ben Larson¹, Jon Tischler², Mamdouh Mohamed³, Anter El-Azab⁴

¹ Mat. Sci. & Tech. Div., Oak Ridge National Laboratory, Oak Ridge, TN 37830, USA

² Advanced Photon Source, Argonne National Laboratory, Argonne ,IL 60439, USA

³ Computational Solid Mechanics Laboratory, KAUST, Thuwal, Saudi Arabia

⁴ Nuclear Engineering and Materials Engineering, Purdue University,
West Lafayette, IN 47907, USA

Formulating a predictive understanding of deformation in ductile materials represents a scientific grand challenge involving the statistical dynamics of interacting dislocations and dislocation densities as they evolve through complex, heterogeneous microstructures on mesoscopic length scales. We have investigated the initial stages of deformation in uniaxially compressed Cu through combined 3-dimensional x-ray microscopy (3DXM) experimental measurements and dislocation dynamics (DD) computational simulations. 3DXM with submicron resolution has been used to make high spatial (0.5 μm) and angular (0.005 degrees) resolution measurements of local lattice rotations in 1% compression-deformed single-crystal Cu over a $\sim 25\mu\text{m} \times 25\mu\text{m} \times 10\mu\text{m}$ volume on Sector 34-ID-E of the Advanced Photon Source. To test our ability to predict initial-stage ductile deformation in Cu on an absolute basis, these measurements have been compared quantitatively with DD simulations of compression for a nominally $10\mu\text{m} \times 10\mu\text{m} \times 10\mu\text{m}$ volume of Cu using the microMegas discrete dynamics code and coarse-graining the simulations to the 0.5 μm three-dimensional spatial resolution of the 3DXM experimental measurements. Absolute comparisons between experimental measurements and DD simulations of local lattice rotations, spatially resolved geometrically necessary dislocation densities, and spatial correlations of the geometrically necessary dislocation densities will be presented. Good quantitative agreement (on a statistical basis) observed between the 3DXM measurements of these quantities in Cu and the DD simulations, without adjustable parameters, will be discussed along with the outlook for future directions.

This research was supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division and by the Center for Defect Physics an Energy Frontier Research Center. The Advanced Photon Source is supported by the Department of Energy, Scientific Users Facility Division.

Multiplication mechanisms and topology changes of interacting dislocation densities investigated by Discrete Dislocation Dynamics

Markus Stricker, Daniel Weygand

Institute for Applied Materials, Karlsruhe Institute of Technology, Kaiserstr. 12,
76131 Karlsruhe, Germany

The plastic deformation of crystalline structures such as metals is based on the movement of individual dislocations and during the process complex networks evolve. The further deformability of the specimen depends on the mobile dislocation density which is either produced by artificially introduced Frank-Read sources in the beginning or by naturally formed dislocation sources as a result of glissile reactions [1].

In Discrete Dislocation Dynamics (DDD) simulations [2], most of the time the influence of these natural sources is neglected or negligible [3], although their contribution to the accumulated dislocation density as well as overall plastic deformation is approx. 15% (Fig. 1, green), suggesting that they are rather active sources.

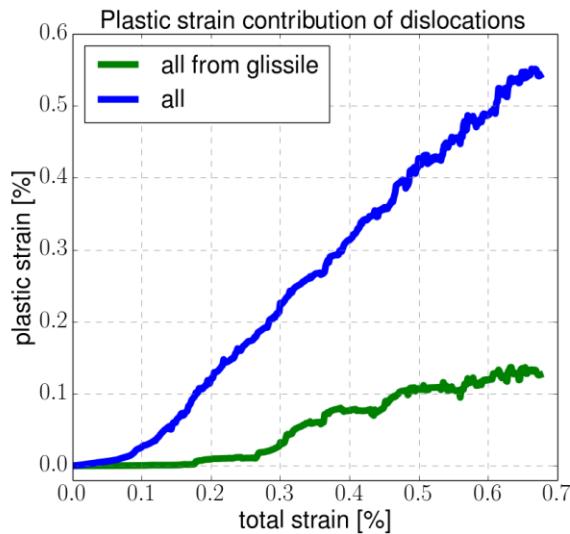


Figure 1: Plastic strain contribution from all dislocation resulting from glissile reactions (green) and total plastic strain produced by dislocations (blue) in tensile direction.

We track the activity of these sources during various loading conditions, different initial configurations (e.g. artificial and relaxed) and with different specimen sizes by DDD simulations and map their occurrence accordingly. An in-depth analysis of the resulting microstructures and their influence on plastic deformation of different specimen configurations as well as the dependency on sample dimensions is presented.

The financial support for the research group FOR1650 “Dislocation based Plasticity” funded by the DFG is gratefully acknowledged.

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The Discrete-Continuum Model: An important breakthrough to simulate the mechanical properties of dislocated crystals with complex boundary conditions

R. Gatti¹, O. Jamond^{1,2}, A. Roos², B. Devincre¹

¹ LEM, CNRS–ONERA, 92322 Châtillon, France

² DMSM, ONERA – The French Aerospace Lab, 92322 Châtillon, France

Plastic deformation of crystalline materials is the result of the collective movement of dislocations, in response of their mutual interactions, external applied loading and interactions with boundaries such as free surfaces, interfaces or grain boundaries. The dislocation microstructures emerging from such dynamics are intrinsically heterogeneous and the way they affect the mechanical properties is a puzzling problem. Therefore, the development of effective models for the study of this multiscale problem is a challenge in materials science.

A reliable tool to simulate crystal plasticity at the mesoscopic scale is the Discrete-Continuum Model (DCM). The DCM is based on a coupling between 3D Dislocation Dynamics (DD) simulations and Finite Element (FE) method. In particular, the DD simulation code is in charge of the dislocation microstructure evolution and dislocation short-range interactions, while long-range internal stress, displacement field, and boundary conditions (including surface and interface effects) are handled by the FE simulation code.

The DCM, which was proposed first in 1999 [1], has been significantly improved during the last two years [2]. It is now possible to handle problems with very large number of dislocations (the performances of the DCM algorithm overcome the multipole algorithm gain with large number of segments), to use non-regular FE meshes, to precisely take into account the influence of finite or periodic boundary conditions and consider isotropic and anisotropic elasticity.

Here, the new capabilities of the DCM are presented and illustrated with recent calculations made for Cu micro-samples and a SiGe nanostructure. With these examples, we show how the DCM is suitable to study plastic deformation in micro- and nano-objects. In particular, the calculation performed for the SiGe nanostructure highlights the attractive capability of running DD simulation in a full FE framework, using anisotropic elasticity.

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Numerical Simulation of Glide Dislocations in Persistent Slip Band

Miroslav Kolář¹, Jan Kratochvíl²

¹Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Trojanova 13, 120 00 Prague, Czech Republic

²Faculty of Civil Engineering, Czech Technical University in Prague, Thákurova 7, 166 29 Prague, Czech Republic

This contribution deals with the material imperfections in nanoscale having the line character, i.e. the crystallographic arrangement of atoms is disturbed along the dislocation line. Dislocations are modeled as smooth closed or open planar curves evolving in time and space [1]. Their motion is driven by the mean curvature flow

$$Bv = T\kappa + F,$$

where v denotes the normal velocity, κ is the mean curvature and F is the sum of all force terms acting on the dislocation curve in the normal direction. In this model B denotes the drag coefficient and T stands for the line tension.

In this work two unlike dislocations gliding in parallel slip planes in the channel of the persistent slip band are considered. The interaction between the dislocation and the channel wall is represented by elastic field of rigid dipoles, which act as potential wells. As the dislocations are pushed by the applied stress between two walls in the opposite directions, they bow out and attract each other forming a dipole. With the increasing stress the dislocations become more and more curved, until they separate. The objective is to determine the passing stress in the channel needed for the dislocations to escape one another and compare the generated stress field in the stress and strain controlled regimes. In the stress controlled regime the stress in the channel induced by boundary conditions is assumed to be uniform. In the strain controlled regime the sum of elastic and plastic strain is taken to be uniform. The stress control provides an upper estimate of the passing stress, whereas the strain control yields a lower estimate.

For numerical simulations we explore the parametric approach and semi-implicit flowing finite volume method [2]. However, the parametric approach itself exhibits unintended behavior, since during the time evolution, the grid points tend to accumulate in certain segments of the curve and can be sparse in some other segments. We overcome this problem by adding the tangential velocity to the parametric equations, which moves the grid points along the dislocation curve. Since the tangential terms do not affect the shape of the evolved curve, we can achieve better numerical stability.

This work is partly supported by the project No. P108/12/1463 *Two scales discrete-continuum approach to dislocation dynamics* of the Grant Agency of the Czech Republic.

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Dislocation-Dynamics based constitutive equations for crystalline plasticity of BCC metals at low temperature

Ghiath Monnet¹, Ludovic Vincent², Benoit Devincre³

¹EDF, MMC, ²CEA, SRMA, ³LEM, ONERA

Based on recent Dislocation Dynamics (DD) simulations, we propose a set of constitutive equations for crystalline plasticity in iron at low temperature. Assuming that the flow stress is controlled by the mobility of screw dislocations, the equations account for the strain rate sensitivity to the applied stress, temperature and microstructure parameters, such as the dislocation density and the average length of screw dislocation segments. The model differs from the Kocks-Mecking formalism in the sense that strengthening is not always conditioned by the dislocation line tension. It is shown that the difference in mobility between screw and non-screw dislocations impacts the average spacing and the strength of obstacles, which become a function of the temperature. This crystalline law is used in homogenization computation and in Finite-Element simulations to predict the mechanical response to tensile load of iron polycrystals and single crystals as a function of temperature. The predicted temperature dependency of the yield stress of polycrystals and of the critical stress of single crystals is in close agreement with experimental results. Furthermore, the model offers a smooth transition towards the Kocks-Mecking formalism known to capture the main physical features of plastic deformation in the athermal regime.

Discrete dislocation analysis of dislocation interactions with voids and precipitates

Lynn B. Munday, Joshua C. Crone, Chi-Chin Wu, Jaroslaw Knap

Army Research Laboratory, Aberdeen Proving Grounds, MD, 21005, USA

Material defects alter the evolution of dislocations by directly impeding their motion and perturbing the homogenous elastic fields of the bulk crystal. The small scale plasticity occurring in the vicinity of crystal defects is dependent on the motion of individual dislocations and is therefore well suited to models where plasticity is explicitly captured by the motion of discrete dislocations. In this work we study small scale plasticity near micron sized voids and impenetrable precipitates using the discrete dislocation approach of van der Giessen and Needleman[1] where the linear elastic fields due to dislocations in an infinite bulk crystal are superimposed onto the linear elastic fields produced by an auxiliary boundary value problem (BVP) containing the corrective image tractions on free surfaces and polarization stress due to the difference in material properties. The dislocation dynamics (DD) are simulated with ParaDiS from Lawrence Livermore National Lab [2], and the corrective BVP is solved using a parallel finite element (FE) code developed at ARL [3]. Both codes execute independently while a two-way parallel communication of elastic fields is performed through a distributed shared memory based virtual file driver. This allows ParaDis to perform dynamic load balancing to address the heterogeneous nature of dislocation motion and multiplication while the FE BVP solver utilizes a static domain decomposition strategy. In this presentation, we will discuss details of the DD-FE simulator and timings for the various components of the coupled DD-FE simulator including the FE linear solver.

We will use the FE-DD code to simulate dislocations interacting with inhomogeneities in three dimensions. Paradis allows us to model high dislocation densities in 3D and the parallel FE code will allow us to simulate large domains with finely resolved inhomogeneities. These simulations will be used to determine strain hardening mechanisms in crystal plasticity associated with Orowan strengthening and forest hardening. The role of inhomogeneity shape, size and density on the strain hardening mechanisms will also be studied. We would also like to study the effect of dislocation nucleation from the void or precipitate and its role in forest hardening.

This work was supported in part by a grant of high performance computing time from the US Army Research Laboratory DoD Supercomputing Resource Center at Aberdeen Proving Ground, Maryland.

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Anisotropic elasticity in dislocation dynamics

S. Aubry, A. Arsenlis

Lawrence Livermore National Laboratories, Livermore, CA (USA)

The dislocation dynamics (DD) method models dislocations behavior, interactions and evolution in BCC and FCC materials. It is used to predict the strength of a material that varies with pressure, strain rate, temperature and evolving dislocation density by providing input parameters to continuum based approaches. Continuum models based on constitutive equations built using dislocation dynamics and molecular dynamics data have been successfully compared to high energy physics experiments in BCC tantalum and vanadium.

Large scale dislocation dynamics simulations usually involve several millions of interacting dislocation segments. The stress at a point and interaction force between two segments need to be computed many times during simulations. Up to now, DD simulations were restricted to isotropic elasticity calculations because using anisotropic elasticity was perceived as too expensive. We evaluate the cost versus accuracy of using spherical harmonics series to approximate the anisotropic elastic Green's function in calculating stresses and forces between segments. The stress at a point is obtained by analytically integrating the spherical harmonics series once and the forces by integrating it analytically twice. We analyze the convergence and cost of using this approach and describe the elements of a fast implementation.

Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under Contract DE-AC52-07NA27344.

Discrete dislocation dynamics with anisotropic elasticity

Richard LeSar¹, John T. Graham¹, Anthony D. Rollett²

¹Department of Materials Science and Engineering, Iowa State University,
Ames, IA 50011, USA

²Department of Materials Science and Engineering, Carnegie Mellon University,
Pittsburgh, PA 15213, USA

Discrete dislocation dynamics simulations have been generally limited to modeling systems described by isotropic elasticity. Effects of anisotropy on dislocation interactions, which can be quite large, have been ignored because of the computational expense involved when including anisotropic elasticity. We present a different formalism of dislocation dynamics in which the dislocations are represented by steps in the deformation tensor. The deformation tensor is a direct measure of the slip in the lattice caused by the dislocations and can be considered as an eigenstrain.[1] The stresses arising from the dislocations are calculated with a fast-Fourier transform method,[2,3] from which the forces are determined and the equations of motion are solved. Because FFTs are calculated on a grid, there are some uncertainties that will be discussed. A notable advantage of this approach is that there is no computational penalty for including anisotropic elasticity. We will review the method and discuss applications.

This work was supported by the National Science Foundation at Iowa State University under Contract DMR-1308430. The authors acknowledge beneficial discussions with Ricardo Lebensohn of the Los Alamos National Laboratory.

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Statistical properties of the velocity of dislocations

Istvan Groma, Peter D. Ispanovity

Departmen of Materials Physics, Eotvos University Budapest, Hungary

In phenomenological theory of the evolution equation of dislocations quantities like mobile/immobile dislocations are often introduced. These quantities, however, are difficult to define on a quantitative manner. Since they are closely related to the velocity distribution of dislocations for a deeper understanding of the physical origin of the phenomenological dislocation theories it is of key importance to study the statistical properties of the velocity of dislocations.

In the first part of the presentation some analytical properties of the probability distribution of the velocity of dislocations are discussed. It is shown that the distribution has an inverse cubic tail. The theoretical result is verified by discrete dislocation dynamics simulations and experimental results on 2D crystals.

In the second part the time evolution of the velocity distributions obtained by 2D and 3D discrete dislocation dynamics simulations are analyzed during the relaxation of an initially random dislocation system [2] and under monotonic loading [1]. It is demonstrated that the velocity distribution exhibits power law type of scaling properties with a cut off depending on the system size.

Financial supports of the Hungarian Scientific Research Fund (OTKA) under contract numbers K-105335 and PD-105256 and of the European Commission under grant agreement No. CIG-321842 are acknowledged.

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Grain boundary modeling using an elasto-plastic theory of dislocation and disclination fields

V. Taupin¹, C. Fressengeas¹, L. Capolungo²

¹ Laboratoire d'Etude des Microstructures et de Mécanique des Matériaux (LEM3)

Université de Lorraine/CNRS, 57045 Metz, France

² G. W Woodruff School of Mechanical Engineering

Georgia Institute of Technology/CNRS, European Campus 57070 Metz, France

The elasto-plastic theory of crystal defect fields (disclinations and dislocations) [1] is used to describe in a continuous manner the elastic structure of symmetric tilt boundaries in various materials, including copper [2], orthorhombic olivine (a major constituent of Earth's mantle) [3] and quasi-two-dimensional fullerene polynanocrystals. Shear-coupled plasticity is further described in media where dislocation-based plasticity is limited, either by scarcity of the slip systems like in olivine [3], or because dislocation glide is restricted, as in polynanocrystals [4].

The smoothness of the present framework makes it attractive because it allows coping with defect core properties. Attractiveness also derives from its computational efficiency because, unlike atomistic simulations, the numerical scheme does not have to resolve the atomic vibrations with time steps in the femto-seconds. Indeed, the atoms and their fast vibrations are exchanged with the dissipative evolution of smooth dislocation/disclination density fields embedded in an elastic continuum. Thus, more or less standard finite element simulations allow monitoring the dynamics of crystal defect ensembles over time scales in the ms, under realistic loading rates and stresses. The role of slow mechanisms such as diffusion and dislocation climb may therefore be investigated.

The initial structure of the tilt boundaries is built from disclination dipole arrays defined after their atomistic topography. Lattice symmetry breaking in the boundary area induces non-locality of the elastic response of the boundary to applied loading. The corresponding characteristic nonlocal length scale has a very small value, about 0.5 Å in copper, implying that the non-locality of elasticity is limited to the defects core region. Nonlocal elasticity plays a key role in securing the driving force for the migration of the boundary. In addition to accurately retrieving the core energy of the tilt boundaries at all misorientations, the theory correctly captures the order of magnitude of the migration rate (about 0.1 μm/s in copper) and the two-folded dependence of the shear-migration coupling factor on the misorientation angle.

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Numerical Method and Applications for Generalized Disclination Theory

Chiqun Zhang, Amit Acharya

Carnegie Mellon University, Pittsburgh, Pennsylvania, 15213

We utilize a theory of generalized disclination mechanics introduced recently that goes beyond treating standard translational and rotational Volterra defects (dislocations and disclinations) in a continuously distributed approach; it is capable of treating the kinematics and dynamics of terminating lines of elastic distortion discontinuities. In this work, a numerical method, as well as a parallel program, based on finite element method and least square method is developed to solve for stress and energy fields of the generalized disclination system. With this numerical method, an isotropic dislocation problem, an anisotropic dislocation problem and a grain boundary problem are solved by applying generalized disclination dipoles. Furthermore, stress field and rotation field of a star disclination problem (which involves five single disclinations in a pentagon) are also calculated and discussed with this method. The examples show finite stress fields at the dislocation or disclination core area. As a practical application of our approach, we calculate elastic strain energies of interfacial dislocation arrays in bicrystals of *nonlinear*, anisotropic elastic materials (cf. Vattre and Demkowicz, *Acta Materialia*, 2013), including those of high-angle boundaries.

A Fast Fourier Transform Based Elasto-Viscoplastic Model for Polycrystalline Plasticity using Field Dislocation and Disclination Mechanics

L. Capolungo¹, M. Upadhyay¹, V. Taupin², C. Fressengeas², R. Lebensohn³

¹G. W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology / CNRS, Metz, France

²LEM3, Universite de Lorraine / CNRS, Metz, France

³Los Alamos National Laboratory, New Mexico, USA

To account for the role of elastic incompatibilities on the mechanical response of polycrystals, an extension of the infinitesimal-strain based elasto-viscoplastic fast Fourier transform based (EVPFFT) model is derived. Here, the incompatibility fields of interest are associated to the presence dislocation and disclinations. The latter, being rotational line defects, are expected to play a prominent role near material interface where large orientation changes can occur. Note here that scale dependence is necessarily introduced in the description of incompatible fields such that dislocations and disclinations can be in deemed statistical or geometrically necessary depending on the resolution size. The model is able to accommodate plastic deformation via the generation of both geometrically necessary dislocations and disclinations and is referred to as the phenomenological field dislocation and disclination mechanics (PMFDDM) model. The PMFDDM FFT framework derives motivation from the fine-scale field dislocation and disclination mechanics theory [2] and the EVP FFT polycrystal model. Precisely, the original EVP FFT framework [1] that finds its roots in the classical dislocation slip based crystal plasticity is extended to accommodate plasticity through the generation of geometrically necessary disclinations in the presence of statistical disclinations. The latter drive the evolution of the plastic curvature in the material. A phenomenological relationship between plastic curvature rate and couple stresses, similar to the prominent power law constitutive relationship between plastic strain rate and Cauchy stress, is thus introduced. Specific treatment of material interfaces is ensured via the use of Hadamard compatibility conditions.

To simulate the polycrystal response, a first estimate of the initial geometrically necessary dislocation and disclination densities, due to the abrupt change in orientation accross grain boundaries and triple junctions within the polycrystal, is obtained by computing the gradients of lattice orientations obtained from EBSD maps. Then upon loading the structure, the possible role of disclinations to plasticity, localization, cyclic response and size effects is investigated [3].

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Computational modelling of dislocation patterns and strain hardening in deformed metals

Shengxu Xia, Anter El-Azab

Purdue University

We present a novel continuum model of dislocation dynamics that predicts the main features of the crystal deformation at the mesoscale, including the evolution of the dislocation density distribution (dislocation pattern), slip patterns, internal stress and the stress-strain behavior under an arbitrary mechanical loading. The model is based on a set of kinetic equations of the curl type that govern the space and time evolution of the dislocation density in all slip systems. These equations are directly coupled via cross slip and short range reactions and indirectly through the long-range stress field of dislocations. The kinetic equations are coupled to crystal mechanics, stress equilibrium and deformation kinematics, through a staggered finite element scheme customized to capture the crystallographic nature of slip. We present results for the evolution of dislocation density and dislocation patterns, stress-strain behavior and hardening, and explain the role of cross slip and short range reactions in both patterning and hardening. We also present a probabilistic description of the internal elastic lattice rotation, stress and elastic strain fields and compare the statistics of the rotation analysis with discrete dislocation dynamics predictions and X-ray measurements. This work was supported by the U.S. DOE Office of Basic Energy Sciences, Division of Materials Science & Engineering via contract # DE-FG02-08ER46494 at Florida State University and by funding from the School of Nuclear Engineering at Purdue University.

Pair correlations and self-correlations in systems of curved dislocations

Thomas Hochrainer

Universität Bremen, BIME, 28359 Bremen, Germany

Dislocation pair correlations are a key to understanding the emergence and stability of dislocation structures. The finding that pair correlations in relaxed configurations of straight parallel edge dislocations are short-ranged was the key to the development of the statistical mechanics based continuum theory of dislocations of Groma and co-workers [1]. This stimulated the development of continuum dislocation dynamics theories of curved dislocations, which, however, had to first solve purely kinematic questions which are trivial in the point particle like descriptions of straight edge dislocations. Only preliminary investigations of pair correlations have been performed for three-dimensional systems of curved dislocations [2,3].

The kinematics of evolving systems of curved dislocations can be described by a hierarchy of plasticity theories using dislocation alignment tensors obtained by suitable integrations over orientation dependent mesoscopic dislocation densities [4]. We show how this procedure can be transferred to generate tensorial descriptions of pair densities and correlations which avoid higher dimensional correlations as introduced in [2]. This averaging also suggests novel approaches to averaging and evaluating correlations from three-dimensional dislocation configurations. We furthermore show that self-correlations in three dimensional dislocation systems are closely related to dislocation curvatures. The self-correlations therefore lead to line-tension effects in averaged descriptions of dislocations.

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FTMP-based Flow-Evolutionary Hypothesis and Its Application to Self-evolving Dislocation Substructures

Tadashi Hasebe

Kobe University, Nada, Kobe 657-8501, Japan

The study makes an attempt ultimately to reproduce the experimentally-observed inhomogeneous deformation-induce dislocation structures based on FTMP (Field Theory of Multiscale Plasticity)[1,2], where TEM observations for sheared single crystal samples with four typical crystallographic orientations are taken as recent successful examples. Crystal plasticity-based finite element simulations utilizing FTMP-based incompatibility model are conducted in connection with a working hypothesis called flow-evolutionary law, whose manifestation is given as a relationship between the incompatibility tensor and the energy-momentum tensor (duality diagram). The hypothesis provides a generalized law for the evolution of inhomogeneous fields and the attendant local plastic flow accompanied by energy dissipation. Demonstrated here are not only successful reproductions of the orientation-dependent dislocation substructures as shown in **Fig.1**, but also the associated energy flow with the evolved inhomogeneities visualized on the corresponding duality diagram, which also help identify the critical roles of the evolving substructures in determining the attendant mechanical responses.

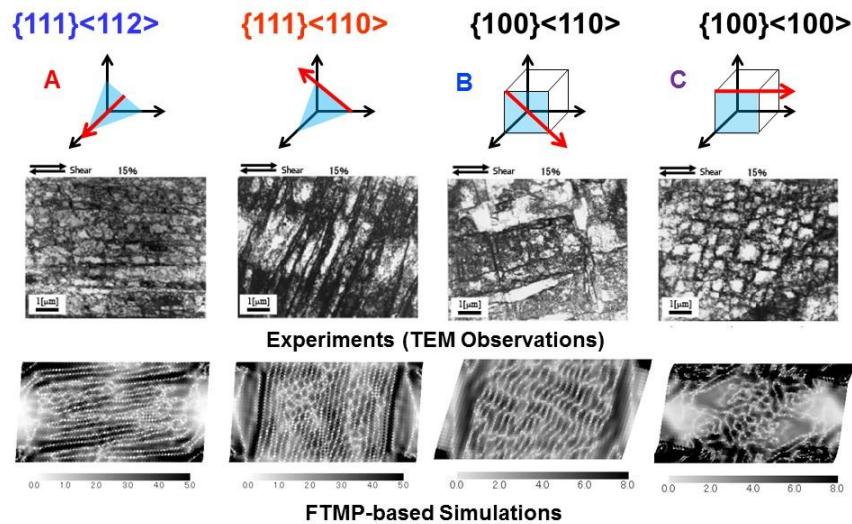


Figure 1: Simulated orientation-dependent dislocation substructures for Fe-Cr alloy single crystal under simple shear, comparing with transmission electron micrographs.

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A Continuum Approach Towards Formation of Persistent Slip Bands During Cyclic Deformation

Stefan Sandfeld¹, Benoit Devincre², Michael Zaiser¹

¹Institute of Materials Simulation (WW8), Friedrich-Alexander-University Erlangen-Nürnberg, Dr.-Mack-Str. 77, 90478 Fürth, Germany

²Laboratoire d'Etude des Microstructures, CNRS / ONERA, 29 avenue de la division Leclerc, BP 72 92322 Chatillon Cedex, France

Fatigue is a multiscale phenomenon involving processes from the atomic to the continuum scale but, despite its huge technological importance, has rarely been addressed from a comprehensive multiscale modeling point of view. In simulations, the physics of fatigue still poses important challenges as material behavior is governed by slip localization and dislocation patterning phenomena which cannot be predicted by standard continuum or atomistic approaches. Most current fatigue models are phenomenological in nature and the physical micro-mechanisms of fatigue leading e.g. to dislocation patterning, strain localisation, crack nucleation/propagation, so far cannot be described by a unified approach [1]. Present-day discrete dislocation dynamics (DDD) simulations for the first time provides a physically based model of emergent dislocation patterning, but cannot access the large cumulative strains associated with failure under cyclic loads.

In this paper we introduce the necessary conceptual steps to overcome this limitation by exploiting recently developed coarse-graining methods that map DDD onto continuum dislocation dynamics (CDD) simulations [2]. CDD simulations represent the same dynamics as DDD simulations in a continuum framework but are in general not limited by the number of dislocations or the accumulated plastic strain, because CDD is a dislocation density-based continuum description. We demonstrate how our continuum model of dislocation dynamics can be calibrated and validated by reference to the DDD models through conversion of the discrete micro-structure into a higher-dimensional density description, which contains additional information about the line orientation and curvature.

Furthermore, we show how the mechanisms that were used in recent DDD simulations for modeling of plastic strain localization during cyclic deformation (as e.g. persistent slip band (PSB) formation) can be transferred to the continuum model. In particular, CDD enables us to simulate the bowing-out of e.g. screw dislocations including the deposition of e.g. edge dislocations, which allows for simulation of PSBs exclusively based on dislocation mechanics of curved lines together with a minimum set of rules for e.g. dislocation annihilation.

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Continuum theory of dislocations: coarse-graining and correlations

P.-L. Valdenaire, A. Finel, Y. Le Bouar, B. Appolaire

Laboratoire d'Etude des Microstructures (ONERA-CNRS)
BP 72, 92322 Châtillon, France

A key issue in the theory of crystal plasticity is the transition between the discrete, where plastic flow is resolved at the scale of individual dislocations, and the continuum, where dislocations are represented by densities. This transition requires the use of coarse-graining procedures, similar to the ones that are used in the statistical mechanic treatment of out-of-equilibrium (or evolving) many-particle systems. Several attempts along this route have been proposed in the recent past. Our aim here is to shed a new light and to clarify the coarse-graining procedure that enables the mathematical transition between the dynamics of discrete dislocations and the transport equations that control the flow of mesoscopic dislocation densities. We emphasize in particular the role of the coarse-graining length on the correlation-induced stresses that emerge as result of the closure of the coarse-grained transport equations.

Power laws distributions as a signature of complexity: models from materials science

G. Ananthakrihsna

Materials Research Centre, Indian Institute of Science, Bangalore, India

Scale invariant power law distributions are ubiquitous to a wide variety of physical, chemical and biological systems ranging from geological to nanometer scales. Despite attempts by best of minds, the origin of power law distributions has remained mysterious. While we will not attempt to solve the general problem, we discuss three different physical situations drawn from materials science where power law distributions are reported. We show that models designed to capture the basic experimental features of the three physical situations automatically predict power law distributions. The three phenomena are the martensitic transformation (elastic), dynamics of peeling of an adhesive tape (visco-elastic) and the Portevin-Le Chatelier effect (plastic).

We first consider a two dimensional model for athermal marteniste transformation. The model includes long-range interaction between transformed domains, inertial effects and dissipation that accounts for acoustic energy. The model predicts experimental features such as thermal hysteresis and, growth and shrinkage of martensite domains under thermal cycling. The model also predicts the power law distribution for the amplitude of the acoustic emission signals during thermal cycling seen in experiments [1]

We next consider the peel front dynamics of an adhesive tape pulled at a uniform speed. The model predicts broad features of the peel dynamics such as the stick-slip motion and the stuck-peeled configurations of the peel front. The model also predicts the power law distribution of acoustic energy reported in experiments.

The third example we consider is the Portevin-Le Chatelier (PLC) effect, a kind of instability found when metallic alloys are deformed in window of strain rates. Three types of bands and the associated serrations are found with increasing strain rate. Analysis of experimental stress signals corresponding to type A serrations show that the stress drop magnitudes follow a power law distribution. Again, the Ananthakrishna model designed to recover the generic experimental features of the PLC effect also captures the power law distribution for stress drop magnitudes.

In all these cases, the power law distributions emerge automatically once attempts are made to capture the generic features of the phenomenon. Surprisingly, in each of these cases, the power law distribution emerges purely from deterministic dynamics.

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Portevin - LeChatelier like phenomena in confined compression of snow

Michael Zaiser, Tom Barraclough, Jane Blackford, Stefan Liebenstein,
Gerhard Weinländer

FAU Erlangen-Nuremberg

Snow is a cohesive-granular material of high porosity which is typically encountered at high homologous temperatures ($> 95\%$ of its melting temperature). Thus, thermodynamically driven microstructure evolution - in particular sintering processes - may occur on the typical timescale of deformation experiments. Shear deformation of snow is associated with strain softening due to the breaking of necks connecting ice granules, but this softening may be counter-acted by age hardening associated with rapid sintering processes which lead to the formation of new necks/bonds. If both competing processes occur on a comparable time scale, complex spatio-temporal deformation patterns may be encountered in the form of stress oscillations and propagating deformation bands.

We present results of confined compression experiments which show such phenomena in the form of compaction bands which during the course of an experiment repeatedly propagate along the compression direction of a laterally confined snow sample. These bands are associated with oscillations in the measured stress strain curve which superimpose on a global hardening trend. The overall phenomenology presents strong analogies with the Portevin-le Chatelier phenomenon encountered in metal alloys in the temperature/strain rate regime where age hardening due to dislocation pinning by moving solutes occurs on a comparable time scale as strain-driven softening due to dislocations breaking free from solute clouds under the action of applied stress.

We formulate a theoretical model which generalizes established frameworks for solid foam plasticity to account for internal length scales associated with the snow microstructure, strain softening processes, and age hardening due to rapid sintering. We demonstrate that by considering typical materials parameters for snow this framework allows to fully reproduce the observed phenomena.

Dislocation Pattern Evolution and Strain Hardening in FCC Metals through Discrete Dislocation Dynamics Simulations

Ahmed Hussein¹, Satish I. Rao², Michael D. Uchic³,
Dennis D. Dimuduk³, Jaafar A. El-Awady¹

¹Department of Mechanical Engineering, Johns Hopkins University,
Baltimore, MD 21218

²UES, Inc., 4401 Dayton-Xenia Rd, Dayton, OH, 45432-1894

³Air Force Research Laboratory, Materials and Manufacturing Directorate,
Wright-Patterson AFB, Dayton, OH, 45433-7812

Strain hardening in crystals and the accompanying dislocation pattern evolution (in the form of cell-like structures) are among the most difficult self-organizing behaviors to predict and explain. Screw character dislocation cross-slip has been typically presumed to play the main role in dislocation cell structure formation. However, many open questions remain regarding this mechanism. Recent molecular dynamics simulations showed that two cross-slip mechanisms, namely, surface and intersection mediated cross-slip mechanisms, exhibit a considerably lower activation energy than the traditionally accepted Friedel-Escaig cross-slip mechanism. In this work, we present the results of implementing these newly identified cross-slip mechanisms into discrete dislocation dynamics (DDD) simulations of nickel microcrystals, ranging in size from 0.5 to 10 microns in diameter. The conditions for each mechanism are discussed, along with their statistics and frequencies. The results show that dislocation cell structures form in simulation cells having diameters greater than 5 microns, as the dislocation density increases with increasing plastic strain. Smaller simulations cells however do not show any considerable cell formation at small strains as compared to the larger cells. These findings agree with recent experimental observations at the same crystal sizes.

Quantification and Comparison of Random Structures

Robert MacPherson¹, Jeremy Mason², Benjamin Schweinhart³

¹Institute for Advanced Study, Princeton, New Jersey 08540, USA

²Boğaziçi University, Bebek, Istanbul 34342, Turkey

³Princeton University, Princeton, New Jersey 08544, USA

Random structures abound at all length scales in materials science. This includes the contact graph of atoms in a metallic glass and the covalent bonds in a chalcogenide glass at the atomic scale, and dense dislocation networks and the bonding of cross-linked polymers at the nanometer scale. Examples at the micrometer scale include the structure of aerogels and the grain boundary network of a polycrystal, and at the macro scale the packing of granular materials and the branching pattern of a tree.

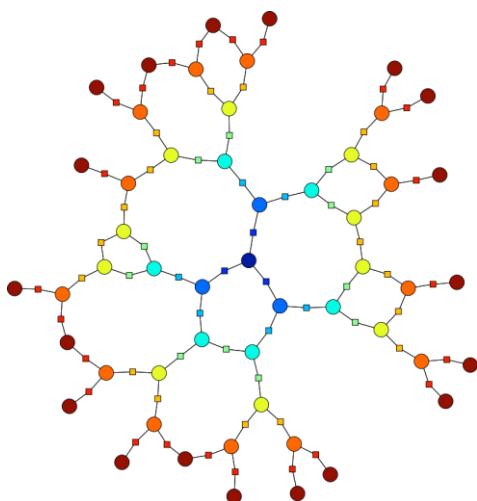


Figure 1: Swatch of a dislocation network, colored by distance from the base point

One feature of all of these random structures is that they defy characterization by the usual approach used in crystallography, that is, by the identification of a periodic unit and the classification of defects as deviations from periodicity. Nevertheless, some means of characterization is clearly necessary. How else would one identify the changes in atomic disorder when annealing a metallic glass, or the changes in a dislocation network resulting from the activation of cross-slip? While previous researchers have proposed a variety of techniques, any given one is usually applicable to only a few of the above examples, and none of them is able to completely characterize the connectivity of a generic random structure.

Our approach is to map a small portion of the structure to a colored graph, known as a swatch, that

gives a complete description of the local connectivity. By considering the probability distribution of swatch types, or local environments, we provide a complete characterization of the connectivity of the structure. That is, any question that may be asked about the connectivity may be answered using only this information. Furthermore, our classification admits a natural metric on the space of random structures. This allows us to, e.g., rigorously quantify the difference in the bonding of a metallic glass from a crystalline solid, or even to meaningfully compare the connectivity of a dislocation network and an aerogel. Finally, we provide evidence that these proposed quantities are practically computable.

This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE 114. Robert MacPherson and Jeremy Mason gratefully acknowledge support from the Institute for Advanced Study.

Spatiotemporal correlations between plastic events in the shear flow of amorphous solids: from molecular dynamics to mesoscopic models

Alexandre Nicolas¹, Francesco Puosi¹, Joerg Rottler², Jean-Louis Barrat¹

¹Univ. Grenoble 1/CNRS, LIPhy UMR 5588, Grenoble, F-38041, France

²Department of Physics and Astronomy, The University of British Columbia, 6224 Agricultural Road, Vancouver, British Columbia V6T 1Z4, Canada

The slow flow of amorphous solids exhibits striking heterogeneities: swift localised particle rearrangements take place in the midst of a more or less homogeneously deforming medium. Correlations and interactions between plastic events that involve of order 25 particles (in 2D) control the evolution of the strain field on much longer length and time scales. Here we develop a mesoscopic (coarse-grained) model of plastic flow that is systematically linked to atomistic molecular dynamics simulations. We first determine the time-dependent elastic response of an amorphous medium to an isolated plastic event and show that, despite large fluctuations, it can be modeled with the picture of 2D Eshelby inclusions with an elastic Green's function displaying quadrupolar symmetry, viz. $G(r) \sim \cos(4\theta)/r^2$ [1]. We then determine the full spatiotemporal correlation functions $C(\mathbf{r}, t)$ (inset of figure for one value of $t > 0$) between elementary plastic events in a sheared athermal glassy solid (main figure, color scale indicates level of nonaffine strain) [2]. Our mesoscopic description builds upon the picture of localized, short-lived and highly dissipative events observed in the MD simulations by considering elastoplastic blocks of size of a rearranging region. Upon reaching a local yield stress drawn from a disorder distribution, elastic interactions occur instantaneously and the local stress evolves according to

$$\dot{\sigma}(r) = \mu \dot{\epsilon} + 2\mu \int d\hat{r} G(r, \hat{r}) \epsilon_{pl}(\hat{r})$$

We achieve excellent agreement for all aspects of bulk rheology between atomistic simulations and this class of mesoscopic models. Quadrupolar plastic correlations (see figure) are also successfully reproduced, but quantitative agreement of dynamical plastic correlations requires considering additional physics, in particular including the effect of elastic heterogeneity on the propagation of shear waves as well as their finite propagation speed.

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Spatial structure and time evolution of breaking bursts in a fiber bundle model of disordered materials

Ferenc Kun, Zsuzsa Danku

Department of Theoretical Physics, University of Debrecen, H-4010 Debrecen, P.O.Box:
5 Hungary

The fracture of heterogeneous materials proceeds in bursts which can be recorded by optical, acoustic or electromagnetic techniques. Although crackling noise is the major source of information about the microscopic dynamics of fracture, its analysis mainly focuses on the statistics of crackling events considering fracture as a stochastic point-process. Here we investigate the temporal and spatial evolution of single bursts emerging in heterogeneous materials under a constant external load using a fiber bundle model. In the model fibers break due to two physical mechanisms: (i) a fiber breaks immediately when the load on it exceeds the local failure strength; (ii) fibers subject to load undergo an aging process accumulating internal damage and break when their damage exceeds a random threshold value. As a consequence under a constant load slowly damaging fibers trigger bursts of immediate breakings analogous to crackling avalanches in real experiments [1,2].

Computer simulations revealed a complex time evolution and spatial structure of single crackling bursts in the model (see Fig. 1 for an example). We demonstrate that

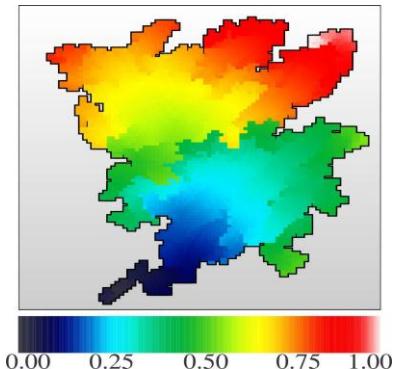


Figure 1: Time evolution of a single burst where the color indicates the time sequence of local breakings.

when the stress redistribution after fiber failures is localized, the average temporal shape of crackling pulses has a right handed asymmetry due to the gradual acceleration of bursts. For long range interaction, however, a symmetric shape with parabolic functional form is obtained. In spite of the compact space-filling internal structure of bursts (Fig. 1), their external frontier proved to be a fractal with dimension $D_f = 1.25$. The same fractal dimension characterizes the geometrical structure of the propagating crack front along which bursts are localized. Our analysis revealed that the pulse shape and spatial evolution of bursts are correlated which can be exploited in materials' testing [2].

This work was supported by the projects TAMOP-4.2.2.A-11/1/KONV-2012-0036 and OTKA K84157.

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Field Dislocation Mechanics in the tectonic and sub-inter-supersonic regimes

Xiaohan Zhang, Amit Acharya

Carnegie Mellon University, Pittsburgh, Pennsylvania, 15217, USA

We explore the potential of modeling both sub-inter-supersonic dislocation motion and dynamic ruptures using Field Dislocation Mechanics (FDM), a non-linear, partial differential equation (PDE) based model of the mechanics of dislocations. A simplified two dimensional FDM model is developed and numerically studied. The model assumes the whole body to be elastic except for a thin layer governed by dislocation plasticity. Dislocations are assumed to move along the layer only. When modeling a fault, the layer is assumed to be elastically weaker than the surrounding and to admit elastic damage on the passage of the rupture front.

One of the main results is that FDM is demonstrated to be able to capture the kinetic relationship of a single dislocation in different velocity regimes (from subsonic to supersonic); qualitative agreement with a Molecular Dynamics simulation of a similar problem is obtained.

The 2-D model is then explored more to show some basic advancements of modeling tectonic phenomenon using FDM. The slip evolution at a spatial point due to the passage of a rupture front is found to be in agreement with short-slip-duration seismological observations. The traction profile shows a strong strengthening effect behind the rupture front as well. A transverse displacement field in qualitative agreement with observations from an earthquake is also shown. These results suggest that FDM is able to address some fundamental issues in dynamic rupture, making it a valuable complementary tool to conventional crack-mechanics based rupture models for the investigation of earthquake related phenomena.

Instabilities & Patterning in Plasticity: Review and Perspectives

Elias C. Aifantis

Aristotle University of Thessaloniki, Thessaloniki GR 54124, Greece

After critically reviewing the early work on plastic instabilities – to which Ladislás Kubin was a major contributor (improving, among other things, the initial models by the author and coworkers on dislocation patterning, persistent slip bands, and Portevin-Le Chatelier bands) – the discussion is focused at the nanoscale. Example problems on size effects, intermittent plasticity and serrated flow are discussed. These require the incorporation of stochasticity in the previously advanced gradient plasticity models. It is also shown that interpretation of related statistical deformation features through usual power laws based on Boltzmann-Gibbs entropy do not hold and one needs to use Tsallis q-entropy considerations for modeling the experimental observations.

A continuum theory for defect dynamics in metallic glasses

Amit Acharya

Carnegie Mellon University

Based on an effort to understand a beautiful and vast literature starting from Kleman and Sadoc, through Nelson and on to recent work of Widom and co-workers, and Takeuchi and Edagawa, we contemplate the modeling of metallic glasses as a 'sea' of geometrically frustrated regular tetrahedra arranged predominantly in clusters of five around 'static' backbones of 5-fold disclination lines. This sea is thought of as punctuated by mobile 4 and 6-fold disclination dipole lines that can be interpreted as dislocation lines (with spread out cores) in the medium. There appears to be evidence that regions of non-pentagonal packing seem to suffer the most plasticity for amorphous materials. I combine these insights based essentially on homotopy theory describing possible lowest-energy static states of the glass and DFT and atomistic simulations for glass structure with the nonlinear pde dynamics of Field Dislocation Mechanics, the 21st century embodiment of the continuous theory of dislocations. The result is a model for dissipative defect dynamics in metallic glasses and similar amorphous materials. With no further assumptions beyond this kinematics and the simplest linear kinetic assumption arising from enforcing positive mechanical dissipation, the model is shown to be capable of demonstrating

- 1) the deterministic origin of what may practically only be considered a stochastic internal stress field;
- 2) dilatancy in plastic flow;
- 3) pressure dependence of plastic flow;
- 4) threshold behavior in the motion of dislocations in response to stress
- 5) the propensity of localized deformation in the form of shear bands due to the evolution of plastic deformation in the model.

Continuum Dislocation Dynamics simulation of dislocation structure evolution in torsion of micro-pillars

Alireza Ebrahimi¹, Mehran Monavari², Stefan Sandfeld², Daniel Weygand³, Thomas Hochrainer¹

¹BIME - Bremer Institut für Strukturmechanik und Produktionsanlagen, Universität Bremen,
28359 Bremen, Germany

²Friedrich-Alexander-Universität Erlangen-Nürnberg, Dr.-Mack-Str. 77, Fürth, Germany

³Institut für Angewandte Materialien, Karlsruher Institut für Technologie, 76131 Karlsruhe,
Germany

Plastic deformation of metals is the result of the motion and interaction of dislocations. Dislocation density based modeling of crystal plasticity remains one of the central challenges in multi scale materials modeling. Continuum dislocation dynamics(CDD) is originally based on a higher dimensional dislocation density tensor. We employ a simplified version of CDD obtained by closing a tensor expansion of the higher dimensional theory at low order which yields a CDD of curved dislocations based on only three internal state variables per slip system [1,2]. These equations define a dislocation flux based crystal plasticity law which does not require distinguishing geometrically necessary and statistically stored dislocations. The evolution equations are solved by a three-dimensional discontinuous Galerkin method guaranteeing the conservation of the total number of dislocations [3]. Different boundary conditions including closed and open boundary conditions are presented. Closed boundary conditions result in dislocation pile ups at the boundaries of the domain; free boundary conditions allow for out-flow of dislocations through the surfaces. We compare the plastic slip and the resulting dislocation microstructure in simulations of torsion and compression of micro-pillars with results of 3D discrete dislocation dynamics simulations. Salient features of the dislocation microstructure can be predicted by the continuum dislocation dynamics theory.

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Free energy of steps on the surface of faceted solids

Rodrigo Freitas, Timofey Frolov, Mark Asta

Department of Materials Science & Engineering, University of California Berkeley,
Berkeley, CA, USA

The properties of solid-liquid interfaces are known to play critical roles in solidification processes. Particularly special importance is given to thermodynamic quantities that describe the equilibrium state of these surfaces. For example, on the solid-liquid-vapor heteroepitaxial growth of semiconductor nanowires the crystal nucleation process on the faceted solid-liquid interface is influenced by the solid-liquid and vapor-solid interfacial free energies, and also by the free energies of associated steps at these faceted interfaces.

Crystal-growth theories and mesoscale simulation methods depend on quantitative information about these properties, which are often poorly characterized from experimental measurements.

Molecular Dynamics simulations provide a natural framework for investigation of solid interfaces, the capillary fluctuation method [1] is one example where the small anisotropy of solid-liquid interfacial free energy of materials with atomically rough interfaces was computed accurately using MD simulations. Properties of steps at faceted solid-liquid interfaces are far less investigated than the properties of atomically rough solid-liquid interfaces. For this reason methods to extract useful thermodynamic information from simulations [2] are rare.

In our work we use the formalism of the capillary fluctuation method to study properties of steps on faceted crystal surfaces. From equilibrium atomistic simulations of steps on (111) surfaces of Copper, fig.1, we compute accurately the step free energy at a temperature close to the melting point. Using thermodynamic integration we were then able to obtain the temperature dependence of the step free energy. We have also computed relevant correlation functions to analyze the characteristics of the atomic diffusion process responsible for the step fluctuations.

This research was supported by the US National Science Foundation. T.F. was also funded by the Miller Institute.

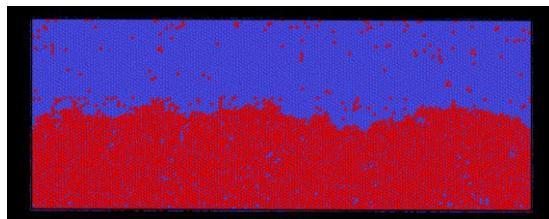


Figure 1: step configuration on a (111) surface of Copper. Red atoms are on the first layer (step).

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Anisotropic geometrical damage for dynamic processes

Ioan R. Ionescu, Jia Li

LSPM, University Paris-Nord, Sorbonne-Paris-Cité, France 99, Av. J.B. Clement, 93430
Villetaneuse, France

We develop here an anisotropic damage model for dynamic processes. The coupled phenomena analyzed here deal with a loading wave which damages the material and changes the propagation properties of material. In this way the speed and the profile of the loading wave is perturbed by the damage processes induced by it. The geometric damage model, represented by micro-cracks growing under dynamical loading, is able to describe the link between the micro and macro-scale characteristic times and the rate of deformation. The micro-crack growth is activated in some privileged directions according to the applied macroscopic loads and the velocity of the micro-crack propagation is estimated by the dynamic stress intensity factor. A discontinuous Galerkin numerical scheme for the numerical integration of the damage model is also proposed. The scheme is robust and very precise. Several two-dimensional boundary value problems are selected to illustrate the model and to analyze the robustness of the numerical algorithm.

Interaction of dislocation triole with standing acoustic wave

Ramil T. Murzaev¹, Dmitry V. Bachurin^{1,2}, Sergey V. Dmitriev¹, Airat A. Nazarov¹

¹Institute for metals superplasticity problems of Russian Academy of Sciences,
450001 Ufa, Russia

²Institute for Applied Materials – Applied Materials Physics, Karlsruhe Institute of
Technology, 76344 Eggenstein-Leopoldshafen, Germany

In crystalline materials under the influence of high amplitude ultrasonic waves the development of fatigue damage occurs, which is directly connected with the peculiarities of the dislocation structure. In this regard, the task of creating materials with good fatigue characteristics includes primarily the study of the mechanisms of formation and dynamics of dislocation structures, mainly dislocation multipoles. The main goal of the work is the study of dynamics of the dislocation tripole interacting with a standing sound wave in a wide frequency range. This phenomenon is not yet well investigated in the literature.

During plastic deformation the dislocation tripole may be formed by impact of a single dislocation with an immobile dislocation dipole. The structure of the dislocation tripole is very multiform. We have considered 15 different stable triole configurations. The calculations were made using 2D discrete dislocation model. For numerical integration of the motion equations the fourth-order Runge-Kutte method was applied.

Only three of the 15 stable configurations of dislocation tripole were found to be mobile under ultrasonic influence. The other dislocation tripole were either immobile, or rearranged themselves into the aforesaid three stable structures. Dynamics of the drift of these configurations were analysed in detail. A criteria, allowing us to determine whether the dislocation triole interacting with an acoustic wave move or not, were formulated. Maximal drift velocity and the maximal frequency as the functions of the oscillation amplitude were also investigated.

Scale-free dynamics in dislocation systems

Péter D. Ispánovity¹, Lasse Laurson², Michael Zaiser³, Stefano Zapperi^{4,5}, Mikko Alava²,
Dániel Tüzes¹, István Groma¹

¹Department of Materials Physics, Eötvös University Budapest, Hungary

²Department of Applied Physics, Aalto University, Espoo, Finland

³Department of Materials Science, University of Erlangen-Nürnberg, Germany

⁴CNR-IENI, Milano, Italy

⁵ISI Foundation, Torino, Italy

Recent experimental and modeling evidences show that micron-scale crystalline materials deform via intermittent abrupt strain bursts. These avalanches caused by the sudden collective motion of lattice dislocations make the deformation process unpredictable at this scale. It is, therefore, of high importance to give a profound understanding of the statistical properties of these dislocation avalanches.

In this talk we explore the behavior of dislocation avalanches in terms of two dimensional discrete dislocation dynamics (DDD). To this end, quasistatic stress-controlled simulations are conducted with three DDD methods differing in the spatiotemporal discretization and the dynamics assumed for individual dislocations. We find that each model exhibits identical avalanche dynamics with the following properties: (i) the avalanche exponent τ is $\tau \approx 1.0$, that is significantly smaller than predicted by mean-field depinning (MFD) theory and (ii) the avalanche cutoff diverges with increasing system size at any studied applied stress level. The latter property is inconsistent with cutoff scaling in depinning systems and with the existence of a critical yield point. We, therefore, conclude that dislocation systems belong to a different universality class than MFD.

In order to understand the origin of the found behavior we also study strain burst scaling in a mesoscopic model of plasticity where the inhomogeneity of the material microstructure is represented by a stochastic yield stress field. Under quite general conditions we find equivalent behavior to that of DDD.

Financial supports of the Hungarian Scientific Research Fund (OTKA) under contract numbers PD-105256 and K-105335 and of the European Commission under grant agreement No. CIG-321842 are acknowledged.

Atomistic Modeling on Elastic Heterogeneities Evolution and Elementary Activations in Metallic Glass

Yue Fan¹, Takuya Iwashita², Takeshi Egami^{1,2,3}

¹Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

²Department of Physics and Astronomy, Joint Institute for Neutron Sciences, and

³Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee 37996, USA

Metallic glasses are emerging as a new category of materials with many promising features, e.g. high irradiation tolerance, high strength, etc. The structure-property relation in metallic glasses, however, is still a challenging and unsolved issue. We investigated the relation between the stability of a metallic glass system and its atomic structure. The stability is observed strongly related to the collective arrangement of atoms, rather than the properties of single atoms. Particularly, in an instantly quenched system, the “soft” atoms with the lowest 5% atomic shear modulus tend to cluster together and show a highly heterogeneous distribution; while in an annealed system, the soft atoms are relatively more homogenously distributed and overall leads to the stabilization of the system.

We further studied the elementary excitations by analyzing the relation between activation energy barriers, atomic displacements and atomic stress changes. It is identified that the elementary activations are elastic-like and highly localized within the first nearest neighbors. A quantitative potential energy landscape for metallic glasses is further constructed. Clarifications of different results obtained in previous studies, as well as implications of the present work, are also discussed.

Dislocation Pattern Evolution and Strain Hardening in FCC Metals through Discrete Dislocation Dynamics Simulations

Ahmed Hussein¹, Satish I. Rao², Michael D. Uchic³,
Dennis D. Dimuduk³, Jaafar A. ElAwady¹

¹Department of Mechanical Engineering, Johns Hopkins University, Baltimore, MD
21218

²UES, Inc., 4401 DaytonXenia Rd, Dayton, OH, 454321894

³Air Force Research Laboratory, Materials and Manufacturing
Directorate, WrightPatterson
AFB, Dayton, OH, 454337812

Strain hardening in crystals and the accompanying dislocation pattern evolution (in the form of Celllike structures) are among the most difficult selforganizing behaviors to predict and explain.

Screw character dislocation crossslip has been typically presumed to play the main role in dislocation cell structure formation. However, many open questions remain regarding this mechanism. Recent molecular dynamics simulations showed that two crossslip mechanisms, namely, surface and intersection mediated crossslip mechanisms, exhibit a considerably lower activation energy than the traditionally accepted FriedelEscaig crossslip mechanism. In this work, we present the results of implementing these newly identified crossslip mechanisms into discrete dislocation dynamics (DDD) simulations of nickel microcrystals, ranging in size from 0.5 to 10 microns in diameter. The conditions for each mechanism are discussed, along with their statistics and frequencies. The results show that dislocation cell structures form in simulation cells having diameters greater than 5 microns, as the dislocation density increases with increasing plastic strain. Smaller simulations cells however do not show any considerable cell formation at small strains as compared to the larger cells.

Frank-Read sources in the Continuum Dislocation Dynamics (CDD) theory: averaging aspects and 3D benchmarks

Mehran Monavari¹, Alireza Ebrahimi², Thomas Hochrainer², Daniel Weygand³, Stefan Sandfeld¹

¹Friedrich-Alexander-Universität Erlangen-Nürnberg, 90762 Fürth, Germany

²University of Bremen, 28334 Bremen, Germany

³Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

The Continuum Dislocation Dynamic (CDD) theory is based on the higher dimensional generalization of the classical Kröner-Nye dislocation density tensor [1]. This theory addresses the problem of statistical averaging of dislocation microstructure properties and provides a framework for correct representation of the evolution of dislocation microstructure. In CDD, dislocation microstructure is approximated through statistical averages of internal variables such as total dislocation density and dislocations curvature.

In this paper we present a mesoscale crystal plasticity framework based on the CDD theory. This framework consists of two parts: a) solving the elastic boundary value problem (BVP) for prescribed boundary conditions together with eigenstrain of dislocation microstructure; b) evolution of the dislocation microstructure in the crystal which is described by CDD [2].

The BVP and CDD problem are solved by the Galerkin and discontinuous Galerkin FEM, respectively, and are coupled through the eigenstrain and resulting stress fields.

An important step in our simulation is obtaining initial values for the continuous dislocation microstructure. Discrete dislocation dynamics models use either given dislocations or a distribution of Frank-Read sources. We discuss different methods for obtaining these initial values for our *continuum* model by e.g. relaxing given dislocation fields or by a continuum version of a Frank-Read source [3]. We study the coarse graining of the time intermittent behavior of Frank-Read sources and compare the evolution and multiplications of dislocations with discrete dislocation dynamics simulations in torsion and tension of 3D FCC micro pillars. Finally, we will also discuss numerical and implementation issues e.g. for our Discontinuous Galerkin finite element implementation, the mesh refinement criterion and the computational efficiency of the method.

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The evolution of plastic flow localization from the micro- to the macro-scale level

Lev B. Zuev

Institute of Strength Physics and Materials Science, SB RAS, 634055, Tomsk, Russia

Using specially designed speckle photography method, the localization of plastic deformation was investigated for a wide range of materials, i.e. metals, alloys, alkali halide crystals, ceramics and rocks [1, 2]. The plastic deformation was found to exhibit a localization behavior at the macro- and micro-scale levels (dislocations and grains). Numerical treatment of experimental evidence was performed. The results suggest that the following relation will hold for the stage of linear work hardening in all materials:

$$\lambda \cdot V_{aw} \approx \frac{1}{2} \chi \cdot V_t \approx Z, \quad (1)$$

where λ is the characteristic spatial scale of deformation macro-localization; χ , interparticle distance in the studied material lattice; V_{aw} , the motion rate of localized plasticity nuclei; V_t , the motion velocity of transverse elastic waves propagating in the deforming solid and Z is a constant. For all materials investigated, $Z \approx 10^{-7} \text{ m}^2/\text{s}$ and $\langle 2\lambda \cdot V_{aw}/\chi \cdot V_t \rangle = 0.99 \approx 1$, which supports the validity of relation (1).

It is also found that for plastic deformation occurring on a dislocation scale level and realizing via the motion of chaotically distributed dislocations the following relation holds true:

$$\langle l \rangle \cdot \langle V_{disl} \rangle \approx Z, \quad (2)$$

which is similar to (1), evidently. Here $\langle l \rangle$ and $\langle V_{disl} \rangle$ are the mean values of the dislocation path and velocity, respectively.

Experimental verification of relations (1) and (2) was provided additionally in the investigations of localized plasticity development in polycrystalline aluminum having grain sizes in the range $10 \mu\text{m} \leq d \leq 10 \text{ mm}$. The relationship $\lambda \cdot V_{aw} \approx Z$ was found to hold true for two regions of the dependency $V_{aw}(d)$ obtained for the studied material. On this base a new approach is proposed for insight into the physical meaning of the well-known Hall-Petch relation.

The relationship (1) suggests that the characteristics of plastic and elastic deformation are closely related [3]. Moreover, the localization behavior of plastic deformation is governed on the different scale levels by the elastic characteristics of the deforming medium. Thus the value Z from relations (1) and (2) is an elastic-plastic invariant of deformation in solids.

It becomes evident that the elastic-plastic strain invariant is of vital importance for gaining of a physical insight into the phenomenon of plastic flow localization. It is significant that (1) relates the characteristics of elastic waves and those of localized plasticity autowaves [2], which allows one to associate plasticity with both crystal defects and ideal lattice properties. The importance of this finding for plasticity model building cannot be too strongly emphasized.

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Numerical Simulation of Dislocation Annihilation by Cross-Slip

Michal Beneš¹, Petr Pauš¹, Jan Kratochvíl²

¹ Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Trojanova 13, 120 00 Prague, Czech Republic

² Faculty of Civil Engineering, Czech Technical University in Prague, Thákurova 7, 166 29 Prague, Czech Republic

Cross-slip is treated as the deterministic, mechanically activated process governed by the applied stress, by the interaction force between approaching screw dislocations of the opposite sign and by the line tension controlled by the persistent-slip band width [1]. The glide dislocations are represented by parametrically described curves moving in slip planes. The simulation model is based on the numerical solution of the dislocation motion law belonging to the class of curvature

driven curve dynamics [2]. We focus on the simulation of the cross-slip of two dislocations Γ_1 and Γ_2 evolving in different slip planes according to

$$B_i v_i = T_i \kappa_i + F_i, \quad i=1,2,$$

where v_i denotes the normal velocity, κ_i the mean curvature of Γ_i , and F_i the sum of all forces acting on Γ_i , B_i is the drag coefficient and T_i the line tension of Γ_i .

Cross-slip leads to annihilation of the dipolar parts of dislocations. In the changed topology each dislocation evolves in two slip planes and the cross-slip plane. The goal of our work is to determine the conditions under which the cross-slip occurs. The simulation of the dislocation evolution and merging is performed by the improved parametric approach. Numerical stability is enhanced by the tangential redistribution of the discretization points [3]. The proposed model predicts the critical annihilation distance and the cyclic saturation stress in agreement with the available experimental data [4].

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A numerical spectral approach for solving elasto-static field dislocation and g-disclination mechanics

Stéphane Berbenni, Vincent Taupin, Komlan Sénam Djaka, Claude Fressengeas

Laboratoire d'Etude des Microstructures et de Mécanique des Matériaux, LEM3, UMR
CNRS 7239, University of Lorraine, Ile du Saulcy, 57045 Metz, France

Recently, a small-distortion theory of coupled plasticity and phase transformation accounting for the kinematics and dynamics of generalized defects, i.e., dislocations and generalized (g-) disclinations, has been proposed [1].

In the present contribution, a numerical spectral approach is developed to solve the elasto-static equations of field dislocation and g-disclination mechanics set out in this theory for periodic media. Given the spatial distribution of Nye's dislocation density and/or g-disclination density tensors in heterogeneous or homogenous linear elastic media, the incompatible and compatible elastic distortions are obtained from the solution of Poisson and Navier-type equations in the Fourier space by using a Fast Fourier Transform method (FFT). The elastic strain/rotation and Cauchy stress tensors are calculated using the inverse FFT. Numerical examples are provided for homogeneous linear elastic isotropic solids. The results include the stress and elastic rotation fields of single screw and edge dislocations, standard wedge disclinations and associated dipoles, as well as 'twinning g-disclinations'. In order to validate the present spectral approach, comparisons are made with analytical solutions using the Riemann-Graves integral operator [2], and with Finite Element results assuming a Gaussian regularization of single dislocation and g-disclination densities.

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A Multiscale Study of Solidification: Interfacial atomistic properties and their consequences at the mesoscale microstructures

Tomorr Haxhimali

Lawrence Livermore National Laboratory, Livermore, California 94550, USA

Here, I will present a thorough multi-scale analysis of solidification in pure and alloy materials. Important phenomena in materials processing, such as dendritic growth during solidification or electro-deposition, involve a wide range of length scales from the atomic level up to product dimensions.

I will initially take a bottom up approach by starting the discussion with describing the atomistic nature of the solid-melt interface.

Above a material dependent roughening temperature the interface is atomically rough which entails that every point of the interface is a site for nucleation. The collective nucleation events make these interfaces subtle to fluctuations that give rise to instabilities, like Mullins-Sekerka, at the nano-scale. The governing equations at the meso-scale describe the propagation of a diffusive field, like molar composition and/or temperature, which magnifies Mullins-Sekerka instabilities at the interface. The system reorganizes itself into a more complex mode of behavior that results in pattern selection in dendritic microstructures.

Below the roughening temperature the interface is atomically smooth which results in a layer-by-layer growth due to isolated nucleation events. A perfect example is Silicon along the $<111>$ interface. I will briefly discuss the consequences of such geometry in the kinetics of this interface for Si nanowire growth [1].

We employ Molecular Dynamics to model the interfacial free energy as a linear combination of the spherical harmonics. For systems with underlying cubic symmetry (like bcc, fcc) the expansion keeps only the kubic harmonics, and hexagonal harmonics for HCP systems.

At the meso-scale we then employ boundary layer method and phase field to study the selected dendrite growth in dendritic microstructures. The phase-field approach, enhanced by optimal asymptotic methods, adaptive mesh refinement and hybrid schemes, copes with a part of the range of length scales, from few tens of microns to millimeters, and provides an effective continuum modeling technique for moving boundary problems.

I will present results for alloys with cubic symmetry like Al-Zn alloys [2] as well as for hexagonal ones like Mg alloys. Also, some recent results for the electro-deposition using phase-field will be shown.

* This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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Modeling of dislocation mechanisms and the influence of the γ/γ' lattice misfit on the dislocation assisted creep of high temperature Ni-base superalloys

S.M. Hafez Haghigat¹, R.C. Reed², D. Raabe¹

¹Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany

²Department of Engineering Science, University of Oxford, Parks Road, Oxford, OX1 3PJ, UK

High temperature creep is one of the life limiting factors for the Ni-base superalloys used in the blades of the gas turbines used for jet propulsion and power generation. We use discrete dislocation dynamics simulations to study the influence of loading conditions and lattice misfit on the plastic strain and its resultant microstructure in the low stress creep regime of these materials. A hybrid glide-climb dislocation mobility law [1] is used to treat the interaction of dislocations in the γ matrix with the γ' particles. This modelling approach allows the necessary contributions to the dislocation climb process to be treated so that dislocation flow can be simulated. Our approach allows an analysis of the propagation of dislocations through the vertical and horizontal channels under the technologically-important case of uniaxial loading, and provides details of locked configurations in vertical channels. Our results demonstrate that for 200 MPa applied along the [111] direction, the creep rate is significantly lower than for loading along [100]. In the latter case, the creep strain increases monotonically due to the propagation of dislocations in the channels oriented perpendicular to the loading direction, the so-called horizontal channel, so that dislocation networks form in agreement with experiment. The anisotropy of dislocations microstructure deposited along the γ/γ' interfaces is investigated in detail for both loading configurations. It is found that the low creep rate for the [111] loading relates to the geometrical prevention of dislocation climb at the γ/γ' interfaces, rather than to the number of active slip systems and their corresponding Schmid factors. Incorporation of the γ/γ' lattice misfit confirms that negative lattice misfit and its resultant misfit stress reduce substantially the climb-assisted dislocation creep. Our detailed microstructure analysis indicates that dislocations are driven to move from the edges towards the centres of cuboidal γ' particles, thus resulting in reduced dislocation interactions near the particle edges and corners.

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Microstructural characterization and petro-physics from natural heterogeneous rocks and the upscaling of properties

Jie Liu¹, Reem Freij-Ayoub², Gerald G. Pereira³, Klaus Regenauer-Lieb^{1,2}

¹Laboratory for Multiscale Earth System Dynamics and Geothermal Research, School of Earth and Environment, The University of Western Australia, M004, 35 Stirling Highway, Crawley, WA 6009, Australia

²CSIRO Earth science and Resource Engineering, 26 Dick Perry Ave., Kensington, WA 6151, Australia

³CSIRO Mathematics, Informatics and Statistics, Private Bag 33, Clayton South, Vic, 3168. Australia

We present a workflow that enables the integrated study of the characterization of complex geometry, fluid transport features and mechanical response at micro-scale, and the upscaling of properties of rocks.

We characterize a microstructure by its volume fraction, the specific surface area, the connectivity (percolation) and the anisotropy of the microstructure. Petrophysical properties (permeability and mechanical parameters, including plastic strength) are numerically simulated based on representative volume elements (RVEs) from microstructural models. The validity of the results from these forward simulations is dependent on selecting the correct size of the RVE. We use stochastic analysis of the microstructures to determine the size of a geometrical RVE [1], and upper/lower bound finite element computations on a series of models with different sizes to determine a mechanical RVE. Upscaling of properties is achieved by means of percolation theory [2]. We detect the percolation threshold by using a shrinking/expanding algorithm on our static micro-CT images of rocks. Parameters of the scaling laws can be extracted from quantitative analyses and/or numerical simulations on the original micro-CT images and the derivative models created by shrinking/expanding the pore-structure. Scaling laws describe how properties obtained at the micro-scale can be used effectively on larger scales.

Different natural rock samples with strong heterogeneity are analyzed. Results show that the strong heterogeneity may cause the scaling parameters different from the values of theoretically random models.

We are grateful to Petrobras' financial support of this research. We thank iVEC for technical support and access to its visualization facilities and supercomputers.

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A mesoscopic stochastic model for micron-scale plasticity

Dániel Tüzes¹, Péter Dusán Ispánovity

Department of Materials Physics, Eötvös University, Pázmány P. stny. 1/a,
H-1117 Budapest, Hungary

Plastic deformation of micron-scale single crystalline specimens is accumulated by large intermittent strain burst (dislocation avalanches) [1]. The size of these bursts is power law distributed, with a cut-off depending on the external shear stress (driving force). At a critical stress value the cut-off tends to infinity, showing analogy with continuous phase transitions. This phenomenon is often investigated numerically in a depinning framework [2–4].

In this poster we investigate the statistical properties of strain bursts with a model that uses dislocation dipoles as the elementary sources of deformation. Due to the properties of dislocations, the interaction is long-range with strong anisotropy. Contrary to previous models, due to the nonpositiveness of the interaction kernel we also allow bursts in the opposite direction of the driving force. After investigating which parameters of this model influence the statistical properties of the plastic response, we highlight the differences and similarities between the results of this model and experimental measurements, 2D discrete dislocation models and other mesoscopic models. In addition, this model gives an effective method to investigate the effect of the specimen size on the size distribution of bursts and leads to an unexpected result in this respect.

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Vacancy-solute clusters and cavities evolution in α -Fe solid solutions

Thomas Schuler, Maylise Nastar

CEA, DEN, Service de Recherches de Métallurgie Physique, F-91191 Gif-sur-Yvette,
France

Carbon (C), nitrogen (N) and oxygen (O) atoms are always present in α -iron (Fe), either as impurities or as alloying elements. In this work we show that despite low solute concentrations and even lower equilibrium vacancy (V) concentrations, V-X (X=C, N, O) clusters form with non-negligible concentrations. The cluster equilibrium distribution is highly dependent upon temperature and concentrations of each species. For vacancy supersaturations (e.g. quenched or irradiated specimens), V-X cluster concentrations increase, and V clusters (cavities) appear.

For each solute, a generalized Hamiltonian is derived on the perfect body-centered cubic lattice including substitutional and octahedral interstitial sites. It is composed of 2-, 3- and 4-body interactions between vacancies and solutes, up to the 8th nearest-neighbour. Interactions are fitted to a whole set of Density-Functional Theory (DFT) calculations of small V-X clusters binding energies, and the predictive capability of the Hamiltonian is checked against another set of clusters. The interaction model is included into a Low Temperature Expansion formalism which yields clusters equilibrium distributions, a valuable information for the analysis of Positron Annihilation Spectroscopy or Resistivity Recovery experiments for instance.

A broken-bond model is then fitted to DFT calculations of X and V migration energies in various environments. It enables the computation of the X and V jump frequencies in any cluster environment. The Self-Consistent Mean Field (SCMF) formalism, extended to systems with two diffusion mechanisms on two different sublattices, uses the Hamiltonian and the broken-bond model to compute thermodynamic averages from which the full Onsager matrix is deduced. From the expression of the Onsager coefficients, one gets the mobility of V-X clusters. The mobility of cavities is measured in Atomic Kinetic Monte Carlo simulations.

In the end, we developed a model at the atomic scale for V-X and V clusters free energies and mobilities. These data can be used as an input for mesoscale simulations, e.g. cluster dynamics, leading to the study of cluster populations evolutions upon annealing and/or irradiation for instance.

This work was supported by the joint program "CPR ODISSEE" funded by AREVA, CEA, CNRS, EDF and Mécachrome under contract n°070551.

A Continuum model for dislocation dynamics incorporating Frank-Read sources and Hall-Petch Relation in Two Dimensions

Yang Xiang, Yichao Zhu

Department of Mathematics, The Hong Kong University of Science and Technology,
Clear Water Bay, Kowloon, Hong Kong

One of the main targets in the continuum plasticity theory is to establish continuum constitutive relations which approximately summarize the underlying discrete dislocation dynamics (DDD).

To facilitate the transition from discrete to continuum in describing the evolution of dislocation systems, we introduce a coarse-grained disregistry function ϕ (CGDF) [1], whose contours with integer value of b – the magnitude of the Burgers vector – characterize dislocation curves shown in Figure 1. This smooth CGDF serves to represent the continuous distribution of dislocations. Some advantages in adopting such way of representation are straightforward: a) The information of materials microstructures necessary for models at the continuum level, such as the dislocation line tangent, curvature, are contained in the CGDF and its spatial derivatives; b) The Kröner-Nye dislocation density tensor can be reproduced in terms of the CGDF; c) The total plastic strain is associated with the integral of this CGDF over the slip plane.

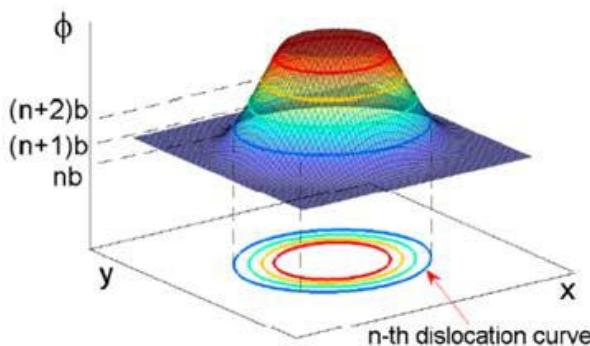


Figure 1: a smooth coarse-grained disregistry function whose contours describe dislocation curves

using our continuum model are shown to agree with results of theoretical predictions and DDD simulations conducted under the same conditions. Also by considering dislocation loop pileups within a rectangular grain, we derive analytical formulas which generalize the traditional Hall-Petch relation into two dimensions without any adjustable parameters. It is shown that the yield stress of a rectangular grain depends not only on the grain size, but also is a function of the grain aspect ratio, whose exact form is associated with the harmonic mean of the length and width of the rectangle. The derived formulas of yield stress are shown excellent agreements with results by our continuum model and DDD simulations.

This work was partially supported by the Hong Kong Research Grants Council General Research Fund grants 605410 and 606313.

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Under the framework described above, we here present a continuum model for dislocation dynamics in one slip plane incorporating the Frank-Read sources as a crucial step towards the full three-dimensional continuum model. The plastic flow is described by an evolutionary equation of the CGDF [2]. The long-range dislocation-dislocation interactions and the local dislocation line tangent effects are both formulated rigorously based on the DDD model in terms of the CGDF [1]. The operations of Frank-Read sources are incorporated in the continuum framework as the source terms of the evolutionary equation whose exact forms are also derived from the DDD model. Simulation results

Modeling polycrystal plasticity using field disclination and dislocation mechanics

V. Taupin¹, C. Fressengeas¹, B. Beausir¹, L. Capolungo², M. Upadhyay²

¹LEM3, Université de Lorraine / CNRS, Metz, France

²G.W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology / CNRS, Metz, France

A mesoscale elastic-plastic theory is developed for the modeling of polycrystal plasticity. It accounts for lattice translational/rotational incompatibility due to the presence of dislocations/ disclinations in the crystal, through polar dislocation/disclination densities [1]. As opposed to statistical dislocation and disclination densities, which do not give rise to net Burgers and Frank vectors, polar defect densities are responsible for long-range elastic strains and curvatures. The spatio-temporal evolution of polar defect densities is provided by their transport equations [1], which involve source terms arising from incompatibilities in the plastic deformation and curvature rates. When modeling a polycrystal, initial polar dislocation and disclination densities composing grain boundaries and triple lines are estimated from gradients in lattice orientations, *i.e.* lattice curvatures, which can be obtained from EBSD maps [2]. When loading a polycrystal, polar defect densities are found to accumulate at grain boundaries and triple lines. This theory has the potential for incorporating grain boundary mechanisms such as grain boundary migration [3] in a crystal plasticity framework. In particular, it can render the competition between dislocation mediated and grain boundary mediated plasticity. In addition, the implications for crystal plasticity include tangential continuity of the mesoscale plastic strain rate and curvature rate tensors on interfaces, which naturally induces nonlocal behavior of a polycrystalline material through grain-to-grain interactions [4].

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A phase field model coupling cracks and dislocations at finite strain

Ruffini Antoine, Finel Alphonse

ONERA, Laboratoire d'Étude des Microstructures, Châtillon, France

In material sciences, the phase field methods are used to describe the evolution of microstructures – such as interfaces, cracks or grain boundaries – into a continuum mathematical formalism. Numerically, these methods are usually more flexible than the multi-body ones and allow the simulation of systems in which space and time scales are extended. It was in this context that, at the beginning of the last decade, the first phase field models of dislocations were elaborated [1,2]. For example, these models are now used to investigate the interactions between dislocations and solid precipitates at the mesoscale.

Another subject of study is the damage of thin film materials which are generally used in microelectronics or optics. Since the thin films are highly stressed (in compression usually), they can delaminate on a part of the substrate and finally buckle. The created structures can themselves induce the delamination of the film along the adherent part of the interface. From a theoretical point of view, the buckling is described by a simplified finite strain elasticity theory (the Föppl and von-Kármán model) while the understanding of the delamination process is based on the concepts of fracture mechanics [3].

However, during the last few years, plasticity has also been shown to occur during buckling and it significantly modifies the process as it is described by these models [4]. Some atomistic simulations have notably revealed that a plastic mechanism can take place in the interface at the base of a straight-sided buckle, modifying its buckling conditions [5]. The problem of the atomistic approach is that it is generally limited to the investigation of systems whose space and time scales appear to be quite far from the real ones, especially in the buckling context. This discrepancy can be reduced by using the phase field methods.

This presentation will therefore describe a continuum numerical model allowing to reproduce the elastic behaviour of a thin film which must be formulated at finite strain. Possibilities for cracking will then be introduced to this model. As an example, we will show that it is able to reproduce the theoretical predictions related to the buckling-driven delamination of a straight-sided buckle. The model will finally be extended by introducing plasticity through a phase field description of dislocations formulated at finite strain. This will be discussed and some examples of simulation will be shown in the buckling context. Obviously, the model presented will be sufficiently general to investigate other situations where cracks and dislocations take place and for which the finite strain effects must be considered.

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Reaction pathway analysis for the partial dislocation mobility in 3C-SiC

Jing Yang, Satoshi Izumi, Ryota Muranaka, Yu Sun, Shotaro Hara, Shinsuke Sakai

Department of Mechanical Engineering, School of Engineering, The University of
Tokyo, 7-3-1 Hongo Bunkyo-ku Tokyo, Japan

As the third generation core semiconductor material, silicon carbide is attracting more and more attention, for its excellent electricity performance in the high temperature due to the wide bond gap [1]. In device manufacture, one of the main difficulties for SiC devices to reach a larger production scale is to understand and to control the residual defects and resulting wafer warpage [2][3]. The existing of wafer warpage is thought highly related to the dislocation nucleation and propagation in the SiC. Therefore, we focus on the dislocation mobility from theoretical approach.

It is well known that in FCC crystal the perfect 60-degree dislocation will dissociate into two partial dislocations: 30-degree and 90-degree partial dislocations. For each partial dislocation, there are two types of dislocation due to which kind of atom composed the dislocation, i.e. Si-core and C-core (Fig1).

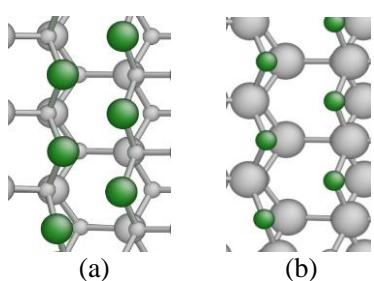


Figure 1: (a) Si-core. (b) C-core.
Stacking faults composed by Si atoms and carbon atoms.

Si-core can move easier than C-core [4]. Furthermore, we attempt to explain this results though the structures' geometry characteristics.

There have been some controversies about which kind of dislocation has high mobility. In this study, reaction pathway analysis based on the nudged elastic band method is applied to study on the mobility of 30-degree and 90-degree partial dislocations in 3C-SiC for both Si-core and C-core. The activation energy was calculated by Vashita potential function, and the dependence of the activation energy on the shear stress was discussed.

The results presented that the activation energies of the Si-core are lower than those of the C-core. This conclusion is consistent with the experimental result that

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Solid phase recrystallization of Si and Ge nanowires

M. Posselt¹, B. Liedke¹, S. Baldauf^{1,2}, Y. Joseph²

¹Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, P. O. Box 510119, D-01314 Dresden, Germany

²TU Bergakademie Freiberg, Institute of Electronic and Sensor Materials, G.-Zeuner-Str. 3, D-09599 Freiberg, Germany

Advanced Si and Ge nanowire transistors can be produced by top-down or bottom-up approaches. In order to obtain the desired electrical properties doping of the nanowires is required. Ion implantation is one of the favored methods to introduce dopant atoms in a controlled manner. If relatively high ion fluences are needed the originally single-crystalline nanowire is amorphized. Subsequently, thermal processing must be used to restore the Si or Ge crystal and to activate the dopants electrically. In planar structures a complete restoration can be achieved by solid-phase epitaxial recrystallization, whereas more complex processes take place in nanowires, due to the significant influence of surfaces and interfaces. In order to understand the solid-phase recrystallization in such confined systems molecular dynamics simulations are performed. Partially amorphized nanowires embedded in a matrix as well as free nanowires and nanopillars are considered. In dependence on whether embedded or free nanowires are investigated several phenomena are observed, such as stacking fault and twin formation, random nucleation of separate crystalline grains, as well as edge rounding and necking. The simulation results are in qualitative agreement with experimental findings.

Figure 1 shows the recrystallization of a free <100>-oriented Si nanowire (length about 16.3 nm) with initially {110} lateral boundaries (width about 2.7 nm). Crystalline seeds exist on both sides of the nanowire. The blue and red colors denote non-crystalline and crystalline regions, respectively. Compared to the initial state (a) the final state (b) shows more crystalline regions and edge rounding due to fast surface diffusion. Atoms belonging to the crystalline part are also shown separately. The recrystallization process leads to stacking fault formation (marked by black lines) which is similar to that observed by TEM after the recrystallization of Si nanowires [1].

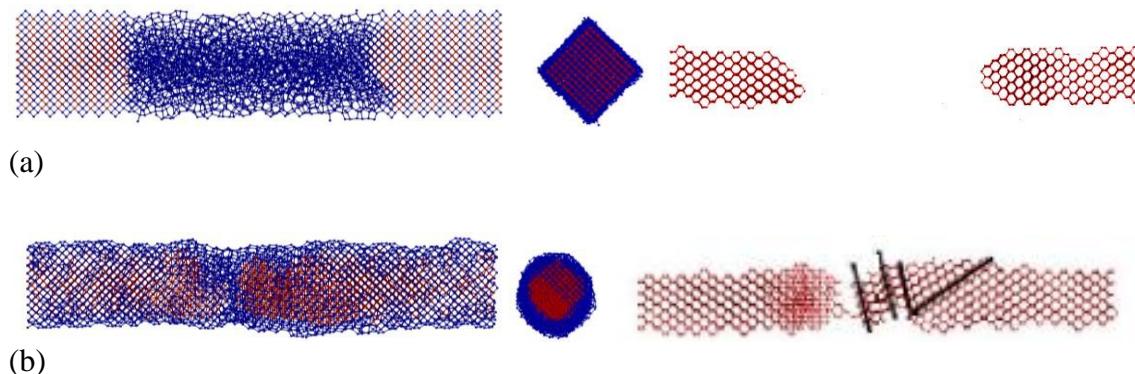


Figure 1 : Recrystallization of a Si nanowire. The figures on the left and in the middle show views into <100>. The figures on the right depict only atoms in the crystalline regions and the view is into the <110> direction.

Large-scale molecular dynamics simulation of microstructure formation during plasma spray process

Tao Wang^{1,3}, Christoph Begau¹, Godehard Sutmann^{1,2}, Alexander Hartmaier³

¹High Performance Computing, ICAMS, Ruhr-Universitt Bochum, Germany

²Jülich Supercomputing Center, Forschungszentrum Jülich, Germany

³Micromechanical and Macroscopic Modeling, ICAMS, Ruhr-Universitt Bochum, Germany

Thermal barrier coatings have become an essential component in nowadays power and propulsion systems by insulating the super alloy from the extremely high operating temperature. During the plasma spray process, both dense and columnar-structured strain-tolerant coatings have been formatted depending on the process conditions. Large-scale molecular dynamics method is used to simulate the plasma spray of copper and refractory ceramics with varying parameters, e.g. plasma temperature, spraying velocity and the size of the jetted clusters. Results show that while the higher plasma temperature and spraying velocities favor the denser structures with fewer defects, the larger size of sprayed clusters introduces more grain boundaries parallel to the coating plane. The microstructure formation map with varying parameters is estimated which would be expected to reach a state of knowledge that allows computational based methods to access the engineering practice conditions. Keywords: plasma spray, solidification, thermal conductivity, coatings

Materials Aging at Mesoscale: Activated Kinetics and Self-Organized Criticality

Sidney Yip

Nuclear Science & Engineering and Materials Science & Engineering
Massachusetts Institute of Technology
Cambridge, MA 02139 USA

There exists a class of materials durability problems where understanding of the microstructure evolution on spatial-temporal scales of micrometers-seconds is lacking. Fundamental phenomena such as creep, corrosion, and fatigue cracking have in common the processes of deformation and flow of inhomogeneous matter out of equilibrium. The challenge of resolving the governing mechanisms currently constitutes a frontier of materials modeling at the mesoscale [1]. In this perspective we describe a time-dependent transition-state theory approach to address two problems, strain-rate dependence of yielding [2], and the transition from logarithmic (primary) to tertiary (damage) creep [3]. In the former we point out an analogy between crystal plasticity and glass rheology, in the latter we suggest an example of self-organized criticality in the form of strain localization. Additionally, we propose a phase diagram in strain-rate and temperature as a mechanism map where thermal and stress activated processes compete [4].

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Low cycle fatigue modeling of dislocation patterning in FCC metals in single and multiple slip by crystal plasticity finite element method

Nicolò Grilli^{1, 3}, Koenraad G. F. Janssens¹, Helena Van Swygenhoven^{2, 3}

¹Laboratory for Nuclear Materials, Nuclear Energy and Safety Department,
Paul Scherrer Institut, Switzerland

²Material Science and Simulations, NUM/ASQ, Paul Scherrer Institut, Switzerland

³NXMM Laboratory, IMX, École Polytechnique Fédérale de Lausanne, Switzerland

Modeling low cycle fatigue in FCC metals is a long-standing problem which has been a topic of research in the past analyzed with different computational methods. The ultimate goal of computational modeling is the prediction of the mechanical behavior and the lifetime of components. The Crystal Plasticity Finite Element (CPFE) method [1] has been used successfully for studying plasticity in metals and is highly compatible with dislocation-based theories. However it has only been applied sporadically to cyclic plasticity because the computational resources needed to solve many cycles are substantial. CPFE can simulate geometries with arbitrary boundary conditions. Current constitutive equations for low cycle fatigue do not fully capture the dislocation structures emerging during cyclic deformation, e.g. the vein-channel structures for single slip cyclic deformation, or cell and labyrinth structures for multiple slip conditions. Modified constitutive laws are proposed that describe the material at a length scale smaller than previous models [2]. Representative volumes with an element size of approximately 200 nm, which is smaller than the periodicity that is typically observed in these dislocation structures, are used in the simulations. The small size of the elements is necessary if one wants to be able to predict the patterning in dislocation structures, which in turn leads to the cyclic mechanical properties. We will present simulations for cyclic shear deformation of single crystals in single and multiple slip orientations up to 100 cycles. The time evolution of the volume fraction of dislocation structures, the strain distribution in low and high dislocation density areas, and local crystal lattice misorientation will be discussed. These quantities will be validated by using various electron microscopy techniques [3] and in-situ synchrotron Laue micro-diffraction [4].

This research is performed using the DAMASK Crystal Plasticity Finite Element open source code of the Max-Planck-Institute for Iron Research.

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**Modeling dislocation climb at the atomic scale
in MgSiO₃ perovskite in the conditions of Earth's lower mantle**

Pierre Hirel, Philippe Carrez, Patrick Cordier

Unité Matériaux et Transformations, CNRS UMR 8207
Université des Sciences et Technologies de Lille 1, 59655 Villeneuve d'Ascq

Convection and plastic deformation in the Earth's lower mantle occur in extreme conditions of pressure and temperature, and at geological times that are reflected in the very low strain rates (10^{-12} to 10^{-16} s $^{-1}$). Although the composition of the Earth's lower mantle is dominated by the MgSiO₃ perovskite, the mechanical properties of this phase, its microstructure and the mechanisms responsible for its plastic deformation are still a matter of debate. Given the thermodynamic conditions, both dislocation glide and climb are expected to contribute significantly to the plastic flow, however the activation energies and rates of these mechanisms are still to be determined.

In this study we utilize atomic-scale calculations to investigate the interaction of vacancies with edge dislocations, an elementary process of dislocation climb. The interaction energies are explicitly computed, and it is shown that contrary to metals where the interaction is almost purely elastic, in MgSiO₃ the vacancy-dislocation interaction is dominated by electrostatic effects due to the ionic character of this material. As a result, ions with different charges have different behaviours: anions (oxygen) are attracted to the dislocation, while cations are repelled. The consequences for dislocation climb are discussed. These results give insight into the importance of dislocation activity in the rheology of the mantle.

This work was supported by funding from the European Research Council under the Seventh Framework Program (FP7), ERC grant N.290424 – RheoMan.

Free energy of dislocations: Collective equilibrium behavior and driving forces for dynamics

Marleen Kooiman, Markus Hütter, Marc Geers

Eindhoven University of Technology, Materials Technology Institute,
PO Box 513, 5600 MB Eindhoven, The Netherlands

Dislocations are an important underlying mechanism for crystal plasticity at small scales. As metals usually contain many dislocations, it is crucial to examine the collective behavior of all dislocations and to obtain the emergent mechanical response of the system. To bridge the micro and mesoscale, we focus on the free energy of dislocation densities. Once calculated, the free energy yields the equilibrium behavior of the system through minimization. Moreover, driving forces for the dynamics of dislocations can be determined from free energy derivatives. Numerous frameworks have been developed that use free energy derivatives in the dynamical equations [1-2]. However, the explicit energy expressions used are still mainly phenomenological in nature.

Here, we present a free energy expression derived by systematic coarse-graining [3]. We have averaged over a grand-canonical ensemble of discrete dislocations, where we restrict ourselves to straight and parallel dislocations. From the obtained grand-canonical partition function, the free energy as a functional of dislocation density profiles is derived by means of a Legendre transform.

The obtained free energy expression consists of the elastic energy in the system, both due to the presence of dislocations and due to applied boundary loading. Moreover, the free energy entails an ideal gas contribution of the dislocations, and a many-body contribution that accounts for screening. The latter is a truly collective term that is not present for a system of discrete dislocations. We show that this many-body contribution can be approximated by a local density approximation.

From the explicit free energy expression, we derive pair correlation functions and the equilibrium pile-up profiles of dislocations on a single slip system. Moreover, we discuss the role of temperature for dislocation systems.

The focus of future research is on the implementation of the current free energy expression in a dynamical framework.

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Thermally-activated dislocation glide from the atomic scale

Laurent Proville¹, David Rodney²

¹CEA, DEN, Service de Recherches de Métallurgie Physique,
Gif-sur-Yvette 91191, France

²Institut Lumière Matière, University of Lyon, Villeurbanne 69622, France

Atomic-scale simulations of the slow and thermally-activated glide of high Peierls stress dislocations remains a challenge but is of fundamental importance to understand plasticity for instance in body-centered cubic (bcc) and hexagonal (hcp) metals and alloys. First, developing realistic interatomic potentials, which reproduce satisfactorily ab initio predictions about dislocation cores and glide processes, is difficult. Second, the average timescale of the glide process, which involves crossing the Peierls barrier by the thermally activated nucleation of kink-pairs, becomes rapidly too slow when the temperature is lowered, to be accessible to direct Molecular Dynamics (MD) simulations. As a consequence, there is still much to be understood and in particular, the well-known discrepancy between atomic-scale simulations and experiments about the Peierls stresses of screw dislocation in bcc metals.

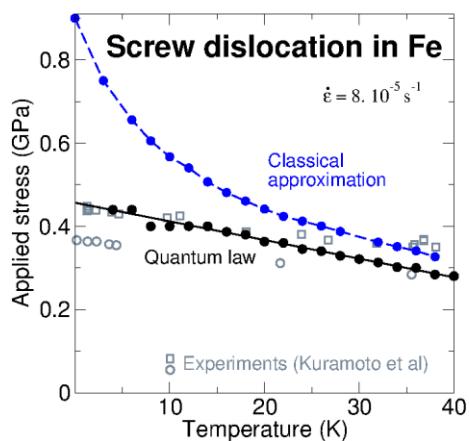


Figure 1: Critical shear stress versus temperature in α -Fe: experimental data from [1], and computed data from classical Orowan law and quantum Orowan law [2].

We present recent advances in modeling the glide of high Peierls stress dislocations. We employ saddle-point search methods (Nudged Elastic Band method) in conjunction with the transition state theory, to predict the pathways and kinetics of dislocation glide. The data computed at the atomic scale allow us to determine the input parameters for transition state theories derived within either classical or quantum statistics. We show in α -iron how the Peierls stress of bcc screw dislocations may be decreased by quantum effects, namely the crystal zero-point vibrations, giving rise at temperatures below 20 K to a large vibrational entropy of kink-pair formation, thus lowering the Peierls barrier. A remarkable agreement is found

when comparing the experimental data [1] with our computations [2]. We will tentatively extend our results to other materials., including Si and Mg.

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A phase field model for dislocation climb

Pierre-Antoine Geslin, Benoît Appolaire, Alphonse Finel

LEM, Onera/CNRS, 29 avenue de la division Leclerc, 92320 Châtillon

Dislocations are linear defects responsible for plastic deformation in crystalline solids. These defects change glide plane by absorbing point defects (climb). Whereas this climb mechanism is inhibited at low temperature, it becomes an essential part of plastic activity at high-temperature (creep). Therefore the analysis of climb dynamics is mandatory to have a better understanding of the creep behavior of metals and alloys. Most of the current modeling techniques for dislocation climb are based on an analytical solution valid under given assumptions [1,2]. First, the dislocation line is generally assumed to be at equilibrium with the surrounding vacancies (local equilibrium assumption). This might be a crude approximation in the case of fcc metals where jogs are high energy defects and can present low concentrations along the dislocation. Second, dislocations are supposed to be far enough from each other such that diffusion is assumed to take place in a hollow cylinder around each dislocation.

To go beyond these assumptions and measure their influence, we first propose an analytical solution for the climb of a isolated dislocation presenting a periodic distribution of jogs. This solution shows that, below a given jog concentration, the local equilibrium assumption can not be valid and the climb rate drops significantly. Second, we propose a phase-field model for dislocation climb to investigate the climb behavior of complex dislocation microstrctures. This model incorporates all the necessary features of dislocation climb, including a dynamic coefficient which controls the kinetics of vacancy absorption/emission at the dislocation core. We show how this parameter can be chosen to reproduce the climb behavior of a weakly jogged dislocation using the analytical solution mentioned before. We use this phase-field model to study the climb behavior of random dislocation distributions and compare it with the simple solution assuming vacancies diffuse in a hollow cylinder around each dislocation.

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Atomistic study of dislocation mobility and obstacle hardening in bcc-Fe: versatility of embedded atom method potentials

S.M. Hafez Haghigat¹, R. Schäublin², J. von Pezold¹, C.P. Race^{1,3}, F. Körmann¹, M. Friák^{1,4}, J. Neugebauer¹, D. Raabe¹

¹ Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany

² Ecole Polytechnique Fédérale de Lausanne (EPFL), Centre de Recherches en Physique des Plasmas, Association Euratom-Confédération Suisse, CH 5232 Villigen PSI, Switzerland

³ School of Materials, University of Manchester, Manchester, M13 9PL, United Kingdom

⁴ Institute of Physics of Materials, Academy of Sciences of the Czech Republic, v.v.i., Žižkova 22, 616 62, Brno, Czech Republic

In crystalline materials the mobility of dislocations and their interactions with obstacles determine the material strength due to dislocation plasticity. Atomistic simulation using the embedded atom method (EAM) is the method of choice to study the kinetics and mechanisms of dislocations. In this study four commonly used EAM potentials for bcc-Fe, namely Ackland et al. (1997), Mendelev et al. (2003), Chiesa et al. (2009) and Malerba et al. (2010), are critically evaluated with respect to their description of the dynamic behavior of $\frac{1}{2} a_0 <111>$ edge and screw dislocations [1]. In the specific case of edge dislocation we find that there is a strong correlation between the dislocation core structure and its glide stress. Analysis of the dislocation migration reveals that the dominant migration mechanism is via progressing straight line segments of the dislocation. This is further confirmed by the excellent qualitative agreement of nudged elastic band calculations of the Peierls barrier with the dynamically determined critical shear stresses. In the second part, the interaction of a $\frac{1}{2} a_0 <111>\{110\}$ edge dislocation with different microstructural defects such as nano-sized obstacles [2,3], second phase precipitates [4] and other dislocations [5] will be discussed. We detail the formation and unzipping process, and the strength of the $<100>$ binary junction through interaction between two $\frac{1}{2} a_0 <111>$ dislocations of edge and screw character. Effects of temperature and strain rate on the unzipping of the junction are quantified. The critical stress, at which the edge dislocation is detached from the screw dislocation, decreases when the temperature increases from 10 to 300 K, whereas it increases with increasing applied strain rate, or dislocation speed. The interaction mechanism and strength of the $a_0 <100>$ binary junction as an obstacle to the edge dislocation are compared to that of other types of defect, namely nano-sized voids, Cu and Cr precipitates and dislocation loops in Fe. The binary junction strength is in the lowest range, comparable to that of a coherent Cr precipitate. However, it appears that the sensitivity of results to the selected empirical potential can be significant and shouldn't be overlooked.

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A 3D dislocation dynamics analysis of the development of size effects at high temperature during micropillar compression of LiF [111] single crystals

H.-J. Chang¹, J. Segurado^{1,2}, R. Soler¹, J. M. Molina-Aldareguía¹, Javier Llorca^{1,2}

¹IMDEA Materials Institute, 28906 Getafe, Madrid, Spain

²Department of Materials Science, Polytechnic University of Madrid, 28040 Madrid, Spain

Compression tests of [111] LiF micropillars with a diameter in the range 1 to 5 μm did not show any size effect on the flow stress [1]. However, more recent experimental data have shown that a strong size effect (“smaller is stronger”) develops progressively as the test temperature increases. At 250°C, the micropillars of 1 μm in diameter were twice stronger than those with 5 μm in diameter [2]. 3D discrete dislocation dynamics (3DDD) of the micropillar compression tests were carried out in order to understand the emergence of a size effect in the flow stress as a function of temperature. Micropillars of diameters in the range 1 to 4 μm and an aspect ratio of 2 (in agreement with the experiments) were studied. The top and bottom surfaces of the circular micropillar were impenetrable to dislocations while the dislocations could leave the micropillar through the lateral surfaces and image stresses on the Peach-Koehler forces were taken into account. The three hard slip systems, [-10-1] (0-10), [0-1-1] (100) and [110] (001), that are activated during compression of LiF along the [111] direction were included in the 3DDD model, as well as the anisotropy in the mobility between edge and screw dislocations, typical of LiF. The evolution of the lattice resistance and of the dislocation mobility with temperature were obtained from theoretical considerations based on experimental results of LiF single crystals [2]. Frank-Read sources were randomly distributed in the three slip systems and the initial dislocation density was equivalent to the experimental one ($\approx 2.5 \cdot 10^{13} \text{ m}^{-2}$).

The results of the 3DDD simulations were able to capture the emergence of the size effect on the flow stress of the [111] LiF micropillars with temperature. This was due to the reduction of the lattice resistance, which become comparable to the size-dependent contribution to the flow stress at 250°C. The changes in the dislocation mobility with temperature only played a secondary role in this respect. Finally, the influence of temperature on the dislocation structures was ascertained from the 3DDD simulations.

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Dislocation Interactions in a Continuum Dislocation Dynamics Formulation

Katrin Schulz¹, Severin Schmitt¹, Doyl Dickel¹, Peter Gumbsch^{1,2}

¹ Institute for Applied Materials (IAM), Karlsruhe Institute of Technology, Kaiserstr.12,
76133 Karlsruhe, Germany

² Fraunhofer Institute for Mechanics of Materials (IWM), Wöhlerstr.11, 79108 Freiburg,
Germany

The strive for advanced materials with well-defined microstructures has also led to an increasing effort towards a physically based description of the motion of dislocations as the cause of plastic deformation and the origin of materials failure. Several dislocation based continuum theories have been introduced, but only recently have rigorous techniques been developed for performing meaningful averages over systems of moving, curved dislocations, yielding evolution equations for a higher order dislocation density tensor, see [1].

In order to reduce the computational complexity of the theory, a simplified theory has been developed [2], which more readily allows for numerical implementation. In order to construct a self-consistent coarsening, several issues have to be resolved including calculation of the stress field of a system of dislocations, correlation functions, and boundary conditions.

Accurate solutions have been found for one dimensional systems [3]. Fully two- and three-dimensional systems will be compared to ensemble averages over discrete dislocation distributions. A continuous field approach including stress interactions perpendicular to the slip planes is introduced and an overview of results for a distribution of one-dimensional glide planes in two-dimensional elastic media is presented. Several aspects of numerical homogenization are analyzed and discussed. Using comparisons with Discrete Dislocation Dynamics (DDD) in a few simple systems, the multi-component stress field which must be considered for dislocation density motion is discussed and enhanced by a statistical model for the representation of dipole interactions in the continuum formulation.

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Protocols for designing H resistant alloys through multiscale modelling: The HeMS Project

Pedro E. J. Rivera

Department of Materials Science and Metallurgy, University of Cambridge

Hydrogen is a ubiquitous element that harms advanced alloys, fostering embrittlement and decreasing component life. There is renewed interest in the topic due to the need for hydrogen storage required for emerging technologies. Hydrogen in steels represents a challenge due to the complexity of the interactions associated to it, the difficulty in establishing the mechanisms through which it alters mechanical properties, and the ability to detect it. Multiscale modelling therefore represents an ideal tool for overcoming these challenges. After reviewing our recent contributions to the computer aided design of novel ultra-hard steels resistant to hydrogen embrittlement [Materials and Design 43 (2013) 499–506], we embark in outlining our multiscale modelling based approach to hydrogen embrittlement and alloy design: the HeMS project (www.hems.ox.ac.uk).

HeMS combines density functional theory, atomistics and micromechanical approaches to gain fundamental understanding into the mechanisms governing hydrogen embrittlement. Employs thermokinetics modelling for microstructural design and computational plasticity for describing microstructure evolution upon exposure to hydrogen. Adopts statistical and artificial intelligence techniques for examining the results of models and experiments. And develops new experimental techniques to determine hydrogen migration in complex steels. This presentation summarises our previous achievements in alloy design, and our on-going work to control hydrogen embrittlement through understanding of its multiscalar effects.

Hydrogen Effects on Dislocation Dynamics and Metal Plasticity

R. B. Sills^{1,2} and W. Cai¹

¹Department of Mechanical Engineering, Stanford University, Stanford, CA 94305, USA

²Sandia National Laboratories, Livermore, CA, 94551, USA

Hydrogen in solid solution can modify the behavior of metals in numerous, seemingly contradictory ways. For instance, hydrogen is believed to enhance localized plasticity while simultaneously decreasing overall ductility. Dislocation dynamics (DD) simulations can provide insight into these effects. While hydrogen modifies dislocation behavior in multiple ways, we focus on two major effects: changes in the driving forces on the lines and modification of the dislocation mobility. In the limit of fast diffusion, where the solute distribution is always in equilibrium with the dislocation stress fields, we show that the elastic stress field due to the solutes can be decomposed into near-core and far-field components (see Fig. 1). The near-core field can be well approximated by a single line of dilatation below the dislocation, and the far-field stresses can be determined by calculating the dislocation stress field with a modified Poisson's ratio. The dislocation mobility in the presence of hydrogen solutes can be determined using atomistic simulations. Using 3D DD simulations that incorporate these effects in an FCC metal, we predict the effects of hydrogen on the behavior of dislocation populations and the stress-strain curve.

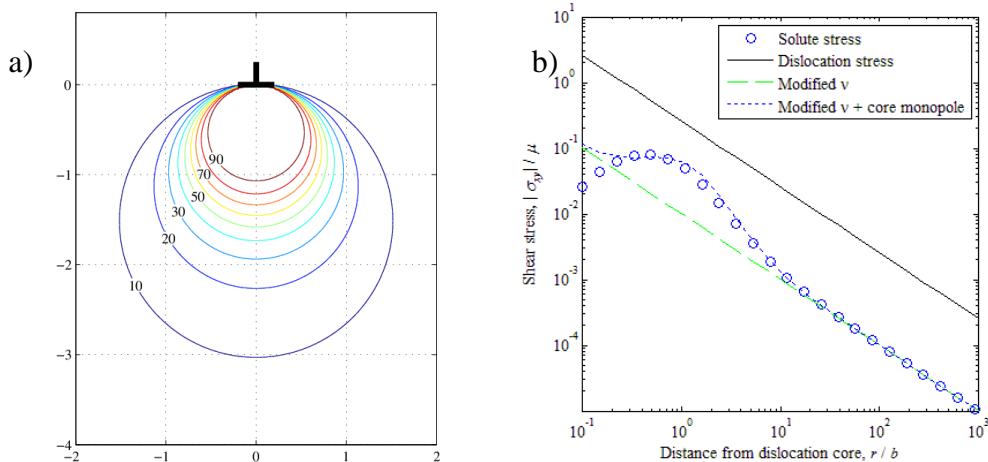


Fig.1: (a) H concentration, c/c_0 , where c_0 is the stress-free concentration, under an edge dislocation in Pd [1]. Grid spacing is b , the Burgers vector magnitude. (b) Shear stress σ_{xy} along the glide plane due to the solute atmosphere [1]. *Modified v* was calculated using the dislocation stress expression with a modified Poisson's ratio and *Modified v + core monopole* adds to this result the stresses due to a solute monopole below the dislocation core. The *Dislocation stress* field is also shown for reference. $c_0=1$ at. % in these figures.

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Effect of microstructure on hydrogen trapping in bcc Fe-Ti-C steel - A quantitative parameter study

Peter Lang, Pedro E.J. Rivera-Diaz-del-Castillo

Department of Materials Science and Metallurgy, University of Cambridge, Cambridge,
CB3 0FS, UK

Hydrogen embrittlement is one of the most devastating and unpredictable, yet least understood, mechanisms of failure experienced by engineering components. H has the tendency to segregate at microstructural defects such as dislocation cores, grain boundaries and interfaces on incoherent particles. Hydrogen, itself as interstitial component, can be trapped by these or other sorts of traps, e.g. substitutional impurities. Such interactions take place at scales ranging from electronic to the microstructural realm. Since the trapping mechanism of H was suggested by Darken and Smith [1] in 1949, hydrogen trapping has been substantiated, experimentally and theoretically. Recently published works by Fischer [2] and Svoboda [3] present equations for the role of several sorts of traps in Fe based alloys. By applying their concepts in the framework of thermo-kinetic simulation we present computational studies including the diffusion process of H, dependent on the depth and molar volume of different kinds of traps. Combining phase transformation kinetics to trap models we calculate the ratio of trapped to non-trapped (free) amount of H. H atoms, able to diffuse through the metal, may recombine to form hydrogen molecules, which develop pressure within the bulk. This pressure can increase to levels where hydrogen induced cracking may occur. To reduce the extent of damage, the microstructure should consist of a homogeneous distribution of hydrogen traps, which will distribute the H atoms innocuously. We will demonstrate that the trapping effect on diffusion of H in pure iron is negligible, whereas the variation of microstructural defects in Fe-based alloys can have a remarkable influence on the mobility of hydrogen in the bulk. In order to obtain a relatively simple illustrative model, the iron based system is alloyed just with titanium and carbon. Incoherent TiC particles are found to have strong interaction energy with hydrogen.

In the model we take as our main variables the four dominant influencing parameters, namely:

- Grain size.
- Dislocation density.
- Austenitization temperature.
- Dilute Ti and C solutions.

We demonstrate the characteristics of H diffusion in Fe and Fe-based alloys under varying the trap population of the material by usage of thermo-kinetic simulations. It is anticipated by our models, that suitable choice of trap type can reduce the susceptibility to hydrogen induced cracking.

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Cyclic and High-Strain Rate Plasticity in Penta-Twinned Silver Nanowires – Atomistic Experiments and Modeling

Horacio D. Espinosa¹, Rodrigo A. Bernal¹, R. Ramachandramoorthy¹, Maria F. Pantano²
Leonardo Pagnotta², Seunghwa Ryu³, Wei Cai⁴

¹Dept.of Mechanical Engineering, Northwestern University, Evanston, IL, 60208, USA

²Dept. of Mechanical Engineering University of Calabria, Italy

³Department of Mechanical Engineering & KI for the NanoCentury, KAIST (Korea
Advanced Institute of Science and Technology)

⁴Dept. of Mechanical Engineering, Stanford University, Stanford, CA, 94305, USA

In recent years there has been a major thrust to develop novel nanomaterials, e.g., nanowires (NWs), exhibiting unique mechanical and electrical properties. These nanostructures are envisioned as building blocks for the next generation of electronic devices, biosensors, energy harvesting systems and other applications. In this context, identification of scale dependent properties is essential. However, such endeavor has proven challenging from both experimental and modeling perspectives. Here we follow a combined computational-experimental approach to characterize the plastic mechanisms in penta-twinned silver nanowires.

Employing a MEMS-based tensile testing technique, we performed *in situ* TEM tensile experiments. The measurements showed that nanowires exhibit increasing strength and ductility as the diameter of the nanowire is reduced. TEM imaging during mechanical straining enabled the visualization of dislocation structures (plastic zones) nucleating at several localized regions along nanowires. These experimental observations were interpreted by means of molecular dynamics simulations (MD), which reveal atomistic detail of the plasticity mechanisms. We found that penta-twinned Ag NWs deform plastically via surface nucleation of stacking fault decahedrons (SFDs). These stacking fault decahedrons form chains, along the wire length, resulting in multiple plastic zones. The signature of these SFDs, visualized in simulations, was identified in TEM as well.

We also report on recent improvements of our MEMS testing system, namely, closed-loop feedback control to achieve displacement-controlled testing, and low-noise electronic sensing for cyclic and high-strain rate mechanical experiments. We show that the signal-to-noise ratio afforded by the feedback system, results in an unprecedented increase in the resolution of stress-strain signatures, which enables a better mechanistic understanding and a more direct comparison to MD predictions. In particular, we have characterized the cyclic behavior of the nanowires. Load and unload cycles reveal increasing hysteresis with increasing unloading strain, which points to the existence of the Bauschinger effect in nanowires. On the other hand, high strain rate experiments with rates as high as 1/s have been performed, revealing increased hardening and decreased plastic localization with increasing strain rate.

3D mesoscopic simulation of fatigue-crack shielding and blunting in FCC metals

Laurent Korzeczek^{1,2}, Benoit Devincre¹, Arjen Roos², Riccardo Gatti¹

¹Laboratoire d'Etude des Microstructures, ONERA/CNRS, Châtillon 92322, France

²Departement des Materiaux et Structure Metalliques, ONERA, Châtillon 92322, France

When subjecting ductile crystalline solids like FCC metals to low-amplitude cyclic loading, plastic strain localizations can appear which may lead to the formation of cracks and subsequent fracture. Crack propagation then depends on the dynamics and the interactions of the dislocations accumulated and patterned in a plastic zone ahead of the crack tip.

Modeling these phenomena is a long-standing and complex problem. So far, existing models are essentially 2D and only few attempts in 3D have been made. 3D dislocation dynamics (DD) simulations are then needed to quantitatively investigate the plastic flow restraining crack propagation through shielding and blunting mechanisms. Only in 3D the influence of crystal symmetry, exact slip system activity and thermally activated processes like dislocation cross-slip can correctly be taken into account.

To model this complex boundary value problem, the Discrete-Continuous Model (DCM) [1] is used to reproduce the properties of realistic dislocation microstructures in large volume elements (e.g. $40 \times 40 \times 40 \mu\text{m}^3$) with a sharp initial crack and cyclically loaded. In this presentation, the first results of the 3D simulations are presented and compared with results from the literature considering a 2D geometry.

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Role of plasticity-induced crack closure in fatigue crack growth in metals

Jesús Toribio, Viktor Kharin

Department of Materials Engineering, University of Salamanca, Spain

The premature contact of crack surfaces attributable to the near-tip plastic deformations under cyclic loading, which is commonly referred to as plasticity induced crack closure (PICC), has long been focused as supposedly controlling factor of fatigue crack growth (FCG). Nevertheless, when the plane-strain near-tip constraint is approached, PICC lacks of straightforward evidence, so that its significance in FCG, and even the very existence, remain debatable. To add insights into this matter, large-deformation elastoplastic simulations of plane-strain crack under constant amplitude load cycling at different load ranges and ratios, as well as with an overload, have been performed. Modeling visualizes the Laird-Smith conceptual mechanism of FCG by plastic blunting and re-sharpening. Simulation reproduces the experimental trends of FCG concerning the roles of stress intensity factor range and overload, but PICC has never been detected. Near-tip deformation patterns discard the filling-in a crack with material stretched out of the crack plane in the wake behind the tip as supposed PICC origin. Despite the absence of closure, load-deformation curves appear bent, which raises doubts about the trustworthiness of closure assessment from the compliance variation. This demonstrates ambiguities of PICC as a supposedly intrinsic factor of FCG and, by implication, favors the stresses and strains in front of the crack tip as genuine fatigue drivers.

Theoretical study of hydrogen interacting with TiC nanoparticles in iron

Davide Di Stefano¹, Matous Mrovec¹, Roman Nazarov²,
Tilmann Hickel², Christian Elsässer¹

¹Fraunhofer-Institut für Werkstoffmechanik IWM, 79108 Freiburg, Germany

²Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany

Brittle fracture of steels resulting from hydrogen embrittlement (HE) presents a serious industrial problem. One of possible means to lower the HE susceptibility is to reduce the amount of diffusible hydrogen in the material. It is widely believed that nano-sized transition-metal-carbide precipitates (e.g. TiC, NbC, or VC) can provide efficient traps for H. But in spite of various experimental evidences, the trapping mechanisms at the atomic scale are not yet well understood.

In this theoretical study, we investigate the interaction of H atoms with TiC particles in the matrix of body-centered cubic iron using first-principles calculations based on density functional theory (DFT). Our atomic-scale results show that the different possible trap sites, namely at coherent Fe/TiC interfaces, interfacial misfit-dislocation cores, and carbon monovacancies in TiC, exhibit large differences in their trapping strength and effectiveness.

A detailed analysis of the computational results with respect to available experimental results reveals a rather consistent interpretation for the trapping mechanisms.

Ab initio modeling of secondary slip in zirconium

Nermine Chaari¹, Emmanuel Clouet¹, David Rodney²

¹Service de Recherche en Métallurgie Physique, CEA Saclay, Gif-Sur-Yvette 91191, France

²Institut Lumière et Matière, Université Lyon 1, Villeurbanne 69622, France

Both experiments [1] and simulations [2] have demonstrated that, in zirconium, the prism plane is the favored slip plane, where screw dislocations dissociate spontaneously and have a small lattice friction. However, screw dislocations can also deviate from the prism plane to glide either in the first order pyramidal plane or in the basal plane. This cross-slip phenomenon has been evidenced with Transmission Electron Microscopy [3], but a detailed understanding is still lacking. Here we investigate dislocation glide in both pyramidal and basal planes using atomic-scale simulations based on a combination of ab initio calculations and empirical potential calculations with the Mendelev potential [4]. We show that surprisingly, both slip systems share the same energy barrier, which is explained by the fact that, in both cases, the dislocation passes through the same metastable configuration with a complex core structure.

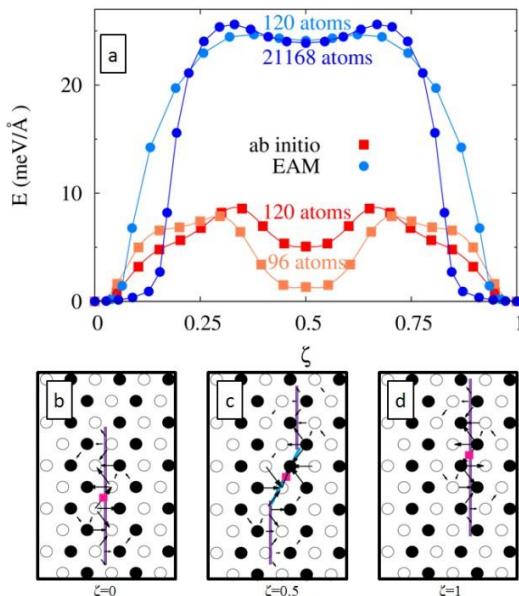


Figure 1: (a) Peierls barrier for pyramidal slip. Differential displacement maps show the dislocation core structure at its initial (b), intermediate (c) and final position (d).

We used the NEB method to determine the Peierls barrier of a screw dislocation initially spread in the prismatic plane and gliding either in a pyramidal plane (fig.1a) or in a basal plane [5]. In both cases, the minimum energy path passes through the same intermediate metastable configuration where the dislocation spreads in the pyramidal plane (Fig.1c). This spreading is rationalized by a metastable stacking fault in the pyramidal plane which corresponds to an elementary twin with a thickness of 2-atomic layers.

The metastable core may thus be described as two partial dislocations spread in two neighbor prismatic planes joined to a nano-twin by a dipole of disconnections.

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MD simulations of defect accumulation and the early stage of crack nucleation in titanium alloys during fatigue

D. S. Xu, H. Wang, R. Yang

Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China

It was recognized more than 50 years ago that for metals and alloys, defects start to accumulate from the very early stage during fatigue, even at the first cycle of fatigue deformation. However, due to the lack of method to observe the *in situ* defect behavior during fatigue at the atomic scale, it is not very clear up to now how defects produced and accumulated, what is the nature of such defects and how they lead to crack formation. The situation becomes worse for titanium alloys used as the rotation components in jet engines, where crack nucleation period constitutes the major part of the component life. Deeper understanding of the defect accumulation and crack nucleation mechanisms is crucial for the design of new materials and components. In the last a few years, large scale molecular dynamics simulations have been carried out to investigate the deformation of titanium alloys, such as dislocation nucleation, interaction and point defect formation by their reaction under various conditions. It was found that dipolar dislocation reaction is an effective way of reducing the number of mobile dislocations, resulting in the hardening of the slip system due to the exhaustion of mobile dislocations. At the same time, the defects formed can be sites for further dislocation nucleation upon continuous fatigue deformation, resulting in deformation localization in the slip bands, and point defects accumulate as deformation proceeds. The strength of the crystals becomes substantially reduced with the presence of large amount of dislocations and other defects, and the strength decreases continuously as the density of defects increases. The factors influencing defect nucleation and accumulation upon dislocation reaction and implications to fatigue failure are discussed.

Physical modeling on size-dependent yield strength with dislocation pile-up and surface effects in finite single-crystal samples

Bo Pan, Yoji Shibutani

Department of Mechanical Engineering, Osaka University, Suita, 565-0871, Japan

Experimental and theoretical researches have shown their explanations of size-dependent relationship between steeply increasing yield strength and decreasing sample size [1-2]. But few researches focus on describing the dislocation pile-up effect and the surface effect in single-crystals on the size effect.

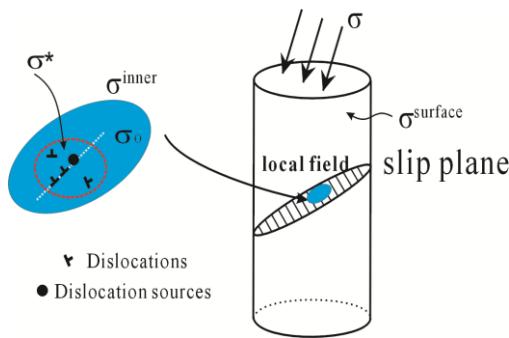


Figure 1: A schematic sketch of stresses state by considering both the surface effect and the micro effect of inner microstructures. The external stress needs to bypass the surface stresses and then be regarded as the applied stresses applied on the inner field to activate inner microstructures.

In this work, a physical model of the yield strength of finite single-crystals at the micrometer scale is derived from the inner microstructure effect and the surface effect as shown in Fig.1. The yield stress σ can be written as $\sigma = \sigma_0 + \sigma^* + \sigma^{surface} = \sigma^{inner} + \sigma^{surface}$, where σ^* and σ_0 are the stresses affected and not affected by dislocations, respectively [3]. Based on the principle of minimum potential energy, the surface stress $\sigma^{surface}$ can be derived as:

$\sigma^{surface} = \gamma O_0(1-\nu)/A$, where γ is the surface energy density, O_0 , A are the perimeter and area of the initial cross section and ν is the Poisson's ratio. According to the dislocation pile-up configuration, the inner strength σ^{inner} can be obtained by considering the effect of microstructures, such as effective length of

dislocation source $\bar{\lambda}_{max}$, dislocation pile-up length L , dislocation density ρ_0 , the number of dislocation sources and so on. It can be expressed as: $\sigma^{inner} = (\alpha\mu b/\sqrt{L\bar{\lambda}_{max}} + \tau_0 + 0.5\mu b\sqrt{\rho_0})/SF$, where τ_0 is Peierls-Nabarro force, α is the geometric parameter, SF is the Schmidt factor, also μ and b are the shear modulus, and the Burgers vector, respectively. In this case, the stress of the filed can be finally obtained as

$$\sigma = \sigma^{inner} + \sigma^{surface} = (\alpha\mu b/\sqrt{L\bar{\lambda}_{max}} + \tau_0 + 0.5\mu b\sqrt{\rho_0})/SF + \gamma O_0(1-\nu)/A \quad (1)$$

It is shown that the “Hall-Petch” relation holds even in the single-crystal, and the number of dislocation pins is a significant factor in the size effect [4]. The process of simulations indicated that the starvation of dislocation sources is one reason for the observed size effect. Moreover, an explicit relationship between the stacking fault energy and the effect of dislocation pile-up was determined in this study: materials with low stacking fault energy will exhibit an obvious dislocation pile-up effect. Furthermore, it can be found that the surface effect from the geometries and the inner strength from the inner microstructures interplay each other, and both influence on the yielding strength, which has the size-dependent characteristic.

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Modeling thermal activation of dislocation glide in cementite at low temperature

Nils Garvik, Philippe Carrez, Patrick Cordier

Unité Matériaux et Transformations, UMR CNRS 8207, Université de Lille 1, 59655
Villeneuve d'Ascq Cedex, France

For a better understanding of mechanical properties in pearlite, we propose to study plastic deformation in cementite. Under extreme deformation, iron carbide Fe_3C (orthorhombic structure, described in the following using *Pnma* space group) exhibits lamellar structure refinement of pearlitic steels [1]. At low temperature and high stress, experimental results show that cementite can deform with [100] dislocations spreading on (010) with dissociation in two partial dislocations separated by a stacking fault [2].

Due to experimental limitations, we propose a numerical model of dislocation core structures and mobility, through an evaluation of associated critical resolved shear stress (CRSS). Our calculations rely on a Peierls-Nabarro-Galerkin model to describe complex core structures at the atomic scale using, as an input, first-principles calculations for generalized stacking fault (GSF) energies [3]. It should be pointed out that how carbon atoms are allowed to relax during GSF energies calculations has a strong effect on stacking fault energies (i) but also on dislocation core structure (ii).

- i) Restoring force, derived from stacking fault energy, are in good agreement with previous ideal shear stress calculations [4,5].
- ii) Dislocation core structures are in agreement with experimental observations, with a dislocation of Burgers vector [100] spread in (010). Moreover, the dissociation width and partial Burgers vectors are found in good agreement with experimental data [2].

We identify two potential slip systems [100](010) and [001](100). In the low temperature, high-stress regime, cementite deformation is driven by the thermally activated motion of dislocations over the Peierls barriers through the nucleation and propagation of kink-pairs. We use the line tension model to describe kink-pair geometry [6,7] and the temperature dependence of the critical resolved shear stress (CRSS) of those two slip systems.

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M111 dislocation of high Peierls stress in BCC Ta

Sanghyuk Yoo¹, Keonwook Kang¹, Christopher Weinberger², Wei Cai³, Vasily V. Bulatov⁴

¹Dept. of Mech. Engr., Yonsei University, Seoul, 120-749, S. Korea

²Dept. of Mech. Engr., Stanford University, Stanford, CA94305, USA

³Mech. Engr. & Mechanics, Drexel University, Philadelphia, PA 19104, USA

⁴Lawrence Livermore National Laboratory, Livermore, California 94550, USA

Dislocation mobility is a key factor to influence plastic behavior of materials, and can be measured by Peierls stress calculation. Peierls stress (PS) is the critical stress at which an infinitely long dislocation starts to move at 0K, and is regarded as intrinsic lattice resistance to dislocation motion. Using atomistic simulations, we calculated PS of a $\langle 111 \rangle / 2\{110\}$ dislocation in a model system of BCC Ta with more than 100 different line orientations [1], among which two high PS orientations are identified: one at screw and the other at M111. While the highest PS at screw has been reported several times in many journal articles, the importance of 2nd highest PS at M111 orientation seems to be taken less seriously. In order to show that this observation is universal regardless of interatomic potential models, we have used two typical potential types of FS [2-4] and EAM [5] and the results are compared with ab initio calculations. All simulations results are consistent in that PS at M111 orientation is on the order of several hundreds MPa. This considerably high PS at M111 creates unique faceting motion in dislocation and is believed to be responsible for pre-yielding in BCC materials.

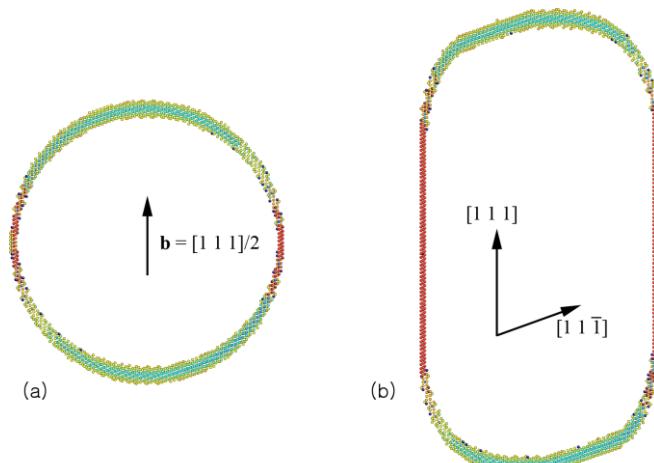


Figure 1: Molecular dynamics images of a dislocation loop of $b=[111]/2\{110\}$ in BCC Ta. (a) Initial circular loop (b) The loop expanded under shear stress of 1 GPa at $T = 10K$. The loop develops in a faceted motion, clearly showing two distinct orientations: screw and M111

This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education (2013R1A1A2063917). The computations in this work were partly performed at the Supercomputing Center/Korea Institute of Science and Technology Information with supercomputing resources including technical support (KSC-2013-C1-026).

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Studying the Effect of Stress Relaxation and Creep on Lattice Strain Evolution of Magnesium Alloy AZ31 under Tension and Compression

H. Wang, B. Clausen, C.N. Tomé, I.J. Beyerlein

Los Alamos National Laboratory, Los Alamos, NM, US

Three approaches for in-situ neutron diffraction measurements, namely, strain holding, stress holding and continuous event-mode, are used to measure the lattice strain evolution of magnesium alloy AZ31 rolled plate under both tension and compression. Stress relaxation or creep induced by holdings is inevitable, especially at loads which are close to the flow stress of the material and affects the results of the measurements. The effect of stress relaxation or creep on the evolution of the lattice strain is studied via comparison with the continuous measured results. To this effect, the experiments are simulated and interpreted using the elastic-visco-plastic self-consistent (EVPSC) polycrystal model in conjunction with an evolving dislocation density (DD) hardening law and a twinning and de-twinning (TDT) twin scheme. The predictions are in reasonable agreement with the corresponding measurements and provide insight into the stress relaxation mechanisms in Mg alloys.

To be presented at International Conference on Multiscale Materials Modeling to be held in San Francisco on October 6 to 10, 2014

Ab initio investigation of the Peierls potential of screw dislocations in bcc iron and its consequences on the dislocation-carbon interaction

L. Ventelon¹, L. Dezerald¹, F. Willaime¹, E. Clouet¹, L. Proville¹, D. Rodney²

¹CEA, DEN, Service de Recherches de Métallurgie Physique, 91191 Gif-sur-Yvette,
France

²Institut Lumière Matière, Université Lyon 1, CNRS, UMR 5306, 69622 Villeurbanne,
France

The high yield stress and the subsequent low ductility in body-centered cubic (bcc) transition metals (V, Nb, Ta, Mo, W, Fe) originate from the core properties of screw dislocations with $\frac{1}{2}\langle 111 \rangle$ Burgers vector, which lead to high energy barriers between two minima. Ab initio electronic structure calculations now allow us to quantitatively describe this barrier, so-called the Peierls barrier. More generally the topology of the 2D Peierls potential of $\langle 111 \rangle$ screw dislocations in all bcc transition metals is being revisited by density functional theory (DFT) calculations. Our DFT results yield 2D Peierls potentials very different from the usually assumed landscapes. We show that iron has a specific and surprising behavior compared to the other bcc transition metals, with a monkey saddle instead of a local maximum located at the hard core, while the energy of the split core configuration is on a high energy peak of the Peierls potential as for the other bcc transition metals [1, 2].

This new picture of the Peierls potential in iron, and in particular the low energy of the hard core, has major consequences on the dislocation-solute interaction in iron. The interaction between a screw dislocation and an interstitial carbon atom is investigated for various solute positions in the vicinity of the dislocation core. It is found that this interaction is strong enough to locally induce an inversion of the stability of the hard versus easy core configurations. A low energy configuration is indeed found where the solute atom is trapped at the center of the dislocation core in the hard core configuration, forming a carbon centered regular trigonal prism similar to the cementite building unit. These new findings have an important impact on the carbon enrichment on dislocations and on the effect of carbon on dislocation mobility.

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Predicting the Rate of Dislocation Cross Slip in FCC Metals

William P. Kuykendall¹, Keonwook Kang², Jie Yin³, Wei Cai^{1,3}

¹ Department of Mechanical Engineering, Stanford University, Stanford, CA 94305, USA

² Department of Mechanical Engineering, Yonsei University, Seoul120-749, South Korea

³ Department of Materials Science and Engineering, Stanford University, Stanford, USA

Cross slip is of fundamental importance for dislocation multiplication, strain hardening, fatigue, and dynamic recovery processes. Because cross slip in FCC crystals is a rare event on the atomistic time scale, it is a challenge to accurately predict the rate of cross slip from atomistic models. A major difficulty arises from the fact that multiple stress components influence the cross slip energy barrier. For the first time, we computed the energy barrier for homogenous cross slip of screw dislocations in FCC metals (Ni[1] and Al) as a function of three stress components, including the Schmid and Escaig stresses on the cross slip plane, and the Escaig stress on the original glide plane. These calculations required the development of a modified string method for stability at high stress conditions. The energy barrier data computed for hundreds of stress combinations are found to be well described by a one-dimensional function of an “effective stress”, which is a linear combination of the three stress components. The regions in the stress space in which different cross slip mechanisms (e.g. Friedel-Escaig and Fleischer) operate are delineated. The effect of jog on the stress dependence of cross slip energy barrier is also discussed.

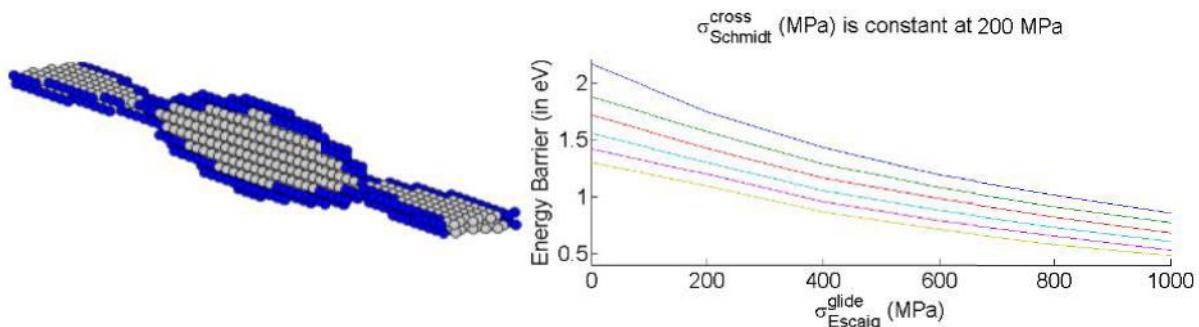


Figure 1: Left: Atomistic simulation of cross slip by the Friedel-Escaig mechanism. Right: The energy barrier (in eV) for homogenous cross slip as a function of increasing Escaig stress on the glide plane (x-axis) and increasing Escaig stress on the cross slip plane (different curves, lower curve is higher stress, in increments of 200MPa, starting at 0 MPa). The Schmid stress on the cross slip plane is fixed at 200 MPa. Other stress components are zero.

This work was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-SC0010412.

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Molecular dynamics simulation of dislocation motion in high-entropy alloys

S. Q. Wang

Shenyang National Laboratory for Materials Science, Institute of Metal Research, CAS,
Shenyang 110016, P. R. China

As the development of superalloys is close to their application limit, the high-entropy alloy is emerging as the most promising candidates for next-generation high-temperature materials [1]. Toughness and ductility are the two key factors for structural application of a material. All of the two properties are closely related with the dislocation movement in the solid. The dislocation structure and property in FCC CoCrFeMnNi and BCC AlCoCrFeNi high-entropy alloys are studied by computer simulations in this work. Different to the usual crystalline solids, high-entropy alloy is paracrystalline phase in which there are neither long-range translational nor rotational symmetries but only a certain fixed neighboring relationship among its lattice sites. Lattice distortions are everywhere in paracrystals [2]. Figure 1 shows the typical paracrystalline lattice of AlCrCuFeTiZn high-entropy alloys.

The atomic configurations of conventional edge and screw dislocations in FCC CoCrFeMnNi and BCC AlCoCrFeNi are built by the first-principles ground-state geometric optimization within the density-functional theory based on the bulk models of these phases [3]. The distribution of strain field around a single dislocation of each types is analyzed.



Figure 1: Paracrystalline lattice in AlCrCuFeTiZn high-entropy alloys.

Molecular simulations are performed using the Morse pair potentials created by Chen's lattice inversion method for the quantitative predictions of dislocation mobility in these two high-entropy alloys. A edge dislocation dipole is created by removing a layer of atoms in the rectangular box of FCC CoCrFeMnNi and BCC AlCoCrFeNi. The periodic boundary condition is used, and a Parrinello-Rahman shear stress is applied to make the dislocation motion [4]. The effects of lattice distortion to the dislocation movement in FCC CoCrFeMnNi and BCC AlCoCrFeNi high-entropy alloys are comparatively studied.

This work was supported by the National Basic Research Program of China (No. 2011CB606403) and the National Natural Science Foundation of China (No. 50971119).

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Grain Scale Models of Plasticity in BCC iron: Describing the Role of Temperature, Strain Rate and States of Stress on Yield

Christopher R. Weinberger¹, Hojun Lim², Corbett C. Battaile², Lucas M. Hale³, Jonathan A. Zimmerman³

¹Drexel University, Philadelphia, PA

²Sandia National Laboratories, Albuquerque, NM

³Sandia National Laboratories, Livermore, CA

Plasticity in BCC metals, including iron, is known to exhibit strong temperature and moderate rate sensitivity in their flow stresses, and the orientation dependent flow stresses in single crystals deviate from the well known Schmid Law. In a related presentation (by Jonathan Zimmerman), atomistic simulations are described that predict the kink-pair activation enthalpy as a function of stress in BCC iron.

Through an appropriate normalization technique, a universal law that describes the orientation dependent yield stresses is developed, and these results can be integrated into higher length-scale models.

We will describe the integration of these results into a crystal plasticity model for BCC iron that captures the experimentally observed rate and temperature dependence as well as the atomistically parameterized stress dependence. The model is able to correctly reproduce the stress dependent yield observed in experiments that cannot be explained by a simple Schmid Law. This model is also used to investigate how to integrate hardening from dislocation-dislocation interactions with the stress-dependent lattice resistance. Using strain hardening behavior fit to experiments from the literature, the model is then used to investigate the role of temperature on the shape of the yield surfaces for both single- and poly- crystals. Our results show that the polycrystalline behavior of BCC iron yield surfaces quickly converges to the standard Von Mises yield surface as temperature is raised above 0K, with no noticeable differences above ~100K.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Probing Micro-Mechanics of Flow in Metals through Crackling Noise and Mean Field Theory

Xiaoyue Ni¹, Gabriele Vajente², Eric Quintero², Fei Sun³, Rana Adhikari², Karin A. Dahmen³, Julia R. Greer¹

¹Division of Engineering and Applied Sciences, California Institute of Technology,
Pasadena, California 91125-8100, USA

²Department of Physics, California Institute of Technology, Pasadena, California
91125-8100, USA

³Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green
Street, Urbana, Illinois 61801-3080, USA

One important aspect of mechanical behavior of materials is establishing a link between micro-mechanics of crystalline deformation and macroscopic plasticity. This is in part because testing theoretical predictions at the appropriate length scale is challenging because of the limited strain sensitivity in nano-mechanical instruments. We developed a methodology to study the internal dynamics of materials driven by defect activity when the sample is subjected to macroscopic deformation. This setup is based on a Michelson interferometer, with the target displacement resolution of order 10^{-15} m/ $\sqrt{\text{Hz}}$ in the range between 10 and 10^3 Hz. We focus on “crackling noise”, which arises from a nonlinear conversion of energy from slow varying external condition to high-frequency random events that are correlated with defect activity: dislocations or shear transformation zones. We aim to reliably obtain the crackling noise data from a variety of materials and interpret it in the context of micro-mechanics and defect activities at the micro-structural level. Statistical Mean-Field Theory (MFT) is used to both analyze the data and to develop predictions about across-the-scales behavior in terms of proximity to critical stresses.

Lattice dynamics and solid-state plasticity experiments at high pressures and strain rates

Bruce A. Remington

Lawrence Livermore National Laboratory

Experiments are being developed on high power lasers and intense x-ray sources, such as the Omega laser at LLE, the Janus and NIF lasers at LLNL, and LCLS at SLAC to study lattice dynamics and solid-state plasticity at high pressures and strain rates. These experiments probe the plastic response of materials to high pressure (50-500 GPa), high strain rate ($10^6 - 10^{10} \text{ s}^{-1}$) deformation. Three classes of experiments in tantalum, a model bcc metal, will be described. Dynamic diffraction experiments with a time resolution of ~0.1 ns or shorter are being developed to probe the microscopic lattice response of samples to a strong shock. [1,2] In particular, the time scale for the onset of plasticity and the rate of the 1D to 3D lattice relaxation are a direct measure of how rapidly dislocations can be generated and transported on sub-nanosecond time scales. [3] Macroscopic plastic flows at high pressure and strain rate can be generated that span a few tens of nanoseconds by using the Rayleigh-Taylor or Richtmyer-Meshkov fluid instabilities. [4,5] Finally, shock driven samples are also recovered so that the residual microstructure caused by the shock and subsequent plastic flow can be examined by SEM, TEM, and other laboratory techniques. [6,7] Results from all three classes of experiments will be compared with simulations using various models of flow stress, and a multi-scale model for bcc strength. [8,9] The mechanisms for plastic deformation and flow vary, depending on the sample pressure, temperature, and strain rate due to the shock or ramp compression. Given the small sample sizes and short time scales of the experiments, MD simulations also provide a valuable guide to the lattice level dynamics, and exhibit significant sensitivity in the predicted results to the interatomic potential. [10,11] Results from the three classes of experiments summarized above will be described, comparisons to theory and simulations given, and a path forward suggested.

This work was performed under the auspices of the Lawrence Livermore National Security, LLC, (LLNS) under Contract No. DE-AC52-07NA27344.

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Grain boundary dynamics from atomistic simulations

C. Brandl¹, D. Perez², T. C Germann²

¹Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM-WBM),
Karlsruhe, Germany

²Los Alamos National Laboratory, Theoretical Division, Los Alamos, USA

The motion of grain boundaries is crucial for the evolution of microstructure both in processing and in application. In experiments, the grain boundary motion is usually studied at relatively high homologous temperature during long times under small mechanical loads. But grain boundary motion is also shown to be a deformation mechanism occurring at high stresses and relative low temperatures, as for example in deformation studies of nanocrystalline metals and shock loading. Using molecular dynamics simulations and transition search methods (string method), the interface motion of grain boundaries is used to elucidate the role of atomistic structure (morphology) and velocity-driving force relation (mobility) for two different driving force mechanisms: elastic anisotropy and shear coupled motion.

As function of temperature and driving force, the grain boundary mobility shows a complex nonlinear behavior beyond the conventional conjecture of Arrhenius-like temperature-dependence in mobility and linear velocity-driving force relation. The velocity-limiting mechanisms range from the pinning-depinning transition at low temperature, through rare-event dynamics of critical “kink- pair” disconnection nucleation along intrinsic grain boundary dislocations, to fluctuating randomly diffusive grain boundary motion at low driving forces and high temperatures. The interfaces’ dynamics are discussed in context of previous atomistic studies and necessary ingredients for a mesoscale model of GB motion.

Experimental investigation of metals at high strain rates

Jonathan C. Crowhurst, Michael R. Armstrong, Bryan W. Reed, Joseph M. Zaug, Harry B. Radousky, Damian C. Swift, Roger W. Minich, Nick E. Teslich, Mukul Kumar

Lawrence Livermore National Laboratory, Livermore, California 94550, USA

Materials at extreme strains and strain rates continue to present both formidable theoretical and experimental challenges. Shock compressed solids are a particularly relevant example. Shock waves have been used for many years to obtain, on the basis of fundamental conservation laws, highly precise material-specific relationships between volume and pressure. However, the detailed physics of shock waves, at even fairly low stresses, and in simple metals, is still imperfectly understood. This has motivated our efforts to characterize the behavior of various metals under high strain rates and to make comparisons to previous results established at lower strain rates, as well as to recent theoretical results.

In this presentation, we will discuss our measurements on aluminum, iron and tantalum thin films. To obtain these data we have used a table-top scale laser to drive shock waves in polycrystalline samples of thicknesses of $\sim 1 \mu\text{m}$, combined with an ultrafast interferometer to measure free surface histories with a time resolution of $\sim 10 \text{ ps}$. For aluminum [1], we will compare our assumed steady wave data at strain rates of up to 10^{10} s^{-1} to literature data up to $\sim 10^7 \text{ s}^{-1}$ and show that the well-known fourth power scaling relation of strain rate to shock stress is maintained even at these very high strain rates. For iron [2], we will show that at strain rates of $\sim 10^9 \text{ s}^{-1}$: 1. The $\alpha \rightarrow \epsilon$ transition begins very soon (within $\sim 100 \text{ ps}$) after the arrival of a large elastic precursor and is essentially complete within a similar time period thereafter. 2. The deviatoric stress before the transition begins can exceed 3 GPa. 3. The majority of the material transforms at stresses up to $\sim 25 \text{ GPa}$, or nearly twice as large as inferred in longer time scale experiments; and, 4., the separate P1 and P2 waves seen at lower strain rates are not observed. We will also discuss our recent results obtained from tantalum thin films and how they compare with those obtained on other shock wave platforms.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344 with Laboratory directed Research and Development funding (12ERD042).

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Temperature and high strain rate dependence of tensile deformation behavior in single crystal iron from dislocation dynamics simulations

Meijie Tang, Jaime Marian

Lawrence Livermore National Laboratory, Livermore, California 94550, USA

We conduct dislocation dynamics (DD) simulations of Fe periodic single crystals under tensile load at several high strain rates and temperatures. The simulations are connected to the atomistic scale via recently-calculated, temperature-dependent dislocation mobility relations. We explore strain rates from 10^4 to 10^6 s⁻¹ at temperatures of 100, 300, and 600 K. We compute the flow stress as a function of strain rate and temperature and find very good agreement with experimental data for Fe, suggesting that strain hardening is the dominant materials response mechanism in the range of conditions explored here.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Multiscale modeling of high-rate plastic deformation of polycrystalline bcc metals

Robert E. Rudd¹, A. Arsenlis¹, N. R. Barton¹, R. M. Cavallo¹, A. J. Comley²,
B. R. Maddox¹, H.-S. Park¹, C. Plechaty¹, S. T. Prisbrey¹, C. E. Wehrenberg¹,
B. A. Remington¹

¹Lawrence Livermore National Laboratory, Livermore, California 94550, USA

²AWE, Aldermaston, Reading RG7 4PR United Kingdom

Multiscale strength models for high-rate deformation have been developed for tantalum and vanadium starting with atomic bonding and extending up through the mobility of individual dislocations, the evolution of dislocation networks and so on until the ultimate material response at the scale of an experiment. [1] These models are based on an information-passing, hierarchical strategy starting with density functional theory, and going through classical molecular dynamics and dislocation dynamics to produce a constitutive model well suited for use in finite element and other continuum simulations. In parallel with the development of the multiscale strength models, high-rate plastic deformation has been the subject of increasing experimental activity. High energy laser platforms such as the National Ignition Facility offer the possibility to study plasticity at extremely high rates in shock waves and, importantly, in largely shock-free ramp-compression waves. [2] Experiments have been conducted on tantalum and vanadium at pressures of ~ 100 GPa and strain rates of $\sim 10^7$ /s. [3] In-situ x-ray diffraction also can provide information about the shear stress in a metal undergoing rapid deformation. These experiments have been conducted on Ta also at pressures of ~ 100 GPa. [4] Remarkably, the predictions of the multiscale model agree well with the experiments without adjustable parameters. Here we review the construction of a multiscale strength model, and report on what aspects of the multiscale model have been tested by these experiments, especially work hardening and dislocation mobility. [5] This is primarily a modeling talk, with some discussion of experimental validation. We consider experiments and simulations of deformation of polycrystalline Ta to study the role of Hall-Petch effects under extreme conditions. We also consider the orientation dependence flow stress in single crystal tantalum, and compare it to the MS model predictions. Finally, we discuss whether the MS model needs to be extended to include homogeneous nucleation. While the dynamic experiments generate integrated data, coupled with the detailed microphysics of the MS model simulations they are beginning to provide a compelling picture of the mechanisms of high-rate/high-pressure metal deformation.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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High-Temperature Discrete Dislocation Plasticity

Amine Benzerga

Texas A&M University, USA

A framework for solving problems of dislocation-mediated plasticity coupled with thermally-activated point-defect diffusion is presented. The dislocations are modeled as line singularities embedded in a linear elastic medium while a concentration field, as in continuum diffusion theory, represents the point defects. Plastic flow arises due to the collective motion of a large number of dislocations. Both conservative (glide) and nonconservative (diffusion-mediated climb) motions are accounted for. A variational principle is used to derive the coupled governing equations for point-defect diffusion and dislocation climb. Superposition is used at each instant to obtain the mechanical fields in terms of the infinite-medium solution for the discrete dislocations and an image field that enforces the boundary conditions while the point-defect concentration is obtained by solving the stress-dependent diffusion equations on the same finite-element grid. Aspects of the formulation are general but its implementation in a simple plane strain model enables the modeling of high-temperature phenomena such as creep, recovery and relaxation in crystalline materials. With emphasis laid on lattice vacancies, the creep response of planar single crystals in simple tension emerges as a natural outcome in the simulations. An adaptive time stepping scheme is used thus enabling to bridge the widely disparate time scales for dislocation glide and climb. A large number of boundary-value problem solutions are obtained which depict transitions from diffusional creep to power-law creep, in keeping with longstanding phenomenological theories of creep.

Tuning Ideal Tensile Strengths and Intrinsic Ductility of BCC Refractory Alloys

Liang Qi, Daryl Chrzan

Department of Materials Science and Engineering, University of California, Berkeley,
CA 94720, USA

Group 6 metal-based (Mo and W) refractory alloys are candidates as structural materials for many high-temperature applications. However, the lack of ductility at room temperature limits their applications. An important theoretical ductility criterion for these alloys is whether their nominally perfectly crystalline structures ideally fail by cleavage or shear deformation under tensile strain along [100] directions. Pure Mo and W fail by cleavage under [100] tension so that they are intrinsically brittle. Based on first-principles calculations and virtual crystal approximations (VCA), we found that decreasing electron numbers by alloying can make these alloys theoretically fail by shear instability and hence transform them into intrinsically ductile materials. This transition can be explained by a Jahn-Teller distortion, that lowers the total energy by splitting the degenerate energy levels of symmetry-related and partially-occupied orbitals. This discovery provides a guide for alloying processes aimed at increasing the intrinsic ductility of group 6 metal-based refractory alloys. This work is supported by EPRI.

DD Simulations of Temperature Effects on Tungsten Micro-pillar Compression with a Semi-phenomenological Dislocation Mobility Formulation

David Rivera, Giacomo Po, Tamer Crosby, Nasr M. Ghoniem

Department of Mechanical & Aerospace Engineering, University of California at Los Angeles (UCLA), 420 Westwood Plaza, Los Angeles, CA. 90095-1597, U.S.A.

The relation of the yield point and subsequent plastic behavior of BCC metals to the ductile to brittle transition temperature (DBTT) provides a unique opportunity to investigate the link between a clear macroscopically observed phenomenon (DBTT), and defect microstructure. The DBTT has been shown to be largely governed by dislocation mobility [1], or dislocation nucleation from crack tips [2]. This is attributed to the thermally activated kink-pair formation mechanisms governing dislocation motion in the low temperature regime. In this work, a dislocation mobility law is introduced and incorporated into a Dislocation Dynamics simulation package (MODEL), with the aim of elucidating the complex temperature governed interactions between defects which ultimately lead to either a brittle or plastic characterization of a BCC metal. The mobility law was obtained through careful analysis of experimental data found in literature, molecular dynamics simulations, and analytical theory for calculation of dislocation velocities in the high strain rate regime. The behavior of dislocations confined to a Tungsten micropillar is examined as a function of temperature and stress and compared to experimental results. The effects of variations in dislocation mobility are subsequently examined to reveal the pronounced impact temperature and stress combinations have on the plastic deformation of BCC metals.

This work is partially supported by the Air Force Office of Scientific Research (AFOSR), Award No: FA9550-11-1-0282 with UCLA, and by the US Department of Energy, Award Number DE-FG02-03ER54708 with UCLA.

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The subsonic/transonic transition of rectilinear edge dislocations: predictions from a field-based equation of motion

Yves-Patrick Pellegrini

CEA, DAM, DIF, F-91297 Arpajon, France

Atomistic simulations carried out during the last fifteen years have revealed the complexities of the behavior of accelerated edge dislocations. These include dramatic dynamic variations of core size, and depending on the type of loading applied, particular ways of leaping from subsonic velocities and “locking” onto asymptotically stable states of faster-than-shear-wave velocity [1]. So far, no fully satisfactory agreement between available models and such intricate results has been reported, even though useful theoretical information has been gathered.

Dislocation glide motion is that of a phase wave involving no transport of matter over more than atomic distances, accompanied by braking or acceleration wave emission. Because of this, dislocation inertia modelling at high velocities and accelerations escapes the classical Newtonian framework, which precludes using an equation of motion (EoM) with acceleration term proportional to some mass coefficient. A realistic EoM is all the more needed in view of recent advances towards truly dynamic discrete dislocation dynamics simulations [2].

Recently, an approach based on a dynamic extension of the Peierls model delivered an EoM for the dislocation mean position that embodies most of the required wave physics [3]. However, the picture was not complete since an associated equation for the mean dislocation core evolution width was missing.

This talk summarizes our progress on this problem, introducing a new, closed, complex-valued EoM for the latter pair of collective variables [3]. Belonging to the class of retarded functional differential equations, our EoM includes retarded self-interactions, the aforementioned wave-emission effects, and provides fresh theoretical insights about dislocation inertia. Its main current limitation is that it cannot account for supersonic asymptotic steady states.

However, it allows one to investigate numerically the response of edge dislocations in fast-loading conditions of the single- and double-step types previously used in atomistic simulations [1]. In this context, we shall present a study of the subsonic-to-transonic transition of an edge dislocation, in good qualitative agreement with available simulations [1], including some non-trivial predictions for this transition that could be tested by atomistic methods.

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Multiscale Modeling of Forming and Fracture – Industry Perspective

Raja K Mishra¹, Kaan Inal²

¹GM Rand D Center, Warren, MI 48090 USA

²University of Waterloo, Waterloo, Ontario, Canada

Advances in modeling deformation and fracture of granular materials at individual grain scales and their integration into component scale simulations using commercial codes have become enablers for implementing multiscale modeling schemes in the metal forming industry. Now it is possible to compute the forming limit diagram for aluminum sheet from electron backscattered diffraction data and simple tensile test data using crystal plasticity simulation at the grain scale, which can be coupled with anisotropic yield function modeling at a macroscale. The key to this advance has been the availability of new experimental and computational tools. Validation of model predictions with evolving microstructure data obtained through in situ multiaxial deformation tests at dislocation scale and electron backscatter diffraction scale have improved the confidence in constitutive models to capture the physics of deformation accurately. Parallel computing and meshless computing have enabled complex geometries, strain paths, crack tip deformation fields, etc. to be integrated efficiently in large component simulations. Among the benefits of this approach are (i) elimination of numerous and often difficult mechanical tests to calibrate anisotropic yield functions, (ii) ability to simulate evolving forming limit curves for smart forming strategies, and (iii) a microstructure-sensitive inverse design approach for materials development. Furthermore, the multiscale hierarchical approach allows for crystal plasticity model to be informed by lower length scale electronic and atomistic simulations of solute-dislocation interactions. Technological challenges such as eliminating negative strain rate sensitivity in Al-Mg alloys that is responsible for the PLC effect, serrations in room temperature tensile stress-strain curves and defects like stretcher marks on formed aluminum sheet panels can now be addressed through multiscale modeling. Details of the above applications will be presented along with a discussion of new challenges and opportunities in multiscale modeling to enable an “atom to auto” approach in the future.

Quantitative study of the role of twin-parent and twin-twin interactions on the mechanical response of hexagonal materials

P.-A. Juan^{1,2}, S. Berbenni^{2,3}, L. Capolungo¹

¹ G.W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology,
UMI GT-CNRS 2958, France

² Labex DAMAS, ANR-11-LABX-0001-01

³ Laboratoire d'Etude des Microstructures et de Mécanique des Matériaux LEM3, UMR
CNRS 7239, Metz, France

Predicting the evolution of the macroscopic response and internal stress developments in metals necessitates the use of multi-scale approaches. In hexagonal material systems, this need is particularly exacerbated by the activation of twin modes, in addition to slip modes, which render the understanding microstructure evolutions and stress heterogeneity developments more complex. For example, the development of backstresses during twin growth remains partly unexplained and not captured by classical polycrystalline models.

The work to be presented aims at unraveling the role of twinning on the plastic response of hexagonal materials. The first part of the study is dedicated to quantifying the effect of twinning on internal stress development in hcp materials (i.e. Mg, Zr). The second part of the work aims at understanding the role of twin/twin interactions on the macroscopic response of materials.

In part 1, an eshelbian micromechanics approach based on the work of Tanaka and Mori is used to provide first in the elastic case, a relationship between twin morphology and internal stresses in both parent and twin domains. This approach is further extended to the case of elastoplasticity and the work is applied to the case of extruded AZ31 alloy. Prediction of the mechanical response and of average internal stress in the materials reveal the key role of the coupling between parent and twin phases in stress developments.

A second possible contributor to stress developments in hexagonals stems from the interaction between twin domains. Using a novel tool for pattern recognitions in EBSD maps of Zr and Mg, statistics of twin/twin interactions are obtained for different loading conditions. In particular the relative ratio of cozonial and non-cozonial interactions is shown. Atomistic studies are also used to probe the energy states in the loci of twin intersections. From these findings a new constitutive model is developed to predict the effect of latent interactions between twin domains in hcp polycyrtals.

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Direct and phase transformation-assisted grain reorientation in HCP titanium and BCC molybdenum

H. Wang, D. S. Xu, R. Yang

Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China

Under severe plastic deformation, apart from popular plastic mechanisms, like dislocation, twinning, grain boundary sliding, grains in polycrystalline materials are reoriented to release stress rapidly. This is usually connected with unconventional processes. Using large-scale molecular dynamics simulations, we have investigated grain reorientation in titanium and molybdenum with the hexagonal close-packed and body-centered cubic structures, respectively. It is found that, in titanium direct grain reorientation occurs under certain unique combination of grain boundary and loading angle, while in molybdenum grain reorientation is achieved through phase transformation between body-centered and face-centered cubic structures. In this talk, the atomic details of such grain reorientation will be presented together with corresponding experimental confirmation.

A multi-scale model for transformation induced plasticity and the numerical calibration of its material parameters

Thomas Antretter¹, Michael Fischlschweiger², Georges Cailletaud³, Eva Hasenhütl¹, Alexander Sannikov²

¹Institute of Mechanics, Montanuniversitaet Leoben, 8700 Leoben, Austria

²Materials Center Leoben Forschung GmbH, 8700 Leoben, Austria

³Centre des Matériaux, Mines ParisTech, Evry Cedex 91003, France

Transformation induced plasticity (TRIP) in martensitically transforming steels can be attributed to plasticity necessary to accommodate the lower density product phase on the one hand, and to an energetically favorable orientation of martensitic variants in the direction of the prevalent stress state on the other hand. In the proposed model these two effects are treated separately and accounted for by different strain contributions in their respective continuum mechanical description [1]. The effects related to the orientation of martensite variants is, for example, expressed in terms of an orientation strain whose evolution follows the classical framework of viscoplasticity. Experiments [2] indicate that dislocation controlled classical plasticity will only occur in the soft austenite parent phase while the orientation effect is limited to the martensite phase. It is thus necessary to resolve the given external stress state at the level of the individual phases using a scale transition rule as proposed by [3]. The parameters of the constitutive model for the constitutive equations as well as for the scale transition rule can partly be obtained from reference experiments. In addition, representative volume elements exemplarily representing the matrix – inclusion topology of the material in the course of transformation allow evaluating quantities, such as phase stresses, otherwise inaccessible to direct or indirect experimental observation.

The so calibrated material model also contains backstresses related to classical plasticity as well as to the orientation effect and is thus capable of predicting the material response even for non-proportional complex loading histories. Corresponding experiments prove the validity of the presented material model.

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A Mechanistic Study of Intergranular Cracking in Stainless Steels

Harry Pommier², Esteban P. Busso^{1,2}, Thilo F. Morgeneyer², André Pineau²

¹ONERA - National Aerospace Research Centre, 91123 Palaiseau, FRANCE

²Centre des Matériaux, Mines Paristech, CNRS UMR 7633, 91003 Evry, FRANCE

Intergranular cracks are known to initiate within heat affected zones of welded austenitic stainless steel components during service when reheated to the 500-700°C temperature range. In this work, the dominant mechanisms responsible for the nucleation of such grain boundary cracks are investigated experimentally and modelled numerically. An experimental procedure specially designed to reproduce the local conditions leading to intergranular cracking in 316L steels is followed. Here, a tensile residual stress field is introduced at the notch root of a CT specimen by deforming it at room temperature. It is then made to relax during thermal exposure at 550°C for a sufficiently long period of time so as to enable the nucleation of intergranular micro-cavities large enough to be observed by SEM, EBSD techniques and local X-ray tomography.

A novel visco-plastic constitutive material model is proposed to describe the mechanical behavior of the material under such reheat cracking conditions. The material model, formulated assuming large deformation kinematics, accounts for the microstructural evolution (dislocation density and mean twin spacing) and kinematic hardening during deformation through suitably defined internal variables. The model is calibrated from monotonic, cyclic and relaxation test data obtained between 20 and 600°C and is implemented numerically into the finite element method. It is then used to predict the generation of residual stress fields in the near-notch regions of the CT specimens during their pre-deformation at room temperature and their subsequent relaxation at 550-600°C. A good correlation is found between the distribution of the largest residual principal stress component predicted numerically and the experimentally observed intergranular damage.

In parallel to the residual stress predictions, which constitutes the main driving force for intergranular damage, the degradation of the inherent grain boundary properties due to the segregation of impurities such as phosphorus is studied. To that purpose, an existing phosphorus segregation kinetics model is used to predict the critical level of grain boundary phosphorus concentration at the moment when intergranular damage is detected experimentally. The results of this study have led to the development of a new alloy with a sufficiently low phosphorus content to avoid grain boundary embrittlement.

Linking Computational Stacking Fault Energies with Plasticity Mechanisms in High Temperature Carbide Ceramics

Gregory B. Thompson¹, Nicholas De Leon¹, Xiao-Xiang Yu¹,
Billie Wang¹, Christopher R. Weinberger²

¹Department of Metallurgical and Materials Engineering, the University of Alabama,
Tuscaloosa, AL 35487

²Mechanical Engineering and Mechanics Department, Drexel University, Philadelphia,
PA 19104

Ceramics are often associated being hard and brittle, yet certain ceramics exhibit room temperature dislocation propagation as well as significant plasticity, upwards of 30%, at elevated temperature. Metal carbides are one such class of materials. However, due to their refractory nature, extensive testing at elevated temperatures can be prohibitive, which makes these systems particularly well suited for combined experimental and computational investigations to fully elucidate the deformation behavior. In this work, experiments, bending tests and indentation, with density functional theory calculations were combined to elucidate plastic deformation mechanisms. A series of TaC and Ta₂C phases were either indented at room temperature or flexural tested near 2000 deg. C. Of these two phases, Ta₂C exhibits more plasticity. The increase plasticity has been associated with a local metal-metal bond within the unit cell. This bond helps regulate both basal and non-basal slip, with experimentally determined slip quantified via dynamical electron diffraction. Experimental determined slip behavior was consistent with the density functional theory computed slip energy hierarchy. Additionally, the slip behavior between the rock salt group IV HfC and group V TaC is compared. Qualitatively, the TaC exhibited a higher density dislocation than HfC at all temperatures. {110} and {111} slip was observed in both systems, and its prevalence was observed as a function of temperature. The difference of slip plane is explained as differences in stable and unstable stacking fault energies between the two metal carbides.

A Multi-Scale Framework to Simulate Dynamic Recrystallization in Magnesium Alloys

Kaan Inal¹, Anthony D. Rollett², Raja K. Mishra²

¹Department of Mechanical Engineering, University of Waterloo, 200 University Avenue West, Waterloo, Ontario, N2L 3G1, Canada

²Department of Materials Science and Engineering, Carnegie Mellon University, 5000 Forbes Avenue, Pittsburgh, PA, 15213-3890, U.S.A

³General Motors Research and Development Center, 30500 Mound Road, Warren, MI 48090-9055, U.S.A

Warm/hot forming can increase the formability of magnesium alloys as this process increases the number of available slip systems due to thermal activation. When magnesium alloys are deformed at elevated temperatures, deformation is accommodated by slip and/or twinning until a critical value is reached. After this the material often exhibits dynamic recrystallization (DRX), which results in softening instead of hardening of the flow curve and can be detrimental or beneficial to Mg processing depending on the application. In this paper, a coupled approach to model DRX where the crystal plasticity based finite element (CPFEM) method is employed together with a probabilistic model to simulate both nucleation of a new grain and growth of the nucleus. The proposed numerical framework employs the local gradient in the dislocation density tensor in the deformed material to determine the nucleation of recrystallized grains. Furthermore, morphological aspects (length, width, etc.) of deformation twinning are introduced into the numerical analyses. This approach enforces equilibrium and compatibility between the twin zones and the parent matrix throughout the polycrystalline aggregate in the weak finite element sense. Twins are assumed to initiate at stress hot spots on the grain boundaries. These locations are then used as potential nucleation sites for DRX by neglecting any twin growth. Simulations of DRX are performed for AM30 and AZ31 magnesium alloys deformed at high temperatures and the predicted textures as well as the stress-strain curves are compared with experimental data to identify what further refinement of the model would improve accuracy.

Hierarchical multi-scale model: from texture and substructure to evolution of plastic anisotropy and complex hardening

Jerzy Gawad^{1,3}, Philip Eyckens², Albert Van Bael², Dirk Roose¹, Paul Van Houtte²

¹KU Leuven, Dept. Computer Science, Celestijnenlaan 200A, 3001 Heverlee, Belgium

²KU Leuven, Dept. Metallurgy and Materials Engineering, Kasteelpark Arenberg 44, 3001 Heverlee, Belgium

³AGH University of Science and Technology, Mickiewicza 30, Krakow, 30-059, Poland

In this study we investigate how to incorporate micro-scale physical phenomena into simulations on a much larger length scale, such as modelling of sheet metal forming operations. Two important micro-scale processes interact during the plastic deformation: evolution of the crystallographic texture and evolution of the substructure. The two not only influence activity of deformation mechanisms, but also result in macroscopically observable changes in both plastic anisotropy and hardening. Furthermore, they are involved in cross-effects, such as hardening of different slip systems, which becomes critically important if the macroscopic deformation path is changed. From the macroscopic mechanical point of view, the hardening evolves substantially faster than the plastic anisotropy. For this reason it is even not uncommon to assume constant plastic anisotropy in simulations of metal forming processes, but the strain hardening is usually considered inconstant.

In this paper we propose a decoupling scheme that exploits the two disparate evolution rates to accelerate the multi-scale model of multi-step plastic deformation. In essence, we adopt a strategy of approximating outputs of a fine scale model that are relevant for a coarse scale model. To capture the evolution of the homogenized variables, the coarse scale model makes use of computationally inexpensive and short-living analytical approximations, which are adaptively reconstructed at different frequency.

Both the coarse-scale plastic anisotropy and the hardening are derived from a fine scale crystal plasticity (CP) model by means of virtual experiments. The CP considers the development of the intragranular dislocation substructure as well as the evolution of texture under the constraint of nearest neighbor grain-to-grain interaction. The plastic anisotropy at the coarse scale level is modelled by means of a plastic potential function, while the hardening is approximated and extrapolated by low order polynomial interpolation functions. Although a number of virtual experiments have to be conducted to construct the plastic potential function, it can be exploited by the coarse scale model for a relatively large range of macroscopic strain. On the other hand, the hardening model has to be updated more frequently, but the computational cost of an update is considerably lower. Moreover, the hardening can be extrapolated along a recent strain path, and the events of strain path change can be easily captured to trigger a necessary reconstruction of the approximation. We show that the hierarchical model is able to accurately simulate multi-stage deformation processes. The investigated case study consists of equibiaxial stretching followed by uniaxial tension, Bauschinger test and a deep drawing process that involves three subsequent changes of the deformation path.

Molecular Statics and Molecular Dynamics Simulations of Dislocation Behavior in a Model FCC Multicomponent Concentrated Solid Solution Alloy

S.I.Rao^{2,3}, C.Woodward¹, T.A.Parthasarathy², D.Dimiduk¹,
O.Senkov², D.Miracle¹, W.Curtin³

¹Air Force Research Laboratory, Materials and Manufacturing Directorate,
WPAFB, OH 45433

²UES Inc, 4401 Dayton-Xenia Road, Dayton, OH 45432

³Institute of Mechanical Engineering, EPFL, Lausanne, Switzerland

In this work, we explore developments in solid-solution alloys and study their application towards alloy discovery using atomistic simulations. Recent work shows that combining 4 or more elements in nearly equiatomic concentrations, may result in a unique class of single-phase materials having unusually high strengths. Similarly, recent developments in atomistic simulations shows that it may now be possible to simulate the behavior of such multicomponent alloys using interatomic potentials that allow one to mix atoms in any combination within a simulation. In this work, molecular statics and molecular dynamics simulations of $a/2<110>$ screw and edge dislocation behavior for a model FCC $\text{Ni}_{30}\text{Co}_{30}\text{Fe}_{20}\text{Ti}_{20}$ alloy are discussed. The work shows that the single phase FCC lattice is elastically stable. Energies of selected points on the gamma surface for the model alloy are compared to that of pure Ni. The core structure $a/2<110>$ screw and edge dislocations in the alloy are shown to be planar, having significant Shockley partial splitting variations along the dislocation line, resulting from concentration fluctuations. The critical stress to move both $a/2<110>$ screw and edge dislocations at 0°K is of the order of 0.005μ , where μ is the shear modulus, which is a value that is significantly ($\sim 10^2$) higher than that for pure FCC Ni. Molecular dynamics simulation results on the critical stress to move the $a/2<110>$ screw and edge dislocations show that the critical stress decreases rapidly with increasing temperature, in a fashion that is similar to a BCC metal. These molecular dynamics simulation results are also shown to be in reasonable agreement with experimental tensile yield strength data for an analogous FCC alloy.

Accelerated Multiscale Simulations of Incipient Plasticity using Hyper-QC

Ellad B. Tadmor

Department of Aerospace Engineering and Mechanics, University of Minnesota

The quasicontinuum (QC) method is a spatial multiscale method that extends the length scales accessible to fully-atomistic simulations (like molecular dynamics (MD)) by several orders of magnitude. While the recent development of the so-called "hot-QC method" [1] enables dynamic simulations at finite temperature, the times accessible to these simulations remain limited to the sub-microsecond time scale due to the small time step required for stability of the numerical integration. To address this limitation, we develop a novel finite-temperature QC method that can treat much longer time scales by coupling the hot-QC method with hyperdynamics – a method for accelerating time in MD simulations. We refer to the new approach as "hyper-QC" [2]. The temporal acceleration makes it possible to perform multiscale hot-QC simulations at near experimental loading rates for problems such as nanoindentation. An interesting observation regarding the possibility of entropically stabilized dislocations [3], uncovered in a hyper-QC simulation, will also be discussed.

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Molecular Dynamics Simulation Study of the Effect of Temperature and Grain Size on the Deformation Behavior of Poly-crystalline Cementite

Hadi Ghaffarian^{1,2}, Ali Karimi Taheri², Keonwook Kang², Seunghwa Ryu³

¹Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology, Daejeon, Korea

²Department of Materials Science and Engineering, Sharif University of Technology, Tehran, Iran

³Department of Mechanical Engineering, Yonsei University, Seoul, Korea

Molecular dynamics simulations combined with quantitative atomic displacement analyses were performed to study the deformation behaviors of poly-crystalline cementite (Fe_3C). At low temperature and large grain size, dislocation glide acts as the preferred deformation mechanism over grain boundary sliding. Due to the limited number of slip systems at low temperature, poly-crystalline cementite breaks by forming voids at grain boundaries upon tensile loading. When temperature rises or grain size reduces, grain boundary sliding becomes the primary mechanism and plastic deformation is accommodated effectively. Our observation sheds light on the origin of brittle-to-ductile transition in recently fabricated bulk sintered poly-crystalline cementite [1].

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Fast Fourier Transform based Multi-scale Probabilistic Model of Twinning in HCP Materials

M. Arul Kumar¹, Irene J. Beyerlein², Ricardo A. Lebensohn¹, Carlos N. Tome¹

¹Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM, 87545, USA

²Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM, 87545, USA

Deformation twinning is an important deformation mechanism in hexagonal close packed (HCP) materials. It is a multi-scale process that depends on microstructural and mechanical responses at the meso, micro and atomic scales. Deformation twinning can be considered as a sequential process of nucleation followed by propagation and growth. The latter processes are responsible for hardening and texture evolution in HCP materials. In this work we focus on the stresses that are associated with the deformation twinning process. A full-field Fast Fourier Transform (FFT) based elasto-visco plastic formulation is modified to model probabilistic twin nucleation followed by propagation and growth in HCP materials. The local stresses at and in the vicinity of twins are quantified during twin nucleation, propagation and growth. An Mg polycrystal is used as the paradigm for implementing this approach. The findings and understanding from this work are translated to the more computationally efficient mean field models, such as self-consistent models.

Mechanical properties of nano-pillars containing a single homo- or heterogeneous interface

Zachary H. Aitken¹, Garrett J. Tucker², Christopher R. Weinberger²,
Julia R. Greer¹

¹California Institute of Technology, Pasadena, California 91125, USA

²Drexel University, Philadelphia, Pennsylvania 19104, USA

Numerous studies on deformation of sub-micron, single-crystalline pillars have furthered our understanding of confined plasticity dominated by a free surface revealing a ubiquitous size effect. While this is of fundamental importance, most structural materials contain interfaces, such as grain boundaries in homogeneous polycrystalline structures or heterophase interfaces in multi-phase systems, which have important effects on their mechanical properties and can serve as sites for damage initiation. The behavior of lattice defects during post-elastic straining in such materials is thus complicated by the influence of boundaries.

We present experimental and computational results of the influence of a single high-angle grain boundary whose plane normal was inclined at an angle to the loading direction within individual Al nano-pillars subjected to uni-axial compression. We discuss their deformation in the framework of stochastic stress-strain signature indicative of nucleation controlled plasticity, as also revealed by molecular dynamics simulations and post-mortem TEM analysis. We also present experimental and computational results of uni-axial tension of nanopillars containing a single Fe/Fe-W metallic glass heterophase interfaces and explore the effect of interface morphology on their mechanical behavior. We employ molecular dynamics simulations to investigate the atomistic processes occurring at the interface and within the pillar bulk that govern deformation.

Scaling laws in the ductile fracture of metals

M. I. Baskes^{1,2,3}, M. Ortiz⁴

¹Bagley College of Engineering, Mississippi State University, ²Jacobs School of Engineering,

UC San Diego, ³Los Alamos National Laboratory, Los Alamos

⁴Division of Engineering and Applied Science, Caltech

Ductile fracture is the process whereby a material separates across a failure surface through mechanisms, such as void nucleation, growth and coalescence, which entail large amounts of plastic work. Owing to its engineering importance, ductile fracture has been the focus of extensive study since the 60's and one of the main driving forces in the development of nonlinear fracture mechanics. Unlike brittle fracture, where the behavior of the material is ostensibly elastic up to fracture, in ductile fracture the plastic dissipation attendant to void growth and coalescence accounts for a significant—or even dominant—part of the energy budget. Such extensive plastic deformation notwithstanding, failure ultimately takes place by separation across a plane or surface and entails a well-characterized amount of energy per unit area, or specific fracture energy, to operate. In consequence, typical measured specific fracture energies for ductile fracture are much larger than those of brittle solids and exhibit a characteristic temperature dependence that includes a brittle-to-ductile transition at a critical temperature. Recently, Fokoua *et al.* (2014) have performed a continuum optimal-scaling analysis of ductile fracture in metals and have shown that ductile fracture in metals can be explained as the outcome of two competing effects: their relatively low plastic-hardening rates, which enables geometric instabilities such as the necking and strain localization, and strain-gradient plasticity. The essence of their void-sheet construction may be understood as follows. Consider a slab of material of dimensions $L \times L \times H$, where H is the thickness of the slab. The slab deforms under periodic boundary conditions on its side and the other two faces of the slab are given displacements $\pm\delta$. Localize the deformations to a band of thickness a , and we subdivide this band into $\frac{L^2}{a^2}$ cubes of size a . We assume that the outside of the band moves rigidly, so that each cube deforms under periodic boundary conditions on its side with its other two faces displacing by $\pm\delta$. For large δ , we expect a void to nucleate from the center of the cube and the total energy of the voided slab/cube to scale as $E_{slab}^{tot} = \frac{L^2}{a^2} E_{cube}^{tot} = KL^2 \left[\left(\frac{\delta}{a} \right)^n a + l \frac{\delta}{a} \right]$ where K is a material constant, $0 < n < 1$ is the hardening exponent of the metal and $l > 0$ is the characteristic length of strain-gradient plasticity. The first term is due to plastic deformation as the void expands and the second term is due to the increase in surface area. Minimizing E_{slab}^{tot} with respect to a we obtain $a = \delta^\alpha l^{1-\alpha}$, with $\alpha = (1-n)/(2-n)$. Inserting these optimal values into the slab energy gives $E_{slab}^{tot} = KL^2 l^\alpha \delta^{1-\alpha}$, independently of the slab thickness H . In the present work, we carry out a similar analysis at the atomistic level. In so doing we explore whether the continuum scaling behavior extends down to the atomistic level, thus bypassing the need to model strain-gradient plasticity at the continuum level. We use an embedded atom method (EAM) model of Ni that reproduces the elastic and surface properties of Ni reasonably well. The calculations are performed with small orthorhombic single crystal unit cells of size $\sim 7.5 \text{ \AA} \times \sim 8.6 \text{ \AA} \times \sim 6 \text{ \AA}$ and direction $x=[1-10]$, $y=[11-2]$, $z=[111]$, which we scale by $2 < a/a_0 < 14$ in each direction, where a_0 is the cell size in the direction of deformation z . A void nucleus of 13 atoms is placed in each cell before deformation of $\pm\delta$ as above. The 3D periodic cell is relaxed to a minimum using standard molecular statics techniques. The cell energy as a function of a has a distinct minimum (sometimes multiple minima) for $0.25 < \delta/a_0 < 1$. Void growth and dislocation emission are clearly evident in the calculations. The cell scaling at the minimum cell energy has a linear logarithmic derivative $\alpha=0.58$ while the energy similarly scales with δ with $\alpha=0.68$. It is encouraging that the scaling of the cell size and energy are nearly consistent, but the value of $\alpha>0.5$ implies the hardening exponent of nickel $n<1$, which is clearly unphysical.

Increasing grain boundary cohesion to improve ductility of bcc transition metals

D. Scheiber^{1,2}, P. Puschnig¹, R. Pippan³, L. Romaner²

¹University of Graz, 8010 Graz, Austria

²Materials Center Leoben GmbH, 8700 Leoben, Austria

³Erich Schmid Institute, 8700 Leoben, Austria

The properties of grain boundaries (GB)s are of strong relevance for plastic deformation of bcc refractory metals. In fact, brittle crack advance and ductile deformation are two simultaneous and competing processes for which the cohesion of the GBs plays a central role. Molybdenum and tungsten are two metals which exhibit low GB cohesion resulting in a high ductile-to-brittle-transition temperature (DBTT) low toughness and intergranular fracture. In order to lower the DBTT and in this way improve the mechanical properties, it is essential to develop a thorough understanding of the interplay between GB geometry, the segregation of solute elements to the interface and the work of separation.

We present atomistic simulations of GBs in tungsten, molybdenum and ferritic iron. Our approach is based on density-functional theory and the embedded atom method to efficiently obtain reliable GB geometries. We scan over a wide range of GBs, selecting those, which are highly frequent in real polycrystals, and investigating the change of properties (i.e. the geometry, work of separation, GB energy) as a function of misorientation. In this way we provide a comprehensive overview of GB cohesion for pure bcc metals in an unprecedented quality. Furthermore, the segregation of a number of solutes to the GB and the surface and their effect on GB cohesion for Mo and W is studied. Herein we present a new approach which combines the traditional method for studying solute segregation in the highly dilute limit with a first-principle mean field approximation (the virtual crystal approximation) to investigate segregation in highly alloyed metals. We discuss the correlation between segregation and GB cohesion and the implications arising for the DBTT temperature.

This work was carried out within the COMET program of the Austrian Research Promotion Agency.

Size Dependent Strength of Nanoparticles – A Combined Experimental/Computational Study

Dan Mordehai¹, Sagi Chen¹, Roman Kositski¹, Koren Shreiber¹,
David J. Srolovitz², Eugen Rabkin³

¹Department of Mechanical Engineering, Technion, Haifa, Israel

²Department of Materials Science, Engineering, Mechanical Engineering and Applied
Mechanics, University of Pennsylvania, Philadelphia, United States

³Department of Materials Science and Engineering, Technion, Haifa, Israel

It is well established that materials can drastically change mechanical properties when their size is reduced to the nanoscale, mainly because of an increase in surface to volume ratio and of lowering the amount of defects in the lattice. Recently, we suggested employing nanoparticles as specimens to study strength at the nanoscale [1,2]. An ensemble of faceted, single-crystal, mobile-dislocation free nanoparticles is produced on a sapphire substrate via dewetting of thin-films. The nanoparticles were indented with a sharp tip or deformed under compression. In this talk, we show how the combination

between the experimental results and atomically-informed dislocation mechanisms allows us to study mechanical properties at the nanoscale. An indentation size effect is observed experimentally, which is rationalized with molecular dynamics (MD) simulations as the competition between dislocation storage and depletion on free surfaces. Moreover, the dependence of their yield stress under compression on their size can be described by a power law. From both MD simulations and finite elements analysis we conclude that the yield point is dislocation nucleated-controlled and we propose a model to rationalize the power-law dependency. We discuss how the mechanical response of the nanoparticles to compression and indentation depends on material properties and crystal structure,

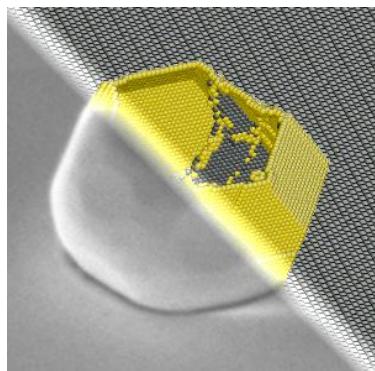


Figure 1: A reproduction of a gold nanoparticle from a SEM image and a molecular dynamics simulation.

which manifests itself through the underlying dislocation mechanism.

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Linking Atomistic, kinetic Monte Carlo and Crystal Plasticity simulations of single-crystal Tungsten strength

David Cereceda¹, J. M. Perlado², Jaime Marian¹
Philip Eisenlohr³, Martin Diehl⁴, Franz Roters⁴, Dierk Raabe⁴

¹Lawrence Livermore National Laboratory, Livermore, California 94550, USA

²Instituto de Fusión Nuclear, Universidad Politécnica de Madrid,
Madrid, 28006, Spain

³Michigan State University, E Lansing, Michigan 48824, USA

⁴Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1,
40237 Düsseldorf, Germany

We present a multiscale model that comprises atomistics, kinetic Monte Carlo and continuum-level crystal plasticity calculations, to simulate the plastic response of tungsten crystals in uniaxial tension tests. Molecular statics calculations are used (i) to study the energetics of kink-pair nucleation as a function of stress for screw dislocation motion, and (ii) to obtain the critical stress deviation from Schmid's law. The atomistic data are used to parameterize a kinetic Monte Carlo model used to simulate thermally-activated screw dislocation motion and to obtain the mobility laws on different slip planes. The dislocation mobility laws obtained from the kMC model are embedded as constitutive law into a dislocation-based crystal plasticity framework, which is used to perform material point simulations and compute the yield strength in single crystal tungsten under different uniaxial loading orientations of the standard triangle.

Modelling Mechanical Behaviour of Quantum Solids using Path-integral Monte Carlo Simulations

Edgar Josué Landinez Borda¹, Wei Cai², Maurice de Koning¹

¹Instituto de Física "Gleb Wataghin", Universidade Estadual de Campinas, UNICAMP,
13083-859, Campinas, São Paulo, Brazil

²Department of Mechanical Engineering, Stanford University, Stanford, CA 94305-4040,
USA

The mechanical behavior of quantum crystals, in which the magnitude of the zero-point kinetic energy is appreciable compared to the energy scale of the interatomic interactions, has become a topic of increasing interest. A system that has received particularly significant attention is crystalline ⁴He, the prototypical bosonic quantum crystal. After initial indications of superfluidity in this crystal [1], extensive experimental effort has been directed toward the mechanical properties of this system. Indeed, observations of elastic stiffening have been linked to dislocation behaviour and the role of isotopic ³He impurities [2,3].

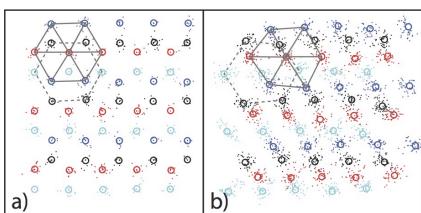


Figure 1: PIMC simulation of homogeneous stacking-fault nucleation in hcp ⁴He under homogeneous shear deformation.

Despite an extensive body of experimental data [4], their interpretation has systematically relied on assumptions concerning the involved fundamental materials parameters, which are inaccessible experimentally. Here, we show how fully atomistic path-integral Monte Carlo (PIMC) simulations [5] can be used to compute such parameters and provide insight into the basic deformation mechanisms involved in systems dominated by quantum effects.

E.J.L.B. and M.K. gratefully acknowledge support from the Brazilian agencies CNPq, Fapesp, Capes and the Center for Computational Engineering and Sciences - Fapesp/Cepid no. 2013/08293-7. E.J.L.B was partially supported by a Santander Graduate Mobility Fellowship. This work was partially supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-SC0010412 (W.C.).

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Unexpected material response in nanoimprinting simulations

Yunhe Zhang, Barend J. Thijssse, Lucia Nicola

Department of Materials Science and Engineering, Delft University of Technology,
The Netherlands

Lithography-free metal imprinting is a promising processing technique whereby a pattern on a rigid punch is transferred onto a metal layer by plastic deformation of the metal itself. We investigate reproducibility and optimal conditions for this process by Molecular Dynamics simulations of an Au thin layer imprinted by a W punch at low processing speeds (9 m/s), using the Zhou-Johnson-Wadley EAM potential.

Many simulations show an unexpected competition between crack formation and dislocation plasticity upon retraction of the punch, which leads in some cases to an imprint and in other cases to a restored, almost flat surface. Surprisingly, the bifurcation of these results can be driven by thermal fluctuations of the atomic velocities alone, see Fig. 1. Other essential parameters are: (1) the crystallographic axis of Au ($<100>$ or $<110>$) that points in the ‘thin’ periodic direction (y), (2) the imprinting depth, (3) the thickness in the ‘thin’ direction.

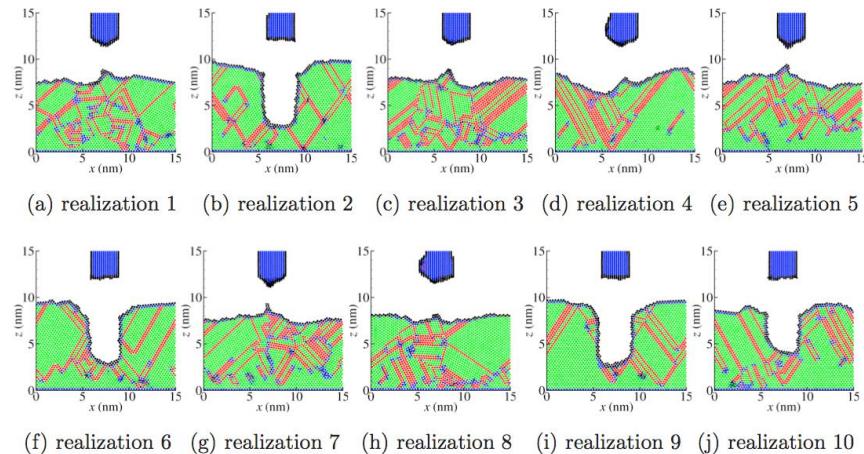


Figure 1:

Final results of ten identical imprinting-and-retraction simulations (300 K), only differing in the Maxwell-Boltzmann atomic velocity samples at the starting points of the simulations. The Au $<110>$ direction points in the periodic direction, perpendicular to the plane of the figure. Green and red atoms have local fcc and hcp symmetry, respectively, illustrating the results of dislocation activity.

Fatigue hot spot simulation of a Ti Widmanstatten microstructure

Benjamin D. Smith^{1,2}, Donald S. Shih¹, David L. McDowell²

¹The Boeing Company, St. Louis, Missouri 63134, USA

²Georgia Institute of Technology, Atlanta, Georgia 30332, USA

A simulated fatigue study has been performed on a Ti-6Al-4V alpha-beta titanium alloy exhibiting a Widmanstatten microstructure. In previous work [1], a crystal plasticity model having a Kocks-type flow rule implemented into an ABAQUS material subroutine has been calibrated to experimental cyclic deformation data. This microstructure-sensitive model has been utilized to identify trends in the fatigue performance of variant Ti-64 microstructures associated with the influence of three key features: the mean colony size, phase volume fraction, and crystallographic texture.

The driving force for fatigue crack formation and early propagation has been quantified through the use of relevant fatigue indicator parameters (FIPs). FIPs are determined through employment of the computed localized stresses and plastic strains induced during the simulations. Three FIPs have been calculated in our fatigue study. The first was the Fatemi-Socie FIP [2], which is related to the maximum plastic shear strain range, $\gamma_{max}^p/2$, and the stress normal to the max plastic shear strain plane, σ_{max}^n , through the following equation:

$$FS = \frac{\Delta\gamma_{max}^p}{2} \left(1 + K \frac{\sigma_{max}^n}{\sigma_y} \right). \quad (1)$$

Here, σ_y is the yield stress and K is a parameter which denotes the material dependence on the stresses normal to the maximum strain plane. The other computed FIPs are variants of the Fatemi-Socie FIP. The second calculated FIP was the grain boundary impingement FIP, which substitutes the net cumulative plastic shear impinging on a grain boundary and the stress normal to this grain boundary interface for the stress and strain based measures for fatigue damage, respectively. Finally, the interlamellar FIP is determined to be equivalent to the Fatemi-Socie FIP resolved onto the interlamellar planes.

Radial correlation statistics have been recruited to study the spatial correlation between favourably oriented slip systems and the maximum FIP locations within the instantiated microstructures. Simulation results suggest that smaller lamellar colonies, reduced alpha-phase volume fraction, and a transverse texture with respect to the loading axis can increase the microstructure's fatigue resistance.

This work was accomplished with financial support of the Boeing Company. The Carter N. Paden Chair in Metals Processing at Georgia Tech also provided supplementary support.

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Screw Dislocations in Layered, Complex Hydrated Oxides

Lu Chen¹, Rouzbeh Shahsavari^{1,2}

¹Department of Civil and Environmental Engineering, Rice University, Houston, TX 77005

²Department of Material Science and NanoEngineering, Rice University, Houston, TX 77005

Dislocations are a common type of defects that significantly influence many mechanical phenomena such as plastic deformation, crystal growth, morphology, or diffusion of materials. While dislocations have been well studied for simple crystalline structures such as pure metals, semi-conductors, ionic materials, and binary oxides, there is very limited knowledge on such defects in complex layered oxides. In this work, we study the mechanisms and the influences of screw dislocations in tobermorite mineral, which is a complex layered oxide material serving as a natural analog of Calcium-Silicate-Hydrate (C-S-H) gel. The latter is the principal source of strength and durability in concrete. We use a cluster-based approach combined with atomistic simulations to investigate the screw dislocation along the interlayer direction of tobermorite (**Figure 1**). An analytical solution of the sextic theory regarding anisotropic materials was implemented to obtain the elastic displacement field. The nonlinear deformations around the core dislocation were accurately captured by atomistic simulations. The final core has a complex 3D structure involving dramatic spiral displacements as well as formation of defected silicate chains resulting from the screw dislocation. Dislocation displacement map indicates an ellipsoid non-planar spreading of the dislocation core extending about 40 Å in the [100] direction and 20 Å in the [010] direction.

This analysis illustrates a low mobility of [001] screw dislocation in tobermorite, since any potential movement will inevitably involve silicate chain breakage. After fitting the atomistic data to classical screw dislocation theories, the core radius is found to be 14.3 Å with a core energy of 53.7 eV/Å. This formation energy and the above observation could be used to compare and predict the prevalent defects along different directions in tobermorite, thus providing fundamental insights on deformation mechanisms governing the mechanical response of C-S-H phases.

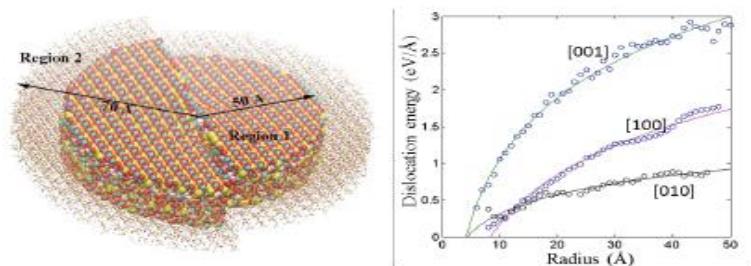


Figure 1. Typical screw dislocation in tobermorite mineral and the corresponding dislocation energies as function of radius.

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Phase Field Crystal Simulation of Strain Effects on Dislocation Movement of Premelting Grain Boundaries at High Temperature

Gao Yingjun, Zhou Wenquan

College of Physics Science and Engineering, Guangxi University, Nanning 530004

The properties of modern materials, especially those of superplastic, nanocrystalline or composite materials, depend critically on the properties of internal interface such as grain boundaries (GBs) and interphase boundaries (IBs). All processes which can change the properties of GBs and IBs affect drastically the behaviour of polycrystalline metals and ceramics. In this paper, using the phase-field crystal model, we investigate the annihilation process of low-angle symmetric tilt grain boundaries (GBs) and dislocations during plastic deformation under conditions where the system approach to the melting point and reach to the temperature at which liquid-solid coexist in simulation, respectively. Our simulation results show that a local premelting occurs around the lattice dislocations as the premelting point is approached from below and the dislocation structure in the premelting region does not change, while the region become significantly larger when the system reach the melting temperature. The deformation performed under the condition of premelting, we can observe that the dislocations of the premelting GB begin to glide under the strain, then those dislocations with opposite Burgers vectors begin to annihilation via the movement, finally the GB is disappeared as well as the premelting region. The annihilation mechanisms of dislocations are similar for premelting conditions. For the temperature reaches to the liquid-solid coexisting region in simulations, the original premelting regions are induced to develop bigger areas of premelting region under the external strain acting. During the process, it can be seen some interactions including the multiplication dislocation pairs, the rotation of dislocation pairs and their annihilation. What's more, the shape of the premelting region changes with the interaction of the dislocations inside of the region, it is observed that the premelting region approaches each other and consolidates together, then decomposes and segregates from each other. Although the shape of the premelting region changes with the applied strain, these regions do not disappear at the end of the simulation, which is totally different to the premelting conditions in lower premelting temperature.

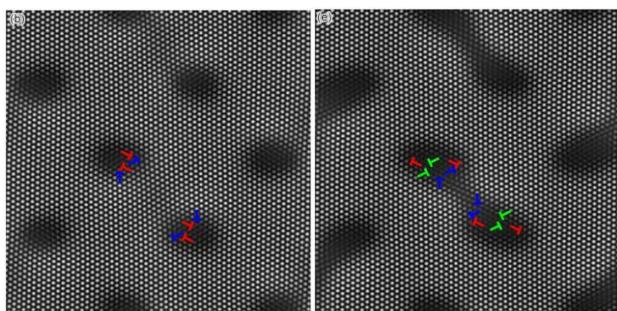


Fig.7 The process evolution of dislocation of GB simulated by using sample C at strain ε (b) =0.045; (e) =0.0510

This work was Supported by National Nature Science Foundation of China (Nos. 51161003 and 50661001) and Nature Science Foundation of Guangxi Province (No. 2012GXNSFDA053001)

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Comparative study of the size of the plastic zone produced by nanoindentation

Yu Gao¹, Carlos J. Ruestes², Herbert M. Urbassek¹

¹Physics Department and Research Center OPTIMAS, University Kaiserslautern,
Erwin-Schr ödinger-Stra ße, D-67663 Kaiserslautern, Germany

²Instituto de Ciencias B ásicas, Universidad Nacional de Cuyo, Mendoza, 5500, Argentina

In 1997 Nix and Gao were the first to calculate dislocation densities caused by a conical indenter [1, 2]. These results were later generalized to a spherical indenter by Swadener et al. [3] using a paraboloid approximation. In 2005 Durst et al. [4] modified this model and concluded that the radius of the plastic zone can be approximated by $R_{\text{plast}} \approx f^* a_c$, where a_c is the contact radius. The factor f is a constant, depending on the material, in the range of $0 \sim 3.5$.

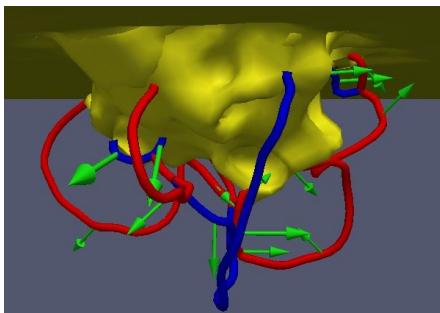


Figure 1: Snapshot of indentation in Fe(100) to a depth of $d=21.4\text{\AA}$. Yellow: deformed surface including unidentified defects. Dislocation lines with Burgers vector $\mathbf{b}=1/2<111>$ are shown in red, those with $\mathbf{b}=<100>$ in blue. Green arrows indicate direction of \mathbf{b} . Dislocations are detected using the DXA algorithm [5]. Visualization has been prepared using Paraview [6]

We use molecular-dynamics simulation to study the size of the plastic zone produced by nanoindentation with a spherical indenter in fcc (Al, Cu) and bcc metals (Fe, Ta) for the low-indexed surface orientations. We study the effects of indenter size, indentation depth, indentation velocity, and target temperature.

Our simulations show that the dislocation structure consist always of two different groups: those that attach to the indentation hole, and those that glide into the substrate or along the surface. We use only the dislocations still attached to the indentation hole to determine the plastic zone. We find that during the indentation process, the f factors are in the range of $3 \sim 4$, and are thus larger than in the Durst model. But after

indenter removal from the substrate, the f factors recede to values in the range of $2 \sim 3$. We find that they do not depend systematically on the crystal structure (bcc or fcc) nor on the surface orientation. The dependence on the indenter radius, indentation depth, indentation velocity and target temperature are only moderate.

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A phase field model coupling cracks and dislocations at finite strain

Ruffini Antoine, Finel Alphonse

ONERA, Laboratoire d'Étude des Microstructures, Châtillon, FRANCE

In material sciences, the phase field methods are used to describe the evolution of microstructures – such as interfaces, cracks or grain boundaries – into a continuum mathematical formalism. Numerically, these methods are usually more flexible than the multi-body ones and allow the simulation of systems in which space and time scales are extended. It was in this context that, at the beginning of the last decade, the first phase field models of dislocations were elaborated [1,2]. For example, these models are now used to investigate the interactions between dislocations and solid precipitates at the mesoscale.

Another subject of study is the damage of thin film materials which are generally used in microelectronics or optics. Since the thin films are highly stressed (in compression usually), they can delaminate on a part of the substrate and finally buckle. The created structures can themselves induce the delamination of the film along the adherent part of the interface. From a theoretical point of view, the buckling is described by a simplified finite strain elasticity theory (the Föppl and von- Kármán model) while the understanding of the delamination process is based on the concepts of fracture mechanics [3].

However, during the last few years, plasticity has also been shown to occur during buckling and it significantly modifies the process as it is described by these models [4]. Some atomistic simulations have notably revealed that a plastic mechanism can take place in the interface at the base of a straight-sided buckle, modifying its buckling conditions [5]. The problem of the atomistic approach is that it is generally limited to the investigation of systems whose space and time scales appear to be quite far from the real ones, especially in the buckling context. This discrepancy can be reduced by using the phase field methods.

This presentation will therefore describe a continuum numerical model allowing to reproduce the elastic behaviour of a thin film which must be formulated at finite strain. Possibilities for cracking will then be introduced to this model. As an example, we will show that it is able to reproduce the theoretical predictions related to the buckling-driven delamination of a straight-sided buckle. The model will finally be extended by introducing plasticity through a phase field description of dislocations formulated at finite strain. This will be discussed and some examples of simulation will be shown in the buckling context. Obviously, the model presented will be sufficiently general to investigate other situations where cracks and dislocations take place and for which the finite strain effects must be considered.

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Revisiting continuum modelling of hydrogen diffusion and trapping in metals for the purposes of hydrogen assisted fracture analysis

Jesús Toribio, Viktor Kharin

Department of Materials Engineering, University of Salamanca, Spain

Addressing the purposes of hydrogen assisted fracture (HAF) analysis, the modelling of hydrogen diffusion in metals with account for hydrogen trapping and relevant physical fields is revisited. Coherent development of continuum model of diffusion and trapping is presented. The flux and mass balance equations in a media with multiple traps are derived from the kinetics principles by means of considering discrete random walk model and its subsequent continuum interpretation. This gives rise to generalised system of partial differential equations of diffusion and trapping. Under definite circumstances, which can be met in engineering HAF cases, certain terms in derived equations become negligible. Dropping them, a series of known specialised models of trapping-affected stress-strain-assisted diffusion are retrieved as approximations of the generalised one and collated as regards their suitability for particular HAF case analyses.

Dislocation mobility laws with several character angles in FCC Aluminum

Jaehyun Cho, Guillaume Anciaux, Till Junge, Jean-François Molinari

École polytechnique fédérale de Lausanne (EPFL)
ENAC-IIC, STI-IMX, Computational Solid Mechanics Laboratory, CH-1015 Lausanne,
Switzerland

The understanding of the collective motion of the line defects called dislocations is important in order to predict plastic deformation of crystalline materials. These can be modeled using several methods, including discrete dislocation dynamics (DDD), molecular dynamic (MD) simulations and the multi-scale *Coupled Atomistic/Discrete-Dislocation* (CADD) [1]. In DDD, the main ingredient to predict dislocation motions is the mobility laws which links dislocation velocities to shear stresses and temperatures. These can be obtained from independent MD simulations [2]. Thus, in CADD coupling, the mobility laws need to match MD. As opposed to 2D, in a 3d framework of CADD, the character angle θ of a dislocation is an important parameter of the mobility laws. These are often assumed to vary monotonically between edge and screw dislocations [3]. However, according to studies based on the Frenkel-Kontorova (FK) model [4,5], the velocities are function of misfit potential (stacking fault energy) $\Upsilon(u)$, material dispersion relations $\omega(k)$ and displacement fields u of a dislocation rather than only a character angle θ . The objective of the presentation is to provide the better mobility law descriptions of a dislocation in FCC Aluminum.

First, the dislocation core structures are studied using MD and confirmed using the variational Peierls-Nabarro method [6], including for mixed character angles. Then, we study dislocation mobility laws for an arbitrary mixed dislocation: we measure the dislocation velocity v under various shear stresses and temperatures. It is observed that v grows quasi-linearly up to the minimum phase velocity v_p of the crystal structure. Then it will progressively saturate to the 1st forbidden velocity (shear wave). This effect can be explained by looking at the waves (more specifically the dispersion relations) dissipating the energy released by the dislocation motion [4,5,7]. Finally, the required information ($\Upsilon(u)$, $\omega(k)$ and u) for the energy balance equation of FK model were obtained from MD and inserted into an extended Ishioka model [5] to produce an estimate of the dislocation mobility laws at several character angles θ .

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A Unified Framework for Localization and Fracture in Extreme Environments

I. Tsagrakis, E.C. Aifantis

Lab of Mechanics & Materials, Aristotle University of Thessaloniki

A unifying thermochemomechanical framework is presented for modeling coupled deformation-heat transfer processes and coupled deformation-diffusion processes under extreme conditions. Small-size or nanoscale specimens are shown to exhibit significantly different behavior than their counterparts at the macroscale. The cases of adiabatic shear banding and hydrogen embrittlement are discussed as examples to illustrate the theory.

Screw dislocation core structure as a function of lattice expansion and contraction in bcc transition metals

L. Dezerald¹, J. Marian², L. Ventelon¹, D. Rodney³, F. Willaime¹

¹CEA, DEN, Service de Recherches de Métallurgie Physique, 91191 Gif-sur-Yvette,
France

² Lawrence Livermore National Laboratory, Livermore, CA 94551, USA

³Institut Lumière Matière, Université Lyon 1, CNRS, UMR 5306, 69622 Villeurbanne,
France

Plasticity in body-centered cubic (bcc) transition metals is governed by the glide of the $\frac{1}{2}\langle 111 \rangle$ screw dislocations. The structure of the dislocation core has an influence on the dislocation glide direction, and has been a matter of debate for several years. Density Functional Theory (DFT) calculations have shown that in pure bcc metals the core structure of $\frac{1}{2}\langle 111 \rangle$ screw dislocations is symmetric, or non-polarized [1], but that in W, it becomes polarized upon alloying with Re [2]. Concomitantly, empirical potentials calculations in Fe and W have shown that the core structure becomes polarized with increasing temperature [3, 4]. In the present work, we investigate the link between lattice variations and dislocation core polarity in W and Fe, as well as in other bcc transition metals.

We first investigated the dependence of the core polarity with lattice parameter using two empirical potentials for Fe: the Mendelev potential [5] and the Ackland potential [6], for which the dislocation core at equilibrium lattice parameter is respectively non-polarized and polarized. Our results show that in both cases the core structure changes from non-polarized to polarized as function of lattice parameter (or as pressure decreases) with a first-order type transition occurring at a negative and positive pressure, respectively. We then used DFT calculations to investigate the core polarization under lattice expansion in bcc transition metals. At equilibrium lattice parameter, the dislocation core is non-polarized in all elements, as expected [1]. But for a few metals non-zero polarity is evidenced in a specific strain range. The present calculations show that there is a general link between pressure and core polarity as in all cases lattice expansion tends to polarize the core.

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Peierls Potential for $\frac{1}{2}\langle 110 \rangle\{110\}$ in MgO: unusual effect of high pressure

Philippe Carrez, Pierre Hirel, Patrick Cordier

1Lab. UMET, UMR-CNRS 8207, University of Lille 1, Villeneuve d'Ascq, 59655 France

Recent studies [1] of $\frac{1}{2}\langle 110 \rangle$ screw dislocation core in MgO showed a major influence of high-pressure on the dislocation core. Based on a generalized Peierls-Nabarro model, it was demonstrated that $\frac{1}{2}\langle 110 \rangle$ core evolves from a planar core in $\{110\}$ at low pressure to a spreading in $\{100\}$ at pressure higher to 50 GPa. Here we revisit these conclusions using full atomistic calculations. Classical rigid pairwise potentials of Buckingham form are used to model both core structure and calculate associated Peierls potentials through Nudge Elastic Band (NEB) method.

As expected from [1], pairwise potentials results confirm that dislocation core evolves from a spreading in $\{110\}$ (at low pressure) to a narrower configuration spread in $\{100\}$ at high pressure. In the same time, it is worth noticing that the stable position of core in the lattice is also evolving. The displacement of stable configuration into the lattice corresponds to an exchange between stable and unstable position according to $\{110\}$ Peierls potentials. Consequently, Peierls potential and/or Peierls stress for gliding in $\{110\}$ do not evolve monotonously with pressure. As such effect could be related to the choice of potential, we will present DFT calculations of periodic dipole arrangement, confirming this unusual change of stable core position with pressure. Further calculations relying on core shell model potentials, taken into account for bonding polarization, show also a remarkable agreement with previous DFT or Buckingham potentials calculations regarding both core spreading and core energy.

This work is supported by funding from the European Research Council under the Seventh Framework Programme (FP7), ERC grant N°290424 – Rheoman.

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Computational Investigations into the Hardness of Metal Carbides

Xiao-Xiang Yu¹, Christopher R. Weinberger², Gregory B. Thompson¹

¹Department of Metallurgical and Materials Engineering, The University of Alabama,
Tuscaloosa, AL 35487

²Mechanical Engineering and Mechanics Department, Drexel University, Philadelphia,
PA 19104

One of the intrinsic properties of ceramics is their high hardness. An *ab initio* computational investigation has been undertaken to elucidate the changes in hardness in metal carbides, with particular attention to sub-stoichiometric anomalous increases in hardness for certain carbides. Investigations into the group IV and V carbides has revealed a monotonic increase in hardness with respect to carbon concentration with the group IV carbides up to a maximum when the metal:carbon ratio is stoichiometric. For the group V carbides, which can promote the precipitation of the vacancy ordered Me_6C_5 phase, increases in hardness are observed experimentally at sub-stoichiometric ratios. Our results, which rule out hardening caused by an increase in bond strength, lends significant evidence towards the increase in hardness being associated with the formation and spacing of Me_6C_5 domains that precipitate out of the MeC matrix grains during cooling. In addition, atomistic simulations have suggested that alloyed Ta-Hf-C ceramics can offer a high melting point and higher hardness than either single metal carbide.

Dislocation diffusion of hydrogen in fcc metal: A molecular dynamics study

Kenji Nishimura, Koji Miyake

National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki
305-8564, Japan

Understanding the diffusion properties of hydrogen in metals, especially interactions between hydrogen and lattice defects such as dislocations, is essential in order to improve the performance and reliability of equipment associated with the production, transportation, storage and supply of hydrogen. In this study, we investigate the effect of an edge dislocation dipole on hydrogen diffusion in face-centered-cubic (fcc) metals using molecular dynamics simulations of palladium-hydrogen as a model system.

Our results predict high hydrogen diffusivity along dislocation lines in Cottrell atmosphere with high hydrogen density after hydrogen accumulation caused by the interactions between hydrogen atoms and tensile hydrostatic stress field created by edge dislocations.

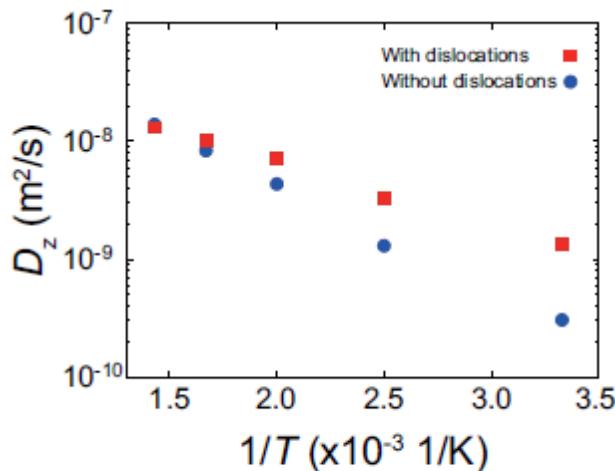


Figure 1: Arrhenius plot of hydrogen diffusivities in palladium with and without dislocations.

dislocation dipole is estimated to be 0.10 eV, which is 38 % smaller than that in the perfect crystal. In the case of 300 K, the hydrogen diffusivity in the system with dislocations is 4.4 times larger than that in the perfect crystal.

A part of this work has been supported by New Energy and Industrial Technology Development Organization (NEDO) under "Advanced Fundamental Research Project on Hydrogen Storage Materials".

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Figure 1 shows the Arrhenius plot of the hydrogen diffusivity in palladium in only one direction, the direction of the dislocation lines. The activation energy of the hydrogen diffusivity in perfect crystal without the dislocations is estimated to be 0.16 eV, which is in excellent agreement with value obtained by means of the first principles calculation [1]. In addition, the value corrected by zero-point energy is 0.24 eV, which is consistent with reported experimental value of 0.23 eV [2]. On the other hand, the activation energy of the hydrogen diffusivity in a system with the edge

First-principles prediction of ductility in rhenium-based alloys from elastic constants, twin boundary energies and surface energies

Maarten de Jong, Liang Qi, Mark Asta

Department of Materials Science and Engineering, University of California, Berkeley,
CA 94720

Hexagonal close packed (HCP) rhenium (Re) exhibits a unique combination of properties that make it a very attractive material for high temperature applications. Most notably, it has no measurable ductile-to-brittle transition temperature, leading to a high ductility over large temperature ranges. The high ductility is related to a dense pattern of twins that form upon deformation. However, the high cost of rhenium and the limited worldwide reserves prohibit its usage in many applications.

In this work we aim to create a replacement strategy for Re. Calculations based on density functional theory are carried out, with the aim of screening for cheaper Re-X alloys while maintaining or improving the beneficial properties of pure Re, especially ductility. Using two ductility parameters for HCP (one based on elastic constants, the other on twin boundary and surface energies) it is shown that solutes to the left of Re in the periodic table increase the ductility, whereas those to the right embrittle Re. Both ductility parameters are shown to give consistent results.

Finally, it is shown that solutes to the left of Re significantly decrease the twin boundary energy whereas those to the right lead to a strong increase. The surface energies vary very little with alloying. We show that these effects can be largely attributed to band filling. It is also shown that the tendency of rhenium to form finely spaced twin boundaries is related to band filling effects and the presence of competing crystal structures that are close in energy to HCP for Re.

Surface Roughness Evolution under Thermo-mechanical Cycling Loads in FCC Metals - Discrete Dislocation Dynamics Simulations

Ahmed Hussein, Jaafar A. El-Awady

Department of Mechanical Engineering, Johns Hopkins University, Baltimore, MD
21218

Discrete dislocation dynamics (DDD) simulations were performed to correlate surface roughness evolution with the evolving dislocation microstructure under thermo-mechanical cyclic loadings. The role of grain-size and initial dislocation densities on the morphology of surface extrusions/intrusions and dislocation substructures are evaluated through systematic large scale 3-dimentional DDD simulations of nickel microcrystals. Cyclic thermal loadings are introduced into DDD simulations through a hierarchical modeling approach in which the thermal stresses arising in the crystal are computed from a finite element model. Cyclic mechanical loads and image fields arising from the evolving free surfaces and grain boundaries are introduced into the DDD simulations by coupling between the finite element method and the DDD framework. Finally, the evolving surface morphology due to dislocation interactions with free surfaces is actively computed from the full displacement field produced by the evolving dislocation-network. A surface roughness measure is developed and several dislocation microstructures of different crystal sizes and initial dislocation densities were simulated for a number of loading cycles. The preliminary results show that the surface roughness character is independent of the dislocation density and number of cycles but changes with crystal size.

Peierls stress, Pile-ups and Inertia effects in Field Dislocation Mechanics

Xiaohan Zhang , Amit Acharya

Carnegie Mellon University

A two dimensional dislocation plasticity model is developed under the framework of Field Dislocation Mechanics (FDM). We address various plane strain dislocation pile-ups problems numerically. The motion of dislocations and their corresponding stress field is studied under various grain boundary conditions. Relation between applied load and the deformation of a grain cell is analyzed as dislocations forming a wall against the grain boundary under shear load. The simplest example of such problems is that all dislocation pile-ups lie on one common slip plane. Such case has been analytically studied by Eshebly Frank and Nabarro, although only for limited types of load conditions. We are able to do more complex cases, for example, multiple layers of dislocations of arbitrary signs under different types of load conditions. Within the same model, some qualitative aspects of FDM are explored including 1) Peierls' stress effect in a translationally-invariant continuum theory like FDM 2) Interaction between dislocations such as dislocation annihilation 3) Dislocation dynamics in the presence of significant material inertia.

Increasing Elongation by Secondary Twinning in Magnesium Nanowires

Chang Ni^{1,2}, Hong Ding², Mark Asta², Xuejun Jin¹

¹Shanghai Jiao Tong University, Shanghai 200240, China

²University of California Berkeley, Berkeley, CA 94720, USA

One great challenge for the application of HCP metals as structural materials is the low ductility, due to the limited number of slip systems in comparison with FCC or BCC structured metals. On the other hand, HCP metals have more twinning systems because of the lower lattice symmetry, where at least five different twinning systems have been reported [1]. In HCP metals increased elongation may be realized when deformation is governed by one twinning system initially, with a second triggered at higher strains.

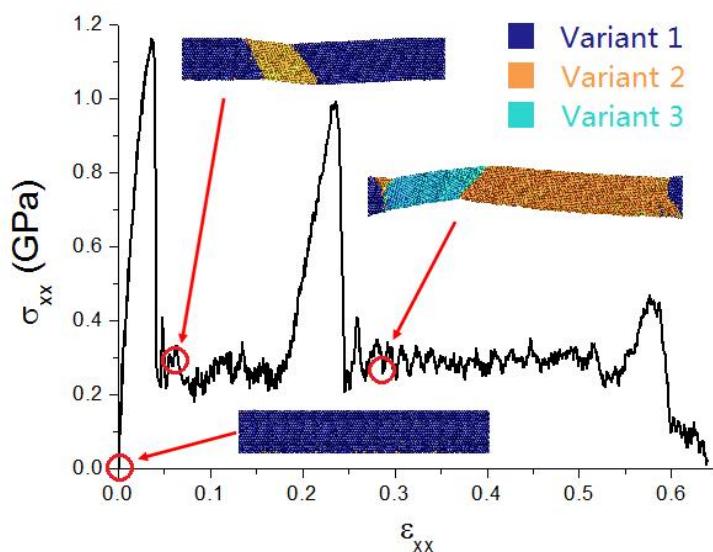


Figure 1: Stress-strain curve of Mg nanowire during tension process. Three snapshots of the nanowire inserted show different variants after twinning. The atoms are colored according to basal plane vector orientation.

In this work, we present simulation results showing the possibility of secondary twinning in HCP Mg nanowires. These molecular dynamics simulations correspond to tensile straining of $<11\bar{2}0>$ -oriented nanowires, and show 60% fracture elongation, as illustrated in Figure 1. The mechanism of secondary twin formation is studied through analyses based on crystallography and local stress state. The deformed nanowires are observed to recover their original configuration after removing the external strain, presenting typical pseudo-elastic behavior.

[1] J. W. Christian and S. Mahajan. Prog. in Mater. Sci, **39**, 1 (1995).

On the effect of dislocation emission on intergranular fracture in Ni

Guoqiang Xu, Michael J. Demkowicz

Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA, 02139

Using molecular dynamics, we investigate crack tip dislocation emission and decohesion during intergranular fracture in Ni. For some grain boundaries, cracks propagate in a brittle-like manner by bond breaking despite copious dislocation emission. Indeed, dislocation emission appears to assist crack advance by bond breaking. This result will be discussed in reference to the Rice-Thompson criterion, which views dislocation emission and decohesion as competing mechanisms during crack propagation.

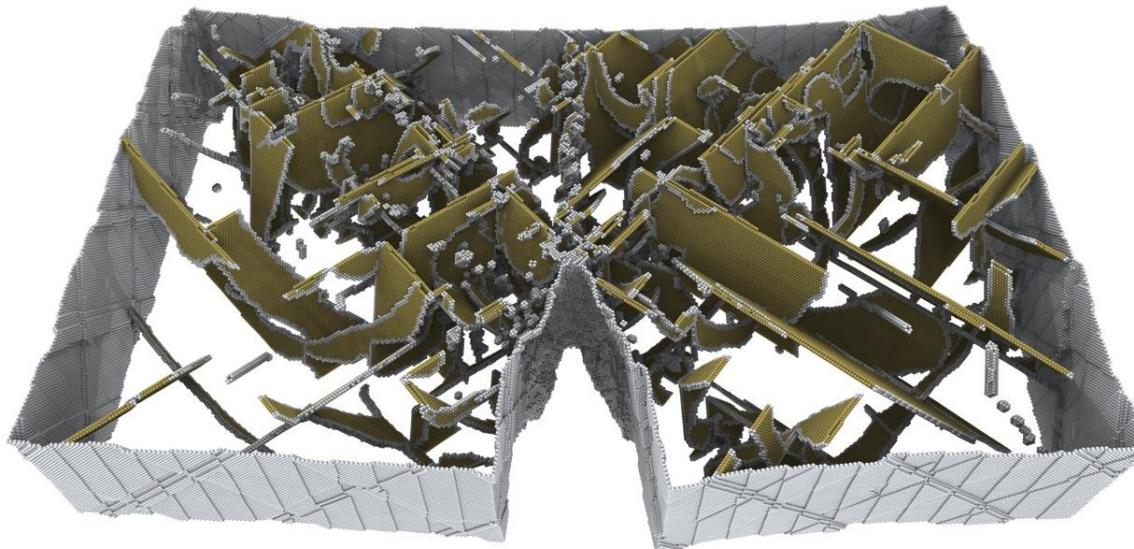


Figure 1: Dislocation emission during brittle-like fracture in a Ni bicrystal.

This work was funded by the BP-MIT Materials and Corrosion Center.

Dislocation-obstacle interactions and effects on glide from atomistic simulations

R. G. A. Veiga, T. Stona de Almeida, J. E. Guimarães Silva, H. Goldenstein

Department of Metallurgical and Materials Engineering, University of São Paulo, Av. Prof. Mello Moraes, 2463, Butantã, São Paulo/SP – 05508-030 – Brazil

The interaction of dislocations with obstacles (atoms in solid solution, voids, precipitates, other dislocations) is expected to play a major role in the strengthening of metallic alloys. In this work, with the aim of modeling dislocation-obstacle interactions and its effects on dislocation glide, we have used the model proposed in Ref. [1] to build a simulation box containing an isolated screw dislocation in bcc Fe with periodic boundary conditions in the glide direction. The separation between the dislocation and its periodic images was 15 nm, corresponding to a dislocation density in the order of $10^{14}/\text{m}^2$.

Three different systems were simulated. The first system consisted of pure Fe (i.e., no obstacle). The second system was Fe-C, with either a random carbon distribution and a carbon Cottrell atmosphere. The Cottrell atmosphere was modeled by Monte Carlo considering that the carbon content was in the range 30-2700 ppm. Finally, we considered a Fe-Cu-Ni system for which we have also used Monte Carlo to model the formation of a Cu-rich precipitate in the vicinity of the screw dislocation.

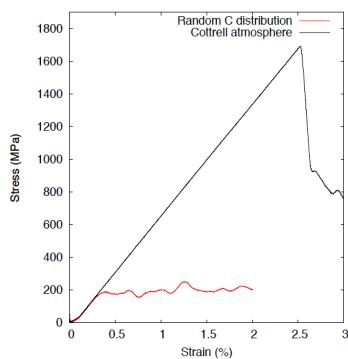


Figure 1: Stress-strain curve for a screw dislocation gliding in the presence of a random carbon distribution and a Cottrell atmosphere.

Dislocation glide in the presence or not of obstacles was simulated by molecular dynamics using the LAMMPS code. Following the same protocol presented in Ref. [2], the bottom of the simulation box was kept fixed while the atoms in the top were displaced in the Burgers vector direction with constant velocity in order to apply a constant strain rate. The simulations were performed in the NVT ensemble for temperatures in the range 70-700 K. As a matter of example, in Fig. 1, one can see the stress-strain curve of a screw dislocation gliding in the presence of a random carbon distribution and a Cottrell atmosphere, considering a carbon content of 2700 ppm.

Funding provided by Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP), grant 2011/19564-6, is gratefully acknowledged.

[1] D. J. Bacon, Y. N. Ossetsky and D. Rodney, Chapter 88 In *Dislocations and Solids*, Elsevier (2009).

[2] C. Domain and G. Monet, Phys. Rev. Letters. **95**, 215506 (2005).

Atomistic Modeling of Dislocation Slip in Alpha-Iron towards the Development of a Multi-Scale Model of Dislocation Plasticity

Lucas M. Hale¹, Jonathan A. Zimmerman¹, Hojun Lim²,
Corbett C. Battaile², Christopher R. Weinberger³

¹Sandia National Laboratories, Livermore, CA

²Sandia National Laboratories, Albuquerque, NM

³Drexel University, Philadelphia, PA

Developing micro- and macro-scale models for yield in body-centered cubic (bcc) metals that capture the underlying physics is important to accurately predict performance and guide design for structural applications of these materials. This has proven challenging due to the complexity associated with the mechanisms for plastic flow in bcc metals. Among these is the observation of non-Schmid slip of dislocations, i.e. that components of the stress state other than those that contribute to the resolved shear stress affect the slip process. In addition, plasticity is known to be thermally activated, and the rate of plastic deformation can be directly connected to the activation enthalpy for dislocation motion. How this enthalpy functionally depends on both the applied stress state and the material resistance to slip is neither trivial nor obvious for materials that violate Schmid's Law.

In our efforts to develop a physically accurate yield model for bcc iron, we perform atomistic calculations to quantify the non-Schmid, stress dependent effects of slip. An atomistic potential for bcc iron is identified that captures the stable compact core dislocation core structure and single peak Peierls barrier (i.e. no metastable split core) consistent with what is predicted from *ab initio* calculations. Using this potential, we evaluate the zero temperature critical resolved shear stress (CRSS) necessary for slip to occur for a variety of different stress states. The CRSS obtained from atomistic simulations is then used to fit a generalized non-Schmid yield law that captures the dependence of the yield stress on shear stresses both parallel and perpendicular to the shear direction, as well as changes in pressure. Of particular significance, we show that atomistic results provide insight on the activation enthalpy for non-Schmid slip, and suggest a functional dependency between enthalpy, the applied stress state, and the CRSS that appears valid across a range of stress states and loading orientations.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Ab initio prediction of screw dislocation motion in bcc transition metals: kink-pair formation enthalpies and Schmid law deviation

D. Rodney¹, L. Dezerald², L. Ventelon², L. Proville², F. Willaime²

¹Institut Lumière Matière, Université Lyon 1, France

²CEA, DEN, Service de Recherches de Métallurgie Physique, France

In body-centered cubic (bcc) metals, plasticity arises from the motion of $\frac{1}{2}\langle 111 \rangle$ screw dislocations. These dislocations are subjected to a lattice resistance that can be described through the two-dimensional energy landscape of the dislocation in the $\{111\}$ plane, the so-called 2D Peierls potential. Here, we employ *ab initio* calculations based on Density Functional Theory (DFT) to determine the 2D Peierls potentials in bcc transition metals: V, Nb, Ta, Mo, W, Fe [1]. We use these potentials to deduce several properties of dislocation glide and in particular, the kink-pair formation enthalpy, as well as the dependence of the Peierls stress on crystal orientation, well-known in bcc crystals for their deviations from Schmid law.

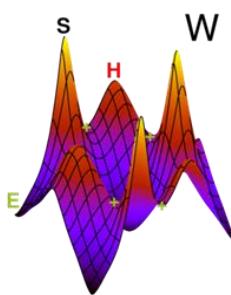


Figure 1: *Ab initio* 2D Peierls potential in W [1].

Dislocations move between Peierls valleys by the nucleation and propagation of kink-pairs. In this work, we calculated the kink-pair formation energy in bcc transition metals using a line tension model parameterized on the 2D *ab initio* Peierls potentials [2], allowing to predict kink properties from *ab initio* calculations performed in cells containing only a few hundred atoms. The formation enthalpies thus obtained show large deviations from isotropic elasticity and, when compared to experimental data, suggest an important contribution of the entropy to the Gibbs formation enthalpy. Moreover, the temperature dependence of the kink-pair enthalpy sheds a new light on the implication of dislocation glide in the brittle-to-ductile transition.

We then used the 2D *ab initio* Peierls potentials calculated under no applied stress to predict the behavior of dislocations under stress. We thus calculated the dependence of the Peierls stress on the orientation of the applied stress with respect to the crystal orientation, allowing us to analyze deviations from Schmid law in various bcc metals. These results are compared to direct *ab initio* calculations of Schmid law deviation, in order to test the validity of using zero-stress Peierls potentials. The calculations show large variations between metals that are discussed with respect to available experimental data.

- [1] L. Dezerald, L. Ventelon, E. Clouet, C. Denoual, D. Rodney and F. Willaime, Phys. Rev. B **89**, 024104 (2014).
- [2] L. Proville, L. Ventelon and D. Rodney, Phys. Rev. B **87**, 144106 (2013).

Getting Real!
**Thermodynamics and Statistical Mechanics from First Principles for Materials
Science and Engineering**

Matthias Scheffler

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin,
Germany

Ab initio (atomistic) thermodynamics [Ref. 1 and references therein] has evolved into a standard practice in important application areas such as, for example, defects in materials, surface reconstructions, corrosion, and sensing. Important ramifications have furthermore established its use in heterogeneous catalysis and electrocatalysis.

Since the late 1990s the above method is being complemented by what is called the “*ab initio* kinetic Monte Carlo” approach, enabling the correct description of the kinetic processes that govern diverse technologically important processes and/or ***the function*** of materials.[1] For short time scales *ab initio* molecular dynamics (MD) helps to identify the relevant processes, but its time span is limited to about one nano second. The *ab initio* kinetic Monte Carlo approach then reaches the realistic range (seconds, minutes, and longer). This enabled the first-principles description and understanding of crystal growth and heterogeneous catalysis.[1]

In this talk, I will examine the critical importance of the accuracy of the underlying interatomic interactions, “the base”, which is many-body quantum mechanics. The range of validity of state-of-the-art approximations (also force fields) will be assessed, and I will address the concept of a “cascade of increasing accuracy”. The latte starts from (sophisticated) force fields and then goes to higher and higher levels of many-electron quantum mechanics and density-functional theory approximations.[2] With respect to the modeling algorithms, I will focus on replica exchange MD, genetic algorithm, and the kinetic Monte Carlo approach. Examples to demonstrate the crucial needs of a reliable description of the interatomic interactions and the significant errors, that result when the interactions (the base of modeling) are not described accurately, come, e.g., from heterogeneous catalysis and biophysics.

- [1] K. Reuter, C. Stampfl, and M. Scheffler, “*Ab Initio Thermodynamics and Statistical Mechanics of Surface Properties and Functions*”, in: Handbook of Materials Modeling, Part A. Methods, S. Yip (ed.), Springer, Berlin (2005). ISBN-10 1-4020-3287-0, p. 149
[2] S. Bhattacharya, S. Levchenko, L. M. Ghiringhelli, and M. Scheffler, Phys. Rev. Lett. **111**, 135501 (2013); and to be published.

Two-scale analysis of composite plates with in-plane periodic microstructures

Kenjiro Terada¹, Seishiro Matsubara¹, Yuki Aoba¹, Norio Hirayama²

¹Tohoku University, Sendai 980-8579, Japan

²Nitto Boseki Co., Ltd., Fukushima 960-2154, Japan

A method of two-scale analysis of composite plates with in-plane periodic microstructures is presented. The overall structure is replaced by an equivalent laminate at macro-scale, each of whose lamina has its own homogenized material properties, and its in-plane, bending and coupling stiffness characteristics can be evaluated by the numerical plate testing (NPT) based on the homogenization theory.

The NPT is realized by finite element analyses with solid elements conducted on the three-dimensional unit cell models with in-plane periodicity constraints only, and the data obtained from the NPT can be used to identify the material properties for all the laminae. Note here that the macro-scale plate is regarded as a laminated composite plate, even if a laminated structure is not assumed for the microstructure.

Our first trial on this development focuses on the linearly elastic materials so that the in-plane, bending and coupling stiffness matrices in the conventional laminate model can be evaluated as macro-scale properties. The second stage of our presentation is extension to NPT with nonlinear materials, in which material properties for each macroscopic lamina are identified with the method of particle swarm optimization or differential evolution with the help of the novel method of NPT conducted on a unit cell discretized with laminated plate elements.

Several numerical examples are presented to demonstrate the processes of NPT and identification of material parameters as well as the homogenization and localization capabilities of the proposed two-scale analysis method.

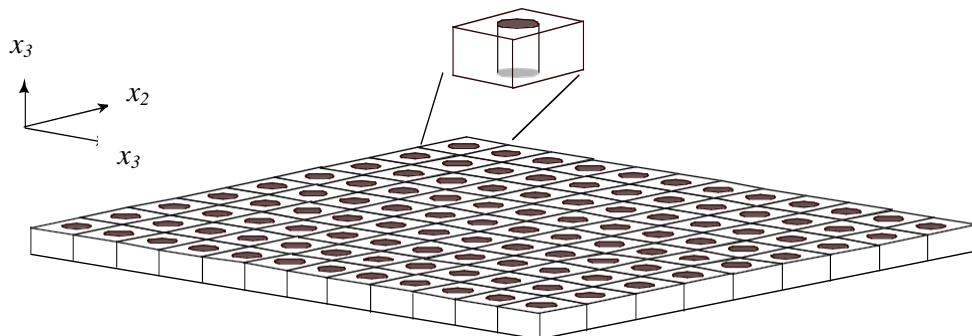


Figure 1: Composite plate with in-plane microstructures

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Siesta-PEXSI: Massively parallel method for efficient and accurate ab initio materials simulation

Lin Lin¹, Alberto Garcia², Georg Huhs³, Chao Yang⁴

¹ UC Berkeley, USA, ² Institut de Ciencia de Materials de Barcelona, Spain, ³Barcelona Supercomputer Center, Spain, ⁴Lawrence Berkeley National Laboratory, USA

We describe how to combine the pole expansion and selected inversion (PEXSI) technique with the SIESTA method, which uses numerical atomic orbitals for Kohn-Sham density functional theory (KSDFT) calculations. The PEXSI technique can efficiently utilize the sparsity pattern of the Hamiltonian matrix and the overlap matrix generated from codes such as SIESTA, and solves KSDFT without using cubic scaling matrix diagonalization procedure. The complexity of PEXSI scales at most quadratically with respect to the system size, and the accuracy is comparable to that obtained from full diagonalization. One distinct feature of PEXSI is that it achieves low order scaling without using the near-sightedness property and can be therefore applied to metals as well as insulators and semiconductors, at room temperature or even lower temperature. The PEXSI method is highly scalable, and the recently developed massively parallel PEXSI technique can make efficient usage of 10,000 - 100,000 processors on high performance machines. We demonstrate the performance the SIESTA-PEXSI method using several examples for large scale electronic structure calculation including long DNA chain and graphene-like structures with more than 20000 atoms.

A coarse-grained Gaussian electronic structure model for molecular dynamics studies of materials

Glenn J. Martyna^{1,2}

¹Physical Science, IBM Research, IBM TJ Watson Lab, Yorktown Heights, NY, USA

²Honorary Professor of Physics, University of Edinburgh, Edinburgh, UK

Computer clock speeds are no longer increasing and increases in computational power are now limited to increases in processor number, unfamiliar territory for computational scientists who have ridden the wave of CMOS-scaling for the past 30 years. In this brave new world, gains in computational accuracy and performance will be driven by methodological development. In this lecture, a non-perturbative treatment of long range forces will be described to allow fast, transferable atomistic simulations is described. There are many physical systems where the non-pairwise additive nature of polarization and dispersion interactions becomes important, in particular, the complex heterogeneous systems of interest in chemistry, biology and biophysics. For example, the dipole moment of water changes from 1.85 Debye in the gas phase to approximately 2.6 Debye in the bulk liquid and attains intermediate values at hydrophobic interfaces due to many-body polarization. Similarly, although the bulk properties of hydrophobic fluids can be modeled using a pair potential, this underestimates the surface tension by 30% due to many-body dispersion interactions. In order to treat both many-body polarization and dispersion interactions in atomic and molecule systems consistently, a coarse grained electronic structure system of quantized Drude oscillators is introduced. Although they obey Gaussian statistics, the system of oscillators generates a surprisingly accurate set of electronic responses as is often the case for models based on Gaussian fluctuations in physics. A simulation method based on quantum path integrals with order O(N) computational complexity is presented to realize the model. Applications to the phase diagram of water and its signature properties, are given.

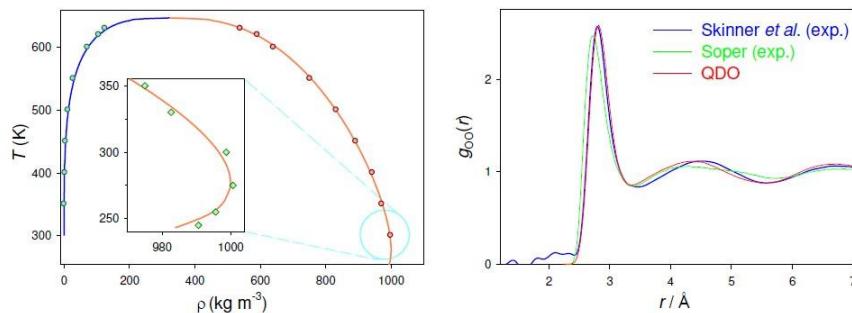


Figure 1: Phase diagram of the Gaussian Coarse-grained water model (left) and its structure at $T=300\text{K}$

A Bayesian Framework for Calibration and Validation of Coarse-Grained Atomistic Models

Eric Wright, Peter Rossky, J. Tinsley Oden

Institute for Computational Engineering and Sciences, Austin, TX 78712

The proposed work addresses issues related to the derivation of reduced models of atomistic systems, their statistical calibration, and their relation to atomistic models, particularly those involved with nanostructured materials. In a general sense, an atomistic description of a material contains a listing of the chemical constituents of the material at the atomic scale, as well as a set of mathematical formulas that quantify intra- and intermolecular interactions between the chemical components of the material. These interactions are usually given in the form of a potential energy ansatz containing a set of free parameters that are calibrated in reference to experimental data and highly accurate, but computationally expensive, quantum chemistry simulations. The potential energy forms, once calibrated, serve as the basis for molecular dynamics (MD) simulations that propagate the system forward in time by numerically solving the classical Newton equations derived from the potential energy formulas. Although much faster than quantum chemistry based computations, the described classical methods, referred to as molecular mechanics methods, become prohibitively expensive for systems of millions or billions of atoms. Thus, the theoretical chemistry community is interested in developing reduced models of atomistic systems that are computationally feasible for systems of meso- to macroscopic size (> 10 nm). Popular routes to model reduction include so-called coarse-graining (CG) methods that reduce the degrees of freedom associated with atomistic calculations by replacing particular groups of atoms with single interaction sites (beads). The reduced models derived from the CG procedure, known as coarse-grained models, involve their own sets of potential energy functions, the free parameters of which are commonly calibrated in reference to atomistic simulation data such that the resulting CG models may reproduce aggregate behaviors of the original atomistic models in MD simulations[1]

We pursue a statistical method for CG model calibration based on principles of Bayesian inference[2], the results of which are dependent on the identification of quantities of interest (QOIs) and their related physical observables. The main issues we address here are the derivation of prior CG parameter probabilities from rigorous mathematical principles, the formulation of likelihood functions with respect to relevant physical observables, computational techniques for sampling CG parameter probability distributions, and the analysis of model uncertainty with respect to chosen QOIs. In order to illustrate these issues, we develop a CG model for a liquid heptane system at standard thermodynamic conditions, calibrate CG parameters according to our Bayesian inference framework, and analyze the accuracy and precision of the model's prediction of the vapor/liquid transfer free energy. We conclude that the selection of calibration observables is vital to the well-posedness and predictive ability of a CG model. We also comment on the implications of our method to problems of model validation and selection.

[1] W. Noid. Perspective: Coarse-Grained Models for Biomolecular Systems. *The Journal of Chemical Physics*, Vol. 139, Issue 9, Page 09090, 2013.

[2] J. T. Oden, R. Moser, O. Ghattas. Computer Predictions with Quantified Uncertainty, Part I. *SIAM News*, Vol. 43, Number 9, November 2010

Assessment of Phase Field Crystal Concepts using Long-Time Molecular Dynamics

K. L. Baker, W. A. Curtin

École Polytechnique Fédérale de Lausanne (EPFL), Institute of Mechanical
Engineering, CH-1015 Lausanne, Switzerland

Accelerated molecular dynamics is used to compute the one-particle probability density in a complex defect consisting of a Lomer dislocation with an equilibrium distribution of vacancies in the core, and the results are considered within the framework of the Phase Field Crystal (PFC) model. The computed one-particle density shows numerous spatially-localized peaks with integrated densities smaller than unity (less than one atom on average) which correspond to a superposition of just a few specific, well-defined atomic configurations with well-defined energies and energy barriers between them. There is no clear path for reconstructing the actual atomic structures from the one-particle density in the absence of knowledge of the multi-particle correlations. The potential energy computed using the one-particle density differs from the actual atomistic energy by nearly 40eV and is distributed among the partially occupied atomic peaks. These results demonstrate, in one non-trivial case, that the PFC model cannot predict the atomistic defect structures, energies of those structures, nor kinetic barriers between those structures. The PFC model thus appears to be limited in its ability to predict atomic defect properties at the quantitative level needed for application to problems in materials science.

Modeling the pressure vessel steel microstructure evolution under neutron irradiation using AKMC in Fe multi component alloys - optimization towards long irradiation times

C. Domain^{1,2}, B. Pannier^{1,2}, C.S. Becquart^{2,3}

¹EDF-R&D, Département Matériaux et Mécanique des Composants (MMC), Les Renardières, F-77818 Moret sur Loing Cedex, France

²Laboratoire commun EDF-CNRS Etude et Modélisation des Microstructures pour le Vieillissement des Matériaux (EM2VM), France

³Unité Matériaux Et Transformations, UMET, UMR 8207, Villeneuve d'Ascq, France

The ageing and the evolution of mechanical properties of pressure vessel steels under radiation has been correlated with the formation of more or less dilute solute clusters. In the dilute Fe alloys, tomographic atom probe analysis show that these clusters are mainly enriched in Cu, Ni, Mn, Si, P. The evolution of these is governed by the migration of the individual point defects which requires a large number of atomistic kinetic Monte Carlo (AKMC) steps to provide the microstructure state obtained after irradiation.

Consequently the simulations are very heavy in terms of computing time. Furthermore, as several substitutional elements (Cu, Ni, Mn, Si, P) and foreign interstitials (C, N) need to be taken into account to describe the alloy, all the possible microstructural objects that can form in the alloys are numerous and complex, their evolution follow very different time scales between the local rearrangement of the clusters and their migration in particular. In this work, some optimization methods and strategies that we have used in our AKMC simulations will be presented and discussed. The microstructure obtained will be compared to experimental results.

This work is part of the PERFORM project.

Kinetics and micromechanics associated with crack growth in brittle materials

S. Djouder, M. Touati, M. Chabaat

Built Env. Research Lab., Department of Structures and Materials, Civil Engg. Faculty,
U.S.T.H.B., B. P. 32 El-Alia, Bab Ezzouar, Algiers, Algeria 16111.

In this study, kinetics and micromechanics associated with crack growth in brittle materials are considered. It is known that crack growth characteristics contain information on the material strength of fracture mechanisms and that there are sufficient experimental data evidencing that in most cases a crack growth is surrounded by a severely Damage Zone (DZ) which often precedes the crack itself. During its propagation, the DZ is characterized by few degrees of freedom (elementary movements) such as translation, rotation, isotropic expansion and distortion. On the basis of a stress field distribution obtained by the use of a Semi-Empirical Approach (SEA), which relies on the Green's functions, these driving forces corresponding to the mentioned degrees of freedom are formulated within the framework of the plane problem of elastostatics.

A number of theoretical models have been proposed for the description of a stress field and kinetics of a damage zone [1, 2]. The traditional one identifies the DZ as a plastic zone and uses the well developed technique of the plasticity theory for the determination of its size, shape, energy release rates etc... According to recent experimental results, some damage patterns do not yield any model of plasticity and the shape of the DZ can be difficult to model. Then, a plasticity criteria is not adequate for damage characterization. However, elastoplastic solution is currently employed due to the lack of other approaches.

Throughout this study, SEM is proposed for evaluating the stress field and the different energy release rates. This approach is based on the representation of displacement discontinuities by means of the Green's function theory [3, 4]. This latest has been used in a purely theoretical context. Herein, we suggest a more realistic model (arbitrary orientations of discontinuities rather than rectilinear ones) for which the result can be obtained using the experimental data and thus avoiding the difficulties of analytical solutions.

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- [2] M. T. K. Takemori, *Polymers Engng. and Sci.*, Vol. **22** (1982) 937-645.
- [3] M. Chabaat, S. Djouder and M. Touati, *Int. J. of Applied Mech. and Mat.* Vol. **3-4** (2005) 243-252.
- [4] A. Chudnovsky, A. Dolgopolsky and M. Kachanov, *Int. J. Solids Struct.*, **23**(1987)1-21.
- [5] B. Budiansky and J. R. Rice, ASME, *J. Appl. Mech.*, **40** (1973) 201-203.
- [6] Yi-Hen Chen, *Int. J. Solids and Structures*, **38** (2001) 3193-3212.

Quantum-Atomic-Continuum-Coupled Model for the Thermo-mechanical Behavior in Micro-nano Simulation

Tiansi HAN, Junzhi CUI

LSEC, ICMSEC, Academy of Mathematics and System Sciences, CAS, Beijing, 100190 China

In order to study the thermo-mechanical behavior of materials in micro-nano scale, a computational model which couples quantum-atomic-continuum natures together is presented in this paper (i.e. QACC model). Unlike traditional methods, the transition region is not needed since the nonlocal mechanical effects are naturally involved in this model. Some necessary assumptions are made when using first principle density functional calculations. Deformations based on Bravais lattice are explicitly derived.

The responses of 3-demensional 25313 copper atoms nanowires under different external loads are simulated in this paper. Stress and strain fields are calculated and dislocation distributions are predicted in the damage process (shown in Figure 1). Numerical results confirm the validity and transferability of this model.

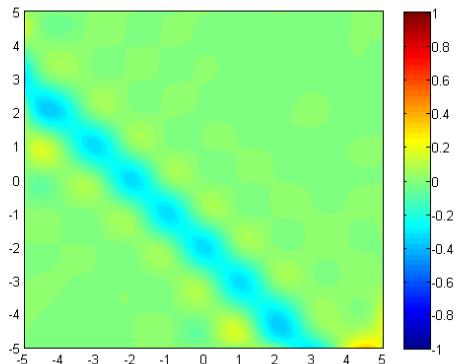


Figure 1 a)

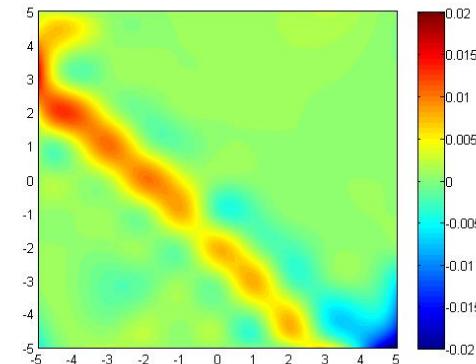


Figure 1 b)

Figure 1 a) xz component of the Cauchy-Green strain tensor and b) xz component of the first Piola-Kirchhoff stress tensor under tension on the middle plane.

This work is supported by the National Basic Research Program of China (973 Program No. 2012CB025904), and also supported by the State Key Laboratory of Science and Engineering Computing. The authors gratefully acknowledge help discussions with PhD. Bowen LI and PhD. Yuran ZHANG.

Getting Real!
**Thermodynamics and Statistical Mechanics from First Principles for Materials
Science and Engineering**

Matthias Scheffler

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin,
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[2] S. Bhattacharya, S. Levchenko, L. M. Ghiringhelli, and M. Scheffler, Phys. Rev. Lett. **111**, 135501 (2013); and to be published.

Two-scale analysis of composite plates with in-plane periodic microstructures

Kenjiro Terada¹, Seishiro Matsubara¹, Yuki Aoba¹, Norio Hirayama²

¹Tohoku University, Sendai 980-8579, Japan

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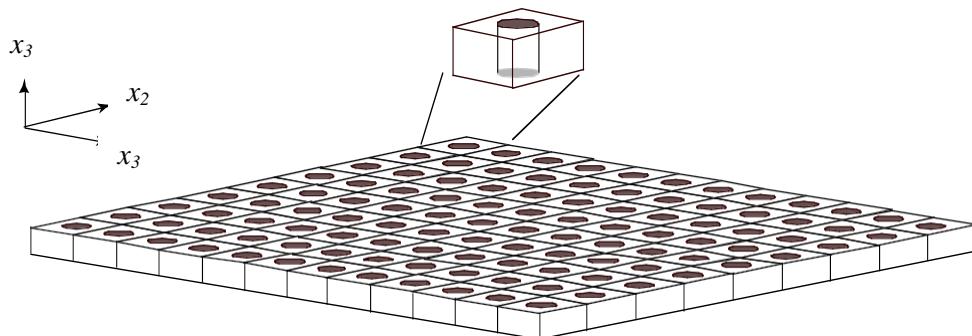


Figure 1: Composite plate with in-plane microstructures

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Siesta-PEXSI: Massively parallel method for efficient and accurate ab initio materials simulation

Lin Lin¹, Alberto Garcia², Georg Huhs³, Chao Yang⁴

¹ UC Berkeley, USA, ² Institut de Ciencia de Materials de Barcelona, Spain, ³Barcelona Supercomputer Center, Spain, ⁴Lawrence Berkeley National Laboratory, USA

We describe how to combine the pole expansion and selected inversion (PEXSI) technique with the SIESTA method, which uses numerical atomic orbitals for Kohn-Sham density functional theory (KSDFT) calculations. The PEXSI technique can efficiently utilize the sparsity pattern of the Hamiltonian matrix and the overlap matrix generated from codes such as SIESTA, and solves KSDFT without using cubic scaling matrix diagonalization procedure. The complexity of PEXSI scales at most quadratically with respect to the system size, and the accuracy is comparable to that obtained from full diagonalization. One distinct feature of PEXSI is that it achieves low order scaling without using the near-sightedness property and can be therefore applied to metals as well as insulators and semiconductors, at room temperature or even lower temperature. The PEXSI method is highly scalable, and the recently developed massively parallel PEXSI technique can make efficient usage of 10,000 - 100,000 processors on high performance machines. We demonstrate the performance the SIESTA-PEXSI method using several examples for large scale electronic structure calculation including long DNA chain and graphene-like structures with more than 20000 atoms.

A coarse-grained Gaussian electronic structure model for molecular dynamics studies of materials

Glenn J. Martyna^{1,2}

¹Physical Science, IBM Research, IBM TJ Watson Lab, Yorktown Heights, NY, USA

²Honorary Professor of Physics, University of Edinburgh, Edinburgh, UK

Computer clock speeds are no longer increasing and increases in computational power are now limited to increases in processor number, unfamiliar territory for computational scientists who have ridden the wave of CMOS-scaling for the past 30 years. In this brave new world, gains in computational accuracy and performance will be driven by methodological development. In this lecture, a non-perturbative treatment of long range forces will be described to allow fast, transferable atomistic simulations is described. There are many physical systems where the non-pairwise additive nature of polarization and dispersion interactions becomes important, in particular, the complex heterogeneous systems of interest in chemistry, biology and biophysics. For example, the dipole moment of water changes from 1.85 Debye in the gas phase to approximately 2.6 Debye in the bulk liquid and attains intermediate values at hydrophobic interfaces due to many-body polarization. Similarly, although the bulk properties of hydrophobic fluids can be modeled using a pair potential, this underestimates the surface tension by 30% due to many-body dispersion interactions. In order to treat both many-body polarization and dispersion interactions in atomic and molecule systems consistently, a coarse grained electronic structure system of quantized Drude oscillators is introduced. Although they obey Gaussian statistics, the system of oscillators generates a surprisingly accurate set of electronic responses as is often the case for models based on Gaussian fluctuations in physics. A simulation method based on quantum path integrals with order O(N) computational complexity is presented to realize the model. Applications to the phase diagram of water and its signature properties, are given.

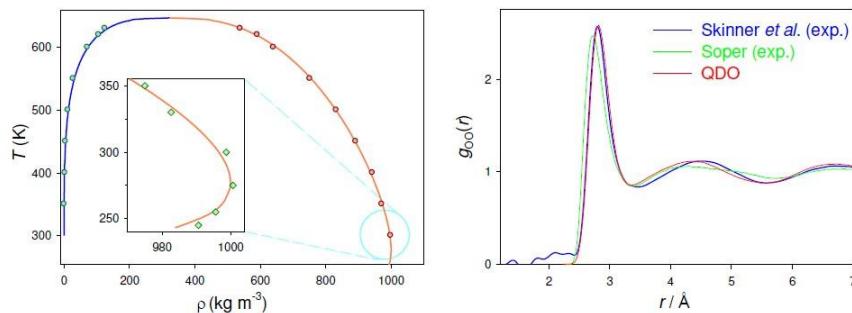


Figure 1: Phase diagram of the Gaussian Coarse-grained water model (left) and its structure at $T=300\text{K}$

A Bayesian Framework for Calibration and Validation of Coarse-Grained Atomistic Models

Eric Wright, Peter Rossky, J. Tinsley Oden

Institute for Computational Engineering and Sciences, Austin, TX 78712

The proposed work addresses issues related to the derivation of reduced models of atomistic systems, their statistical calibration, and their relation to atomistic models, particularly those involved with nanostructured materials. In a general sense, an atomistic description of a material contains a listing of the chemical constituents of the material at the atomic scale, as well as a set of mathematical formulas that quantify intra- and intermolecular interactions between the chemical components of the material. These interactions are usually given in the form of a potential energy ansatz containing a set of free parameters that are calibrated in reference to experimental data and highly accurate, but computationally expensive, quantum chemistry simulations. The potential energy forms, once calibrated, serve as the basis for molecular dynamics (MD) simulations that propagate the system forward in time by numerically solving the classical Newton equations derived from the potential energy formulas. Although much faster than quantum chemistry based computations, the described classical methods, referred to as molecular mechanics methods, become prohibitively expensive for systems of millions or billions of atoms. Thus, the theoretical chemistry community is interested in developing reduced models of atomistic systems that are computationally feasible for systems of meso- to macroscopic size (> 10 nm). Popular routes to model reduction include so-called coarse-graining (CG) methods that reduce the degrees of freedom associated with atomistic calculations by replacing particular groups of atoms with single interaction sites (beads). The reduced models derived from the CG procedure, known as coarse-grained models, involve their own sets of potential energy functions, the free parameters of which are commonly calibrated in reference to atomistic simulation data such that the resulting CG models may reproduce aggregate behaviors of the original atomistic models in MD simulations[1]

We pursue a statistical method for CG model calibration based on principles of Bayesian inference[2], the results of which are dependent on the identification of quantities of interest (QOIs) and their related physical observables. The main issues we address here are the derivation of prior CG parameter probabilities from rigorous mathematical principles, the formulation of likelihood functions with respect to relevant physical observables, computational techniques for sampling CG parameter probability distributions, and the analysis of model uncertainty with respect to chosen QOIs. In order to illustrate these issues, we develop a CG model for a liquid heptane system at standard thermodynamic conditions, calibrate CG parameters according to our Bayesian inference framework, and analyze the accuracy and precision of the model's prediction of the vapor/liquid transfer free energy. We conclude that the selection of calibration observables is vital to the well-posedness and predictive ability of a CG model. We also comment on the implications of our method to problems of model validation and selection.

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Assessment of Phase Field Crystal Concepts using Long-Time Molecular Dynamics

K. L. Baker, W. A. Curtin

École Polytechnique Fédérale de Lausanne (EPFL), Institute of Mechanical
Engineering, CH-1015 Lausanne, Switzerland

Accelerated molecular dynamics is used to compute the one-particle probability density in a complex defect consisting of a Lomer dislocation with an equilibrium distribution of vacancies in the core, and the results are considered within the framework of the Phase Field Crystal (PFC) model. The computed one-particle density shows numerous spatially-localized peaks with integrated densities smaller than unity (less than one atom on average) which correspond to a superposition of just a few specific, well-defined atomic configurations with well-defined energies and energy barriers between them. There is no clear path for reconstructing the actual atomic structures from the one-particle density in the absence of knowledge of the multi-particle correlations. The potential energy computed using the one-particle density differs from the actual atomistic energy by nearly 40eV and is distributed among the partially occupied atomic peaks. These results demonstrate, in one non-trivial case, that the PFC model cannot predict the atomistic defect structures, energies of those structures, nor kinetic barriers between those structures. The PFC model thus appears to be limited in its ability to predict atomic defect properties at the quantitative level needed for application to problems in materials science.

Modeling the pressure vessel steel microstructure evolution under neutron irradiation using AKMC in Fe multi component alloys - optimization towards long irradiation times

C. Domain^{1,2}, B. Pannier^{1,2}, C.S. Becquart^{2,3}

¹EDF-R&D, Département Matériaux et Mécanique des Composants (MMC), Les Renardières, F-77818 Moret sur Loing Cedex, France

²Laboratoire commun EDF-CNRS Etude et Modélisation des Microstructures pour le Vieillissement des Matériaux (EM2VM), France

³Unité Matériaux Et Transformations, UMET, UMR 8207, Villeneuve d'Ascq, France

The ageing and the evolution of mechanical properties of pressure vessel steels under radiation has been correlated with the formation of more or less dilute solute clusters. In the dilute Fe alloys, tomographic atom probe analysis show that these clusters are mainly enriched in Cu, Ni, Mn, Si, P. The evolution of these is governed by the migration of the individual point defects which requires a large number of atomistic kinetic Monte Carlo (AKMC) steps to provide the microstructure state obtained after irradiation.

Consequently the simulations are very heavy in terms of computing time. Furthermore, as several substitutional elements (Cu, Ni, Mn, Si, P) and foreign interstitials (C, N) need to be taken into account to describe the alloy, all the possible microstructural objects that can form in the alloys are numerous and complex, their evolution follow very different time scales between the local rearrangement of the clusters and their migration in particular. In this work, some optimization methods and strategies that we have used in our AKMC simulations will be presented and discussed. The microstructure obtained will be compared to experimental results.

This work is part of the PERFORM project.

Kinetics and micromechanics associated with crack growth in brittle materials

S. Djouder, M. Touati, M. Chabaat

Built Env. Research Lab., Department of Structures and Materials, Civil Engg. Faculty,
U.S.T.H.B., B. P. 32 El-Alia, Bab Ezzouar, Algiers, Algeria 16111.

In this study, kinetics and micromechanics associated with crack growth in brittle materials are considered. It is known that crack growth characteristics contain information on the material strength of fracture mechanisms and that there are sufficient experimental data evidencing that in most cases a crack growth is surrounded by a severely Damage Zone (DZ) which often precedes the crack itself. During its propagation, the DZ is characterized by few degrees of freedom (elementary movements) such as translation, rotation, isotropic expansion and distortion. On the basis of a stress field distribution obtained by the use of a Semi-Empirical Approach (SEA), which relies on the Green's functions, these driving forces corresponding to the mentioned degrees of freedom are formulated within the framework of the plane problem of elastostatics.

A number of theoretical models have been proposed for the description of a stress field and kinetics of a damage zone [1, 2]. The traditional one identifies the DZ as a plastic zone and uses the well developed technique of the plasticity theory for the determination of its size, shape, energy release rates etc... According to recent experimental results, some damage patterns do not yield any model of plasticity and the shape of the DZ can be difficult to model. Then, a plasticity criteria is not adequate for damage characterization. However, elastoplastic solution is currently employed due to the lack of other approaches.

Throughout this study, SEM is proposed for evaluating the stress field and the different energy release rates. This approach is based on the representation of displacement discontinuities by means of the Green's function theory [3, 4]. This latest has been used in a purely theoretical context. Herein, we suggest a more realistic model (arbitrary orientations of discontinuities rather than rectilinear ones) for which the result can be obtained using the experimental data and thus avoiding the difficulties of analytical solutions.

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Quantum-Atomic-Continuum-Coupled Model for the Thermo-mechanical Behavior in Micro-nano Simulation

Tiansi HAN, Junzhi CUI

LSEC, ICMSEC, Academy of Mathematics and System Sciences, CAS, Beijing, 100190 China

In order to study the thermo-mechanical behavior of materials in micro-nano scale, a computational model which couples quantum-atomic-continuum natures together is presented in this paper (i.e. QACC model). Unlike traditional methods, the transition region is not needed since the nonlocal mechanical effects are naturally involved in this model. Some necessary assumptions are made when using first principle density functional calculations. Deformations based on Bravais lattice are explicitly derived.

The responses of 3-demensional 25313 copper atoms nanowires under different external loads are simulated in this paper. Stress and strain fields are calculated and dislocation distributions are predicted in the damage process (shown in Figure 1). Numerical results confirm the validity and transferability of this model.

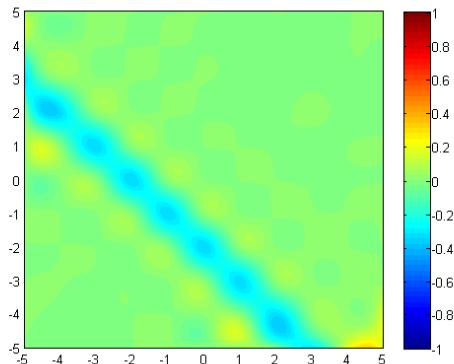


Figure 1 a)

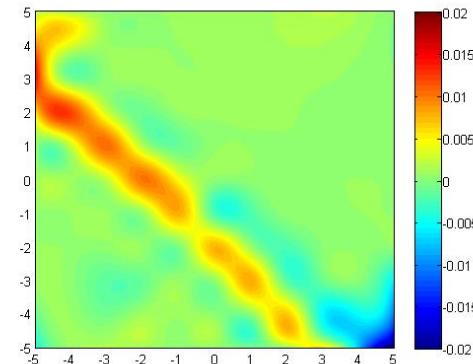


Figure 1 b)

Figure 1 a) xz component of the Cauchy-Green strain tensor and b) xz component of the first Piola-Kirchhoff stress tensor under tension on the middle plane.

This work is supported by the National Basic Research Program of China (973 Program No. 2012CB025904), and also supported by the State Key Laboratory of Science and Engineering Computing. The authors gratefully acknowledge help discussions with PhD. Bowen LI and PhD. Yuran ZHANG.

Extending accelerated molecular dynamics methods to larger and more complex systems

Arthur F. Voter

Los Alamos National Laboratory, Los Alamos, New Mexico, 87545, USA

Many important materials processes take place on time scales that vastly exceed the nanoseconds accessible to molecular dynamics simulation. Typically, this long-time dynamical evolution is characterized by a succession of thermally activated infrequent events involving defects in the material. In the accelerated molecular dynamics (AMD) methodology, known characteristics of infrequent-event systems are exploited to make reactive events take place more frequently, in a dynamically correct way. For certain processes, this approach has been remarkably successful, offering a view of complex dynamical evolution on time scales of microseconds, milliseconds, and sometimes beyond. Examples include metallic surface diffusion and growth, radiation damage annealing processes, and carbon nanotube dynamics. In this talk, I will discuss some recent advances that are extending the range of applicability of the AMD methods to larger and more complex systems. For example, we now understand that the parallel replica dynamics method can give exact state to state dynamics even when the state definitions are not necessarily Markovian, provided the dephasing stage is continued long enough [1]. This provides a clean framework for treating more complex systems where it is difficult to define simple, deep states, or where it is desirable to lump many basins together into one superstate. We have also formulated a new, local version of the hyperdynamics method that gives constant boost as the system size is increased, in contrast to standard hyperdynamics, for which the boost decays towards unity as the system size is increased. We have also been exploring the limiting boost that is possible with hyperdynamics when the bias potential can be designed in an ideal way.

This work was supported by the United States Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, and by the Laboratory Directed Research and Development program at Los Alamos National Laboratory.

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Bifurcation diagram and thermally assisted magnetization reversals in spin-torque driven nanomagnets

Eric vanden-eijnden and Katie Newhall

Courant Institute, NYU, USA

Driving nanomagnets by spin-polarized currents offers exciting prospects in magnetoelectronics, but the response of the magnets to such currents remains poorly understood because they apply a nonconservative force, called spin-transfer torque (STT), on the system. Here we investigate the effect of STT in various parameter regime. In the low-damping regime, we show that an averaged equation describing the diffusion of energy on a graph captures the dynamics of these magnets. From this equation, we can obtain the bifurcation diagram of the magnets, including the critical currents to induce stable precessional states and magnetization switching, as well as the mean times of thermally assisted magnetization reversal in situations where the standard reaction rate theory of Kramers is no longer valid. These results match experimental observations and give a theoretical basis for a Neel-Brown-type formula with an effective energy barrier for the reversal times. For higher values of the damping, results from large deviation theory can be used to identify the pathway and rate of switching of these magnets when the amplitude of the thermal noise is small.

Sampling saddle points on the free energy surface

Amit Samanta

Lawrence Livermore National Laboratory, Livermore, CA 94551, USA

Efficient exploration of the free energy surface (FES) of a complex system at finite temperatures, though often desirable, remains a difficult task. Such explorations involve searching for metastable states and bottlenecks for transitions between these metastable states in the space of coarse grained variables. In this talk, I will present an algorithm for finding saddle points on the free energy surface “on-the-fly” without having to find the free energy function itself. This is done by using the general strategy of the heterogeneous multi-scale method, applying a macro-scale solver, here the gentlest ascent dynamics algorithm, with the needed force and Hessian values computed on-the-fly using a micro-scale model such as molecular dynamics. The algorithm is capable of dealing with problems involving many coarse-grained variables. The utility of the algorithm is illustrated by studying the saddle points associated with (a) the isomerization transition of the alanine dipeptide using two coarse-grained variables, specifically the Ramachandran dihedral angles, and (b) the beta-hairpin structure of the alanine decamer using twenty coarse-grained variables, specifically the full set of Ramachandran angle pairs associated with each residue.

Enhanced sampling of rare events in molecular dynamics simulations by nonlinear manifold learning

Behrooz Hashemian, Daniel Millán, Marino Arroyo

LaCàN, Universitat Politècnica de Catalunya-BarcelonaTech, Barcelona 08034, Spain

Molecular Dynamics (MD) simulation is broadly used across various disciplines, including Materials Science, Chemistry and Biology. Continuous improvements of computational resources enable MD simulations of increasingly complex systems. However, the phenomenal challenge of bridging between the femtosecond time scale of molecular vibrations and millisecond-and-up time scale of conformational transitions remains, and calls for multiscale approaches for of complex molecular systems.

This time-scale disparity in systems with metastability makes it very difficult to obtain accurate sampling, and consequently hinders the connection between simulations and experiments. To overcome this issue, a number of enhanced sampling methods have been proposed, such as Metadynamics [1] and Adaptive Biasing Force [2]. However, the effectiveness of these methods relies on a good set of collective variables (CVs), which need to compactly characterize molecular conformations, capture metastability, and be differentiable. Identifying such a coarse model for the system is far from obvious for complex systems.

We present here a general method, Smooth and Nonlinear Data-driven Collective Variables (SandCV) [3], based on machine learning techniques to identify such CVs from available computational or experimental ensembles, and integrate them in enhanced sampling methods. SandCV is a versatile method and can be non-intrusively combined with the available molecular dynamics implementations. We show how this methodology can deal seamlessly with intrinsic manifolds of complex topology described with multiple parametrization patches.

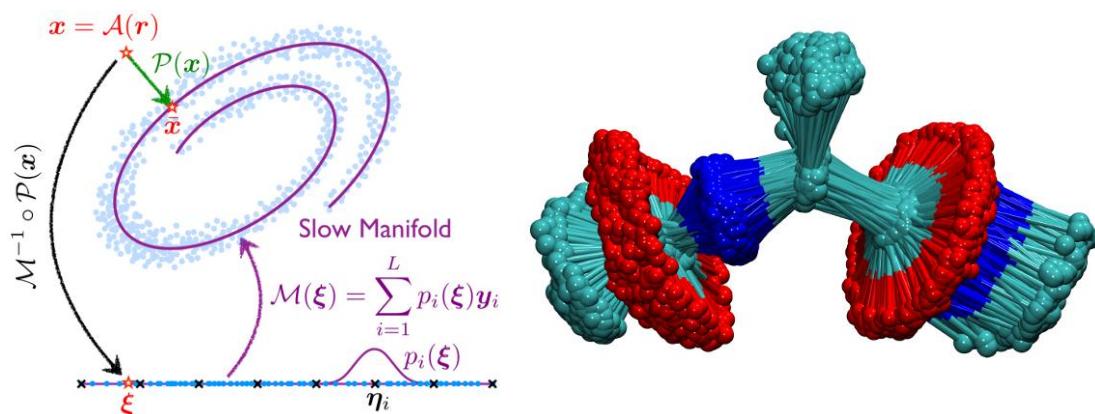


Figure 1: Left: schematic representation of SandCV algorithm. Right: High-dimensional configuration of alanine dipeptide as a benchmark molecule with two collective variables.

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Numerical methods for high-dimensional problems in computational materials science

Johannes Bulin, Jan Hamaekers

Fraunhofer Institute for Algorithms and Scientific Computing SCAI, Sankt Augustin,
Germany

In this talk we present our recent research on numerical methods for high-dimensional problems with applications in the field of atomistic modeling and rational material design. In order to develop new materials with desired properties, theoretical support to predict the relationship between kinds of elements, structures and functions is necessary. Note that recent advances in high performance computing made it possible to perform large scale computational screenings and to obtain very accurate descriptions of complex quantum electronic interactions in the form of potential energy hypersurfaces. However, a global exploration (and approximation) of this surface is very complex due to its high dimensionality. Here, state-of-the-art methods from scientific computing open the possibility to circumvent this so-called curse of dimensionality. This way a large-scale computational screening, e.g. to generate new potential models, will become feasible. We will discuss the application of a hierarchy of state-of-the-art deterministic and stochastic methods known from the field of high dimensional problems for approximation, dimension reduction and global and local optimization. In particular, we will give details on sparse grid based techniques, which, under certain regularity conditions, allow to circumvent the curse of dimensionality at least to some extent. Furthermore, we will discuss the application of high-dimensional approximation and optimization techniques to automatically and efficiently generate appropriate potential models.

A Path Factorization Approach to Multiscale Stochastic Simulations

Manuel Athènes¹, Vasily V. Bulatov²

¹ CEA, DEN, Service de Recherches de Métallurgie Physique, F-91191 Gif-sur-Yvette,
France

² Lawrence Livermore National Laboratory, Livermore, California 94551, USA

A common issue limiting the efficiency of stochastic simulation algorithms is the numerical slowing-down that results from the occurrence of metastable states. Here, an exact algorithm based on a path factorization of the linearized propagator is proposed and applied to anomalous diffusion and to the precipitation of impurities via vacancy diffusion, two model systems in which metastability is important. Paths escaping from the metastable basins can be directly generated owing to the algorithm, which results in a dramatic acceleration of the simulations.

Overcoming Temporal and Spatial Multiscale Challenges in Materials Modeling and Computing

Mitchell Luskin¹, Andrew Binder¹, Pavel Bochev², Derek Olson¹, Danny Perez³, Alex Shapeev¹, Gideon Simpson⁴, Art Voter³

¹University of Minnesota, Minneapolis, Minnesota, USA

²Sandia National Laboratory, Albuquerque, NM 87123, USA

³Los Alamos National Laboratory, Los Alamos, NM 87545, USA

⁴Drexel University, Philadelphia, 19104, PA SA

Predictive computational models for materials must include the interactions of multiple spatial and temporal scales. These scales can be classified as microscopic, mesoscopic, and macroscopic for simplicity, but there are typically structures at many scales with varying degrees of separation. The promise of technologies based on engineered high performance materials make materials modeling an increasing focus of research and development.

Temporal and spatial multiscale challenges appear because the material response of crystalline solids is characterized by the nucleation, dynamics, and pattern formation of defects such as point defects (vacancies, interstitials, impurities), line defects (dislocations), and surface defects (grain boundaries, surfaces, cracks, etc.). To overcome these challenges and reach mesoscopic scales, we will present new mathematical foundations and computational algorithms for spatial coarse-graining (atomistic-to-continuum coupling methods) and temporal coarse-graining (accelerated dynamics methods), as well as methods combining spatial and temporal coarse-graining.

A continuum framework for the treatment of mechano-chemically driven phase transformations with a group/sub-group character

S. Rudraraju¹, A. Van der Ven² and K. Garikipati³

¹University of Michigan

²University of California, Santa Barbara

³University of Michigan, Ann Arbor

We consider the continuum formulation and numerical solution of mechano-chemically driven phase transformation problems that are characterized by a free energy function that is non-convex with respect to strain and composition. The non-convexity demands that at least the first gradients of strain and composition be included in the formulation to ensure mathematical well-posedness, and physically consistent solutions. The corresponding chemical problem was famously treated by Cahn and Hilliard in 1958, while Toupin followed with the nonlinear elasticity problem in 1962. The coupled, nonlinear, initial and boundary value problem has not been solved to our knowledge, mainly because of the smoothness requirement imposed by the higher-order partial differential equation of nonlinear strain gradient elasticity. Here, we draw upon interpolation functions with a spline basis to surmount this difficulty, and also extend them to the Cahn-Hilliard description of the chemical problem. The mathematical formulation is variationally derived, and its numerical implementation is made possible by a weak treatment of higher-order boundary conditions. The use of algorithmic differentiation also makes the exact linearization tractable.

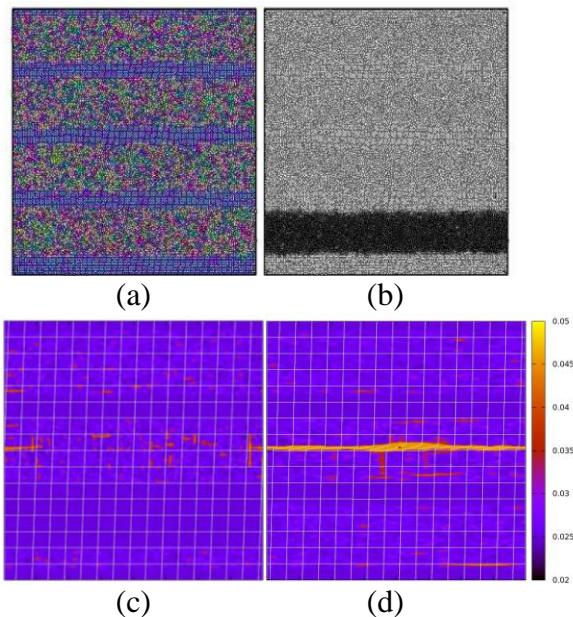
Combined Atomistic/Continuum Modeling of Strain Localization in Metallic Glass

Adam R. Hinkle¹, Michael L. Falk¹, Chris H. Rycroft², Michael D. Shields¹

¹Johns Hopkins University, Baltimore, MD 21218, USA

²Harvard University, Cambridge, MA 02138, USA

The modeling of metallic glass mechanical response, including the prediction of failure, requires the establishment of numerically tractable continuum descriptions of viscoplasticity that incorporate relevant atomistic mechanisms and can be parameterized to metallic glass microstructure. Here we deploy the shear transformation zone (STZ) theory [1] to make quantitative predictions of deformation and failure processes in amorphous solids. This is done in the context of a thermodynamic theory wherein the local disorder is quantified in terms of an effective temperature. [2] Molecular dynamics (MD) simulation is used to parameterize the model. A highly optimized fully Eulerian implementation of the STZ theory is implemented [3] to investigate monolithic metallic glasses and metallic glass crystal composite materials subjected to very large strains, such as those that arise in failure processes such as strain localization. We then perform cross-comparisons between continuum theory and MD predictions using structural parameters that can be independently measured in MD. The onset of failure depends sensitively on the coarse-grained stochastic field that represents the structural inhomogeneity, the details of which determine the mechanical response as well as the onset of instabilities. The properties of this stochastic field are further studied to provide insights into the structure of amorphous solids.



In these images from 3D MD simulations and 2D continuum simulations crystalline layers have been inserted between amorphous regions to create a lamellar composite. In (a) the atoms in MD are colored by potential energy, while in (b) the atoms are light or dark depending on the local shear strain. In (c) and (d) the local values of the effective temperature in the continuum simulation are shown.

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Strain Functionals for Characterizing Atomistic and Other Geometries

Edward M. Kober, Paul M. Welch

Los Alamos National Laboratory, Los Alamos, NM 87545, USA

The development of a set of strain tensor functionals that are suitable for characterizing arbitrarily ordered atomistic structures is described. The approach starts by transforming the discrete atomic coordinates to a continuous and differentiable density function,[1] here using Gaussian smoothing envelopes. The local geometries are then characterized in terms of a Taylor series expansion about each atomic center. From the properties of the Gaussian function, the n-th order derivatives can be directly related to the n-th order moments of the neighboring atom positions. This is similar to an approach used by Zimmerman et al [2], except that the neighborhoods are smooth rather than discrete. The current approach is similar to the Second Order Maximum Entropy (SOME) method, developed by Cyron et al [3] for interpolation in a mesh-free continuum code, where Gaussian functions are used to develop a least-biased definition of a neighborhood. The Cartesian moments can be transformed to solid harmonic functions (also called 3D Zernike functions), which retain radial information compared to other previous analyses based on spherical harmonic functions. Those functions can be further recast in terms of Rotationally Invariant Functions (RIF) that cleanly isolate different types of shape distortions (strains) and orientation factors. Similar RIF descriptions have been previously used for pattern recognition and image processing [4,5]. When fully coupled with the SOME approach, the mapping here would become a unitary basis transformation so that the derived shape factors can be quantitatively related to strains.

Examples of using these RIF basis functions to classify the deformation geometries observed in Molecular Dynamics (MD) simulations of Cu and Ta under strong compression will be shown. The expansions are carried out to fourth order, which is what is required to distinguish between crystal structures. The resulting functionals allow different types of defect structures and deformations to be readily identified, along with the pathways of the deformation processes. The analysis can then be extended to vector quantities (velocities, forces) so that the analogous momentum and stress functions functionals can be defined, leading to a thermodynamically consistent coarse-graining procedure.[1] It can also be extended to tensors, such as the crystal orientation matrices used in finite element simulations of polycrystalline materials. The gradients and higher order derivatives of these functions can then be used to identify and characterize the grain boundaries and higher order junctions.

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In-situ Neutron Measurement and Modeling of Martensitic Phase Transformation

C. N. Tomé¹, Y. Jeong², H. Wang¹, B. Clausen¹, F. Barlat²

¹ Los Alamos National Laboratory, Los Alamos, NM, US

² Pohang University of Science and Technology, Pohang, Republic of Korea

A martensitic phase transformation model is proposed and implemented in a polycrystal plasticity code to describe mechanical response of transformation induced plasticity (TRIP) steel. The transformed martensite domains are introduced as new grains and included in the homogenized effective medium. The stress induced by the martensitic phase transformation strain is accounted for. The phase transformation model is implemented into the framework of an elastic-visco-plastic self-consistent (EVPS) model for polycrystalline materials. The new model is evaluated by comparing simulations of mechanical response, volume fraction evolution, texture evolution, and internal stress evolution to in-situ neutron diffraction measurements of an austenitic stainless steel.

Smart use of Density Functional Theory calculations to drive Newtonian dynamics

M. C. Shaughnessy, R. E. Jones

Sandia National Laboratories, Livermore, CA 94550, USA

We present a method for adaptively creating and sampling a database of density functional calculations in order to simulate large, complex atomistic systems at finite temperatures. The database consists of configurational/cluster-to-force maps and has a metric property via the Kabsch algorithm which we exploit in structuring the database for efficiency and accuracy. Details of the formulation including the correlation between local configuration size and force accuracy, will be discussed, as well as a number of practical applications of the method.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Structural phase transformations in solids - Atomistic insight on mechanisms and interface properties

Ari Harjunmaa, Jutta Rogal, Ralf Drautz

Interdisciplinary Centre for Advanced Materials Simulation Ruhr-Universität Bochum,
44780 Bochum, Germany

Atomistic modelling of the dynamics of phase transformations is a particularly challenging task. If the mechanism of the phase transformation is governed by so-called rare events then the time scale of interest will reach far beyond the capabilities of regular molecular dynamics simulations.

The atomistic rearrangements during solid-solid phase transformations in bulk systems involve massive structural changes including concerted multi-atom processes. The interface between two structurally different phases leads to a complex energy landscape that needs to be explored during the dynamical evolution of the interface. Here, we employ an adaptive kinetic Monte Carlo approach to investigate such processes at the interface between cubic and topologically close-packed phases in transition metals. In particular we investigate the transformation between BCC and A15 in molybdenum. During the dynamical simulations a finite, disordered interface region evolves to compensate the structural mismatch between the two crystal phases. This disordered interface region makes the identification of a single transformation mechanism difficult. Still, from our simulations we extract a layer transformation time which we relate to an effective barrier for the transformation mechanism and discuss the corresponding atomistic processes that we find along the transformation path.

Three-dimensional iso-geometric solutions to Toupin's gradient elasticity theory at finite strains and its application to study of dislocation cores and defects

S. Rudraraju¹, A. van der Ven², K. Garikipati¹

¹University of Michigan, Ann Arbor

²University of California, Santa Barbara

We present, to the best of our knowledge, the first complete three-dimensional solutions to a broad range of boundary value problems for a general theory of finite strain gradient elasticity. We have chosen for our work, Toupin's theory [Arch. Rat. Mech. Anal., 11(1), 385-414, 1962]— one of the more general formulations of strain gradient elasticity. Our framework has three crucial ingredients: The first is iso-geometric analysis [Hughes et al., Comp. Meth. App. Mech. Engrg., 194(39-41), 4135-4195, 2005], which we have adopted for its straightforward and robust representation of C1-continuity. The second is a weak treatment of the higher-order Dirichlet boundary conditions in the formulation, which control the development of strain gradients in the solution. The third ingredient is algorithmic (automatic) differentiation, which eliminates the need for linearization “by hand” of the rather complicated geometric and material nonlinearities in gradient elasticity at finite strains. We present a number of numerical solutions to demonstrate that the framework is applicable to arbitrary boundary value problems in three dimensions. We discuss size effects, the role of higher-order boundary conditions, and perhaps most importantly, the application of the framework to resolve elastic fields around crack tips and dislocation cores.

A concurrent atomistic-continuum study of sequential slip-transfer reactions for dislocation pile-ups at grain boundaries

Shuzhi Xu¹, David L. McDowell^{1,2}, Rui Che³, Liming Xiong³, Youping Chen³

¹GWW School of Mechanical Engineering, Georgia Institute of Technology, Atlanta,
Georgia 30332, USA

²School of Material Sciences and Engineering, Georgia Institute of Technology, Atlanta,
Georgia 30332, USA

³Department of Mechanical and Aerospace Engineering, University of Florida,
Gainesville, Florida 32611, USA

Grain boundaries (GBs) play an important role in determining bulk mechanical properties of polycrystals such as strength, ductility, and resistance to fatigue and fracture [1]. In particular, slip transfer reactions with GBs are complex; dislocations can be reflected, absorbed or desorbed at the interface, and/or transmitted directly, in addition to the possibility of shear-induced GB migration. However, modeling of interface impingement of dislocation pile-ups at grain boundaries has been well beyond the reach of most modeling techniques that seek to resolve atomic level structure during interface reactions due to the accompanying long range stress fields of the pileup, combined with other 3D features of interface structure and mixed dislocation character. In this work, concurrent atomistic-continuum (CAC) simulations [2] are performed to study sequential edge or screw dislocation impingement from a given pile-up on a coherent twin boundary, a Σ_3 (112) incoherent twin boundary, and a Σ_{11} symmetric tilt grain boundary in Cu and Al. Results elucidate the role of specific GB structures and dislocation character in interface absorption-desorption reactions, including evolution of the structure of the interface in the process.

This work is supported by the National Science Foundation as a collaborative effort between Georgia Tech (CMMI-1232878) and the University of Florida (CMMI-1233113). Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of NSF.

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A theory and challenges for coarsening in microstructure

David Kinderlehrer

Carnegie Mellon University Pittsburgh, PA 15213

Cellular networks are ubiquitous in nature. Most technologically useful materials arise as polycrystalline microstructures, composed of a myriad of small crystallites, the grains, separated by interfaces, the grain boundaries. The energetics and connectivity of the network of boundaries are implicated in many properties across all scales of use.

Coarsening is governed primarily by the attempt of the system to decrease the interfacial energy subject to spatial constraints. The recently discovered grain boundary character distribution (GBCD) shows that features of the configuration texture, and more generally, the boundary network is ordered. We discuss a theory for the evolution of this statistic which bridges mesoscopic scales. It gives rise to many interesting questions and challenges: we still have much to learn about these very ancient questions.

Interfaces in Discrete Environments

Nung Kwan Yip

Purdue University

We will discuss some results for interfaces in discrete environment, their pattern formation and dynamics. The discreteness can come from numerical discretization or physical models such as spin systems.

A degenerate Ising model for atomistic simulation of crystal-melt interfaces

Tim Schulze¹, Dmitri Schebarchov², Shaun Hendy³

¹University of Tennessee, USA

²University of Cambridge, UK

³University of Auckland, New Zealand

We consider an Ising-type model for a solid-liquid interface. While the standard Ising model admits only second-order phase transitions as one increases temperature, making it a poor choice for modeling the solid-liquid phase transition, a simple modification of the model introduces a first-order phase transition. This is accomplished by weighting one of the two “spin” states more heavily in the partition function, representing the larger entropy of the liquid phase. This model is combined with micro-canonical Monte-Carlo techniques to simulate systems with solid-liquid phase coexistence. The model will first be illustrated in two dimensions using a simple square lattice before presenting results for the face centered cubic lattice and further generalization to partially melted nano-cluster.

Continuum framework for dislocation structure, energy and dynamics of dislocation arrays and low angle grain boundaries

Xiaohong Zhu¹, Yezun Gu², Yang Xiang³

¹Department of Mathematics, Jinan University, Guangzhou 510632, China

²NANO Science and Technology Program, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong

³Department of Mathematics, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong

We present a continuum framework for dislocation structure, energy and dynamics of dislocation arrays and low angle grain boundaries which may be nonplanar and nonequilibrium. In our continuum framework, we define a dislocation density potential function on the dislocation array surface or grain boundary to describe the orientation dependent continuous distribution of dislocation in a very simple and accurate way. The continuum formulations of energy and dynamics include the long-range interaction of constituent dislocations, local line tension effect of dislocations and the cooperative motion of dislocations, which are derived from the discrete dislocation model. The continuum framework recovers the classical Read-Shockley energy formula when the long-range elastic fields are canceled out. Applications of our continuum framework are presented for dislocation structures on static nonplanar low angle grain boundaries and misfitting interfaces.

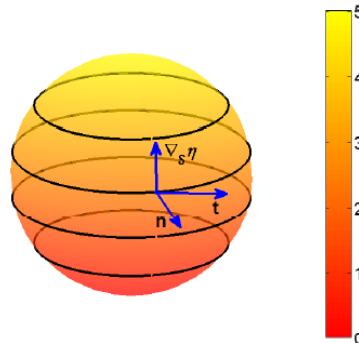


Figure 1: Representation of an array of dislocation loops on a spherical surface using the dislocation density potential function η . The color bar shows the values of η .

This work was partially supported by the Hong Kong Research Grants Council General Research Fund 605410 and 606313.

Analysis of force-based multiscale method

Jianfeng Lu¹, Pingbing Ming²

¹Duke University, USA

²Chinese Academy of Sciences, China

The force based multiscale method that couples together physical models on different scales offer great flexibility for designing consistent multiscale schemes. In this talk, we will study the stability and convergence properties of these schemes. Our result identifies the stability condition for atomistic-to-continuum hybrid method in general dimensions.

Multiscale analysis of non-linear dislocation models

Tom Swinburne

Imperial College London, UK

The discrete, generalized Frenkel-Kontorova (FK) model treats a dislocation line as a chain of nodes, sitting in a periodic lattice potential, interacting through an arbitrarily non-local harmonic force. As the FK model supports a kink mechanism with analytical limits, it has found wide employment since the late 1920s[1].

Despite this popularity, there are very few rigorous results on the transport properties of the FK chain, arguably the main quantities of interest for the dislocation community. In my talk, I will outline a way to derive exact bounds on the transport properties of the FK chain through the novel application of multiscale analysis to the adjoint Fokker-Planck equation[2].

It is found that the free energy barrier is always a lower bound to the true finite temperature migration barrier for this general and popular system, an important result for the large community working on such problems. Numerical simulation confirms the analysis, whilst limiting cases provide a connection the results of transition state theory. The application of these techniques to other problems in crystal plasticity will be discussed.

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A parameter identification problem for random heterogeneous materials

Frederic Legoll

Navier Laboratory, Ecole des Ponts ParisTech, FRANCE

This work is concerned by transport phenomena in porous media, modeled by the Darcy equation. We consider heterogeneous materials, the properties of which are modeled by a random stationary permeability. Based on experimental results, the conductivity, at the microscopic scale, is supposed to be distributed according to a Weibull probability law, the parameters of which are yet unknown. In this work [1], we discuss the identification of the parameters of this microscopic model on the basis of some observed quantities at the macroscopic scale, including the effective (homogenized) permeability.

This is joint work with W. Minvielle, A. Obliger and M. Simon.

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Homogenization of heat diffusion in a cracked medium

Xavier Blanc¹, Benjamin-Edouard Peigney²

¹LLJL, Paris-Diderot University, 5 rue Thomas Mann, 75205 Paris Cedex 13

²CEA/DIF, BP 12, 91680 Bruyères le Châtel, France

We consider the propagation of heat through a periodic cracked medium, exposed to an incoming energy flux. We assume that the cracks are orthogonal to the surface of the material, where an incoming heat flux is applied. The cracks are supposed to be of depth 1, of small width $\alpha\epsilon$, ϵ being the period of the medium and $\alpha \in [0,1)$ is a fixed parameter related to the width of the crack.

Physically, the exchange surface between the medium and the energy source may be greatly modified by the fractures. This may have a significant impact on the energy balance of the considered system. In many situations, the intricacies of the cracked medium are such that it is almost impossible to carry out a direct calculation. Besides, many spatial scales may be involved simultaneously. Full numerical simulations of such multi-scaled media become hence infeasible. That is why we look for an average approach that could capture the effects of cracks in a homogenized medium. The model presented here is simple enough to be coupled to standard FEM codes. The physical idea behind the model is to treat the flux enhancement induced by the crack as a volume source term in the homogenized energy equation. We show this can be rigorously justified by homogenization theory.

The considered linear diffusion problem reads $\partial_t u_e - \Delta u_e = 0$ with Neumann boundary conditions imposed on the surface of the cracked domain Ω_ϵ .

We find that, in the limit $\epsilon \rightarrow 0$, u_e is well approximated by the solution of a limit equation of the form $-\Delta u + \partial_t u = \alpha\chi(x)$ where χ is the indicator function of the cracked zone; u evolves in a homogenized domain where the crack is not described anymore. A full mathematical proof as well as numerical illustrations are presented.

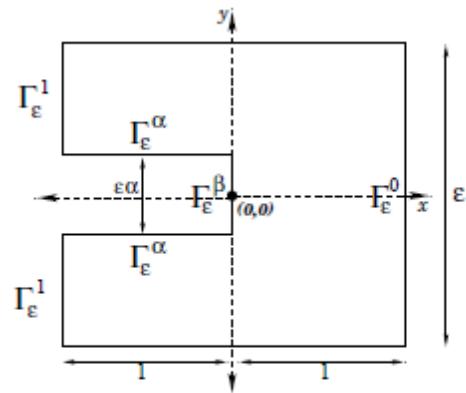


Figure 1: Ω_ϵ

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Multiscale modeling of spin transfer torques in ferromagnetic multilayers

Jingrun Chen, Carlos J. Garcia-Cervera, Xu Yang

UCSB

Ferromagnetic multilayers are essential building units for data storage and manipulation. Recent experiments reveal that the existence of a spin current makes ease of magnetization switching and magnetic domain-wall motion. Starting from quantum mechanics, we derive models at different scales for spin dynamics, which is coupled to magnetization dynamics described by Landau-Lifshitz-Gilbert equation. In the hydrodynamic regime, our model recovers the model derived from linear response theory under the assumption of weak spin-magnetization coupling. Quantitative comparison of our model and experimental data will also be presented.

Comparison of 3D phase field and Peierls-Nabarro modeling of dislocation dissociation, glide and twinning in fcc systems

Jaber Rezaei Mianroodi¹, Bob Svendsen^{1,2}

¹Material Mechanics, RWTH Aachen University, Aachen, Germany

²Microstructure Physics and Alloy Design, Max-Planck Institute for Iron Research, Düsseldorf, Germany

The purpose of this work is the development and comparison of two approaches to the modeling of dislocation dissociation, glide and twinning in fcc systems. The first of these is a phase-field (PF) approach (e.g., [1-2]), while the second is a dynamic generalization of existing static Peierls-Nabarro (PN) models (e.g., [3]). In contrast to [1,2], the current PF approach [4] is based on two phase-fields per glide plane. This is analogous to and consistent with the current PN model based on two disregistry fields per glide plane [5]. In both cases, the corresponding free energy model accounts in particular for the stacking fault (SF) energy of the material determined via *ab initio* means.

Considering periodic systems and employing Fourier methods, both models are applied in a comparative fashion. As an example application of the phase field approach, consider the loading of Al and Cu and corresponding microstructure development in Figure 1.

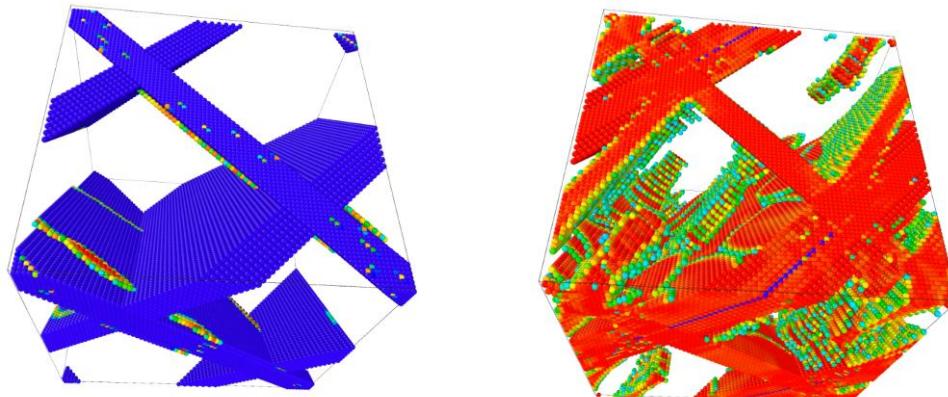


Figure 1. Phase field modeling of dislocation-based deformation in Al (left) and Cu (right) during uniaxial compression. Blue: ideal glide; red: SF/twin; green: dislocation line.

As shown, in case of Cu (right), loading results in the formation of multiple SF layers and twinning. On the other hand, in Al (left), the deformation is governed almost solely by ideal dislocation glide. Analogous results from the PN model and additional examples will be discussed.

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Defect Nucleation in Crystals

T.J. Delph¹, J.A. Zimmerman², H.S. Park³

¹Lehigh University, Bethlehem, PA 18015, USA

²Sandia National Laboratories, Livermore, CA 94551, USA

³Boston University, Boston, MA 02215, USA

Transition state theory is of interest because it allows the prediction of rate and temperature effects upon defect initiation in crystals. More importantly, it is valid for arbitrary loading rates, in particular loading rates achievable in the laboratory and suffers from none of the limitations in this regard inherent in molecular dynamics simulations. We describe here a recently-developed transition state theory model for the initiation of crystal defects. This model makes use of a previous model for zero-temperature defect initiation in combination with multi-dimensional harmonic transition state theory. Harmonic transition state theory requires an accurate determination of the saddle point activation energy. The present model presents a relatively simple means of determining this quantity that does not require an *a priori* assumption as to the nature of the nucleated defect. Moreover various other quantities required by transition state theory are calculated in a rather natural fashion. We apply the model to several examples of defect initiation. The first is that of triaxial stretching of an fcc crystal, for which the relevant defect is spherical cavitation. The other, considerably more complicated, example is that of nanoindentation on the (001) surface of a gold crystal. Here the initial defect is a dislocation that nucleates at five atomic planes beneath the indenter. In both cases, excellent agreement is observed between the model predictions and the results of independent molecular dynamics simulations over a range of loading rates. The predictions of the model may also be compared to available experimental data, and we comment upon efforts in this direction.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Atomistic Modeling at Experimental Strain Rates: Plasticity in Amorphous Solids

Penghui Cao, Xi Lin, Harold S. Park

Department of Mechanical Engineering, Boston University, Boston, MA 02215, USA

We present a new computational approach that couples a recently developed potential energy surface exploration technique with mechanical deformation to study the deformation of atomistic systems at strain rates that are much slower, i.e. experimentally-relevant, as compared to classical molecular dynamics simulations. Examples of the new insights into the plasticity of amorphous solids that are obtained using this new approach will be given, with a particular emphasis on how the shear transformation zone characteristics, which are the amorphous analog to dislocations in crystalline solids, undergo a transition that is strain-rate and temperature-dependent, and how surface effects impact the shear transformation zone characteristics.

Spectral finite-element based methodology for large scale electronic-structure calculations using density functional theory

Phani Motamarri, Vikram Gavini

University of Michigan

Material defects are ubiquitous. They occur in very small concentrations, yet have profound influence on macroscopic properties of materials. The development of a mathematical model which accurately describes such defects presents a unique challenge since such a model must incorporate physics at multiple length scales. This involves resolving the defect core at quantum mechanical scale as well as the long range elastic fields away from the defect. One of the most popular electronic structure theories which can be used to achieve the above goal is Kohn-Sham density functional theory (DFT). However, the complexity of these calculations restricts the computations to sample sizes of the order of a few hundred atoms. To extend the DFT calculations to realistic sample sizes that can accurately capture the long ranged fields generated by defects, an efficient approach that can seamlessly bridge quantum mechanical and continuum scales using single physics (DFT) is highly desirable. The development of real-space electronic structure calculations using a finite-element discretization of DFT is an important step in the above direction. The ability to handle complex geometries, arbitrary boundary conditions and more importantly the coarse-graining nature of basis sets makes finite-elements highly desirable especially in problems involving defects.

Following this line of thought, we first develop an efficient real-space approach to perform electronic structure calculations using an adaptive higher-order spectral finite-element discretization. The key ideas involved are to use an a-priori mesh adaption technique and subsequently employ Chebyshev acceleration strategies in conjunction with special quadrature rules to reduce the computational cost in solving the DFT problem. Our studies show that staggering computational savings of the order of 1000-fold can be realized by using sixth-order finite-element discretization, in comparison to linear finite-elements and compares favorably with other widely used basis-sets. Next, we address the problem of computational complexity involved in solving the DFT problem which scales cubically with number of atoms in the system. To this end, we formulate a sub-quadratic scaling subspace projection technique to conduct large-scale electronic structure calculations using DFT. The proposed methodology takes advantage of the representation of Kohn-Sham Hamiltonian in Lowden orthonormalized finite-element basis constructed using spectral finite-elements in conjunction with Gauss-Lobatto- Legendre quadrature rules. Further, the proposed approach treats both metallic and insulating systems on the same footing by projecting the Kohn-Sham Hamiltonian in a non-orthogonal localized basis constructed from the Chebyshev filtered subspace. We further demonstrate the scaling, efficiency and accuracy of the proposed algorithm on full three dimensional systems involving metallic aluminium nano-clusters up to 3430 atoms and insulating alkane chains up to 8000 atoms using pseudopotential calculations. We also demonstrate the proposed algorithm on all-electron calculations up to 5000 electrons.

Enabling strain hardening modeling via efficient time-integrators in dislocation dynamics simulations

Amin Aghaei¹, Ryan B Sills^{1,2}, Wei Cai¹

¹Department of Mechanical Engineering, Stanford University, Stanford, CA 94305, USA

²Sandia National Laboratories, Livermore, CA 94551, USA

Dislocation dynamics (DD) provides a systematic framework for the simulation of metal plasticity and strain hardening. DD models follow the motion of a network of dislocation lines discretized into segments and connected by a set of nodes, which are the degrees of freedom of the system [1] (see figure 1). In order for DD simulations to provide insight into the strain hardening process, they must be able to reach plastic strains on the order of experimental values (>10%). Despite the development of massively parallel algorithms and codes, this level of plastic strain has been out of reach thus far.

A major cause of this computational gap is inefficient time integration. In order to remove this limitation, we have developed advanced time integration algorithms for 3D DD simulations [2]. We show that DD simulations contain unstable modes, which force explicit time-integrators to take very small time steps, while implicit time-integrators offer much better performance. Unfortunately, there also exist unstable and highly non-linear modes that require a very small time step even when an implicit integrator is used. A significant speed-up is then achieved by the sub-cycling algorithm, in which nodes involved in the unstable and non-linear modes are time- integrated with small time steps while the remaining nodes are integrated with larger time steps. The performance of these advanced algorithms in large-scale DD simulations is evaluated.

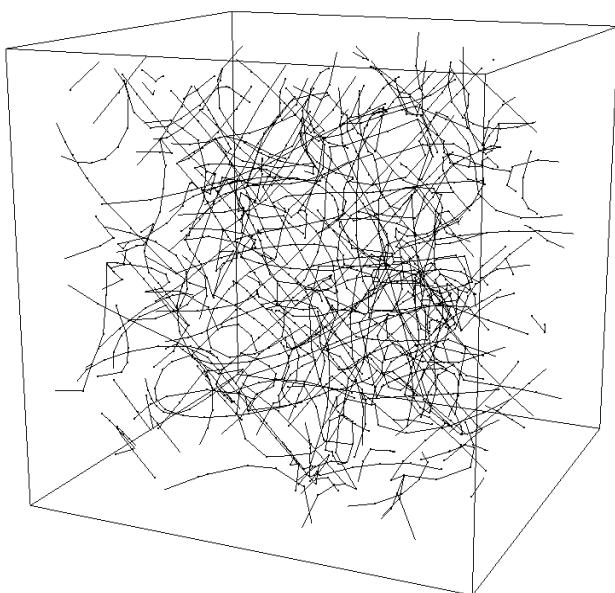


Figure 1: A snapshot of a typical DD simulation of an FCC metal subjected to uniaxial loading.

This work was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE- SC0010412 (AA & WC), and by Sandia National Laboratories (RBS). Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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**A numerical and computational framework for hierarchical multi-scale simulations
on large scale computers**

Jaroslaw Knap, Carrie E. Spear, Kenneth W. Leiter, David A. Powell, Richard C. Becker

Army Research Laboratory

Over the last few decades, multi-scale modeling (MSM) has become a dominant paradigm in materials modeling and simulation. The practical impact of MSM depends, to a great extent, on the ability to utilize modern computing platforms. However, since there are no general numerical and computational frameworks for MSM the vast majority of multi-scale material models are developed on a case-by-case basis. Therefore, we seek to formulate an adaptive numerical and computational framework for MSM on large scale computers. We do not plan to develop a specific method for MSM simulations, but instead, aim to develop a broad and flexible numerical framework for designing and developing such simulations. Our focus is primarily on new scalable numerical algorithms applicable in a wide range of MSM applications. These algorithms fall mostly into the three areas: i) scalable data transfer between parallel applications, ii) adaptive strategies for MSM, and iii) data analytics for MSM. We present a formulation of our numerical and computational MSM framework. Subsequently, we describe development of a new two-scale multi-scale model of composites utilizing our framework.

Acceleration of microscale polycrystal plasticity models using GPUs

A.W.Richards¹, L.J. Vernon¹, M. Knezevic², R.A. Lebensohn¹, R.J. McCabe¹

¹Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

²University of New Hampshire, Durham, New Hampshire 03824, USA

We present a framework for accelerating the computation of microscale polycrystal plasticity models using GPUs, for use with black-box commercial Finite Element (FE) software.

There is growing recognition within the mechanics community of the need to incorporate microstructure evolution into macroscale engineering simulations. However, many microscale models are computationally prohibitive for macroscale finite element simulations of thermo-mechanical forming processes, and other engineering applications.

We have previously demonstrated that Taylor-type plasticity models can be used to accurately predict the microscale texture evolution of cubic materials, and that this model is amenable to a computational speed-up exceeding 100x when using a spectral representation. We presently demonstrate that such computations are ideally suited to GPUs affording additional orders-of-magnitude speed-up, and we devise a scalable computational framework highly suitable for parallelized implementations.

In the present work, we have developed an implementation of the Spectral Taylor model on GPUs using nVidia's CUDA Fortran, constituting a standalone computational application/service. We have also developed a simple, light-weight C-scheduler using Unix sockets to pass data to and from the app, and show how this can be trivially called from within the commercial finite element package Abaqus. As a case study, we have fit the model's plasticity parameters to experimental tension/compression data for a cubic polycrystalline metal, whose initial texture has been characterized via EBSD, and we show results from a macroscale simulation computed on a desktop workstation utilizing single- and dual-GPUs. Further, we show results from a distributed architecture computation, demonstrating how the same implementation can utilize non-local GPUs across a network with absolutely no modifications.

In addition to the accelerated computation of the microscale texture evolution, we emphasize the ability of the method to utilize non-local computational resources; further, we assert that the implementation is sufficiently abstract so as to be compatible with virtually any FEA package that permits user-defined material models, e.g. Sandia National Lab's SIERRA framework, with only trivial modifications.

3D phase field modeling for nanowire growth by vapor-liquid-solid mechanism

Yanming Wang¹, Seunghwa Ryu², Paul C. McIntyre¹, Wei Cai^{3,1}

¹Department of Materials Science and Engineering, Stanford University, Stanford, CA

²Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology, Yuseong-gu, Daejeon, Korea 305-701

³Department of Mechanical Engineering, Stanford University, Stanford, CA 94305, USA

Nanowire (NW) has promising applications in many fields such as integrated circuits, solar cells or solar cells, for its special electronic and optical properties [1]. Vapor-liquid-solid (VLS) process is a widely used NW growth method; however, many fundamental questions including the nucleation failure and growths kinking are still not fully understood. The answers to these questions are important for better control of the NW orientation, yield and quality required for industry applications. Therefore, a 3D computational model studying VLS mechanism that can both capture the realistic NW morphology and reach the experimental time scale is critically needed.

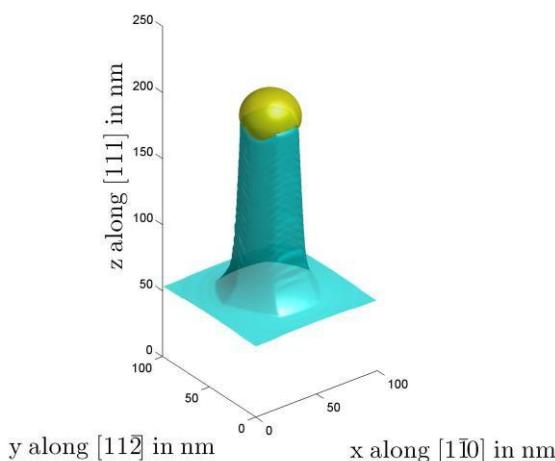


Figure 1: simulation snapshot shows the NW growth along [111] orientation.

We developed a 3D multi-phase field model for VLS NW growth [2]. The model captures the equilibrium catalyst droplet shape on the substrate prior to NW growth. For the NW growth process, the model captures the NW tapering and sidewall facets in good agreement with experimental observations. The model predicts the steady-state NW growth velocity is a linear function of the vapor chemical potential and the inverse of catalyst diameter, providing a confirmation of the Gibbs-Thomson effect in nanowire growth [3]. The model is applied to study the instability of the catalyst droplet on top of the NW, which is important for understanding the onset of growth kinking.

This work is supported by the National Science Foundation under Grant No. 1206511. Seunghwa Ryu acknowledges the support by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT & Future Planning (2013010091).

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Generalized Irving-Kirkwood formula for the calculation of continuum quantities in molecular dynamics models

Jerry Zhijian Yang¹, Xiaojie Wu², Xiantao Li²

¹Wuhan University, Wuhan, 430072, China

²Penn State University, University Park, PA 16802, USA

Continuum mechanics quantities can be computed from molecular dynamics (MD) models based on the classical Irving-Kirkwood (IK) formalism. Practical implementations of IK formulas involve a spatial averaging using a smooth kernel function. The obtained results usually need to be further processed to reduce the fluctuation, e.g., by ensemble or time averaging. In this talk the IK formalism is extended to systematically incorporate both spatial and temporal averaging into the expression of continuum quantities. We will present the results both in Lagrangian and Eulerian coordinates.

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A concurrent parallel multiscale algorithm for large 3d continuum/atomic simulations at finite temperature using lammps

Fabio Pavia, William A. Curtin

EPFL, Lausanne, Switzerland

Deformation and fracture processes in engineering materials combine complex phenomena and often require simultaneous descriptions over a range of length and time scales, with each scale using a different computational technique. Here we present a high-performance parallel 3D computing framework for large multiscale studies that couples an atomic domain, modeled using molecular dynamics, and a continuum domain, modeled through explicit finite element. The method ensures mechanical equilibrium at the interface between the different domains of the model, with the finite elements providing boundary conditions for the atomic simulations. Most importantly, the entire method is implemented using the large-scale parallel molecular dynamics code LAMMPS, thus taking advantage of all the tools associated with this popular open-source code. We demonstrate operation of the code with a study of dislocation glide and bowing around obstacles, for dislocation lengths of ~50nm using fewer than 1,000,000 atoms but with no spurious image forces or errors due to coupling.

Analysis of an energy localization method used in kinetic Monte Carlo simulations of heteroepitaxial growth

Kyle Golenbiewski¹, Tim P. Schulze¹, Peter Smereka²

¹Department of Mathematics, University of Tennessee, Knoxville, TN 37909-1300, USA

²Department of Mathematics and Michigan Center for Theoretical Physics, University of Michigan, Ann Arbor, MI 48109-1109, USA

Heteroepitaxial growth consists of slowly depositing one material onto a crystalline substrate formed from a second material. An important feature of this process is that the natural lattice spacing of the deposited material may differ from that of the substrate's, resulting in elastic strain. Simulation of such growth using kinetic Monte Carlo is often based on rates determined by differences in elastic energy between two configurations. This, however, is computationally challenging due to the long range nature of elastic interactions. Adopting an atomistic approach, we consider a method in which the elastic field is updated using highly accurate local approximations, though the energies themselves are far less accurate. Namely, we approximate the elastic energy barrier by constraining the displacement field with an atom removed to agree with the displacement field when the atom is present outside some local region. In order to gain insight into this energy localization method, we appeal to a continuum analogue of the discrete mechanical system. For the scenario of an isolated island sitting on an unbounded and otherwise flat film on a flat substrate, we extend earlier results done on a 2D system to 3D.

Frozen Gaussian approximation for wave propagation in periodic media

Xu Yang

UC Santa Barbara

Unlike the Gaussian beam method (GBM), frozen Gaussian approximation (FGA) is a semiclassical approximation to high frequency waves with Gaussians of fixed width. It was called Herman-Kluk approximation in quantum chemistry, and used for solving the Schrodinger equation. In this talk, we generalize the idea, derive and analyze the accuracy of FGA for waves propagating in periodic media, modeled by the Schrodinger equation with a lattice potential. Assuming the existence of band gap, we are able to obtain the effective dynamic equations of electrons within each energy band, and prove the first order accuracy of FGA.

Semiclassical Models for Quantum Systems and Band Crossings

Lihui Chai, Shi Jin, Qin Li

UCSB

We derive the coupled semi-classical Liouville system for the Schrödinger equations with band crossings to describe the inter-band transitions semi-classically. The main idea is using the Wigner transform and the basis representation, retaining the off-diagonal terms in the Wigner matrix which cannot be ignored near the point of band crossing. The coupled Liouville systems are able to describe the inter-band transition phenomena very well and consistent to the adiabatic approximation if the adiabatic assumption holds. A domain decomposition method that couples these non-adiabatic models with the adiabatic Liouville equations is also presented for a multiscale computation. Solutions of these models are numerically compared with those of the Schrödinger equations to justify the validity of these new models for band-crossings.

An efficient rescaling algorithm for simulating the evolution of precipitates in an elastic media

Shuwang Li¹, Amlan Barua¹, Xiaofan Li¹, John Lowengrub²

¹LDepartment of Applied Mathematics, Illinois Institute of Technology,
Chicago 60616, USA

²Department of Mathematics, University of California at Irvine, Irvine CA 92697, USA

In this talk, we present a space-time rescaling scheme for computing the long time evolution of multiple precipitates in an elastically stressed medium. The algorithm is second order accurate in time, spectrally accurate in space and enables one to simulate the evolution of precipitates in a fraction of the time normally used by fixed-frame algorithms. In particular, we extend the algorithm recently developed for single particle by Li [1] to the multiple particle case, which involves key differences in the method. Our results show that without elasticity there are successive tip splitting phenomena accompanied by the formation of narrow channels between the precipitates. In presence of applied elastic field, the precipitates form dendrite-like structures with the primary arms aligned in the principal directions of the elastic field. We demonstrate that when the far-field flux decreases with the effective radius of the system, tip-splitting and dendrite formation can be suppressed, as in the one particle case. Depending on the initial position of the precipitates, we further observe that some precipitates grow while others may shrink, even when a positive far field flux is applied. We will also explore the possibility that like single precipitates, multiple precipitates may tend to attractive self-similar configurations under appropriate growth conditions

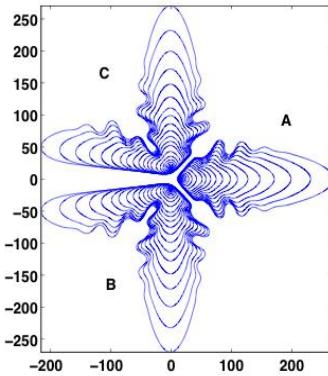


Figure 1: Three precipitates develop dendritic structures under applied shear strain.

The authors thank support from NSF.

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Scalable parallel kinetic Monte-Carlo without approximation

Tomas Oppelstrup¹, Vasily V. Bulatov¹, David Jefferson¹, Luis Zepeda-Ruiz¹ and George H. Gilmer²

¹Lawrence Livermore National Laboratory, Livermore, California 94550, USA

²Colorado School of Mines, Colorado 80401, USA

Summary: We employ the Time Warp optimistic parallelization scheme to an atomistic kinetic Monte-Carlo simulation. This method of parallelization is free of approximation and delivers the same trajectory as a serial execution, while mitigating communication latencies and temporal load imbalance through speculative execution. On even moderately sized lattice gas models we obtain 1000-fold speedup compared to serial execution.

Kinetic Monte-Carlo (KMC) is a widely used simulation method in materials science, statistical mechanics, biology, etc. A KMC simulation propagates by discrete events, which move or otherwise change the state of one or more of the simulated objects (e.g. atoms). The events happen at rates given by distribution functions prescribed by each particular KMC model. There is no global time stepping, and in most cases each event require updating only a small subset of the simulated system. This structure makes KMC adapt automatically to the time scales present in the system. This particular feature has made it possible to simulate for example coarsening and radiation damage over time scales spanning many orders of magnitude, and makes KMC an ideal tool for simulation of systems with a frequently changing and broad spectrum of time scales.

The event driven nature and often inherent asynchronicity of KMC simulation makes it difficult to parallelize, and large scale parallelization has so far been approximate in nature. This has largely limited KMC simulation to serial computation, which severely limits accessible length scales.

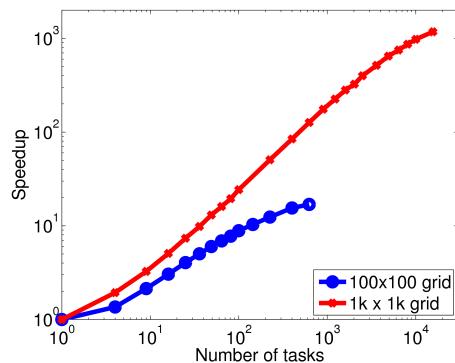


Figure 1: Speedup of lattice gas model compared to serial execution.

In this work, we employ the optimistic parallelization scheme Time Warp[1,2] where the synchronization problem inherent in any parallel computation is handled through speculative execution, and the promise to undo incorrect computations when causality errors are detected. Initial results show that a 1000-fold speedup can be attained in even moderately sized lattice gas problems (see Figure 1). The availability of an exact method for atomistic KMC, free of potential artifacts resulting from approximate schemes, will allow multi-micron length scales to be reached, while retaining the inherent multi-scale time adaptivity of KMC.

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OptiDis: a MPI/OpenMP Dislocation Dynamics Code for Large Scale Simulations

Arnaud Etcheverry¹, Pierre Blanchard¹, Olivier Coulaud¹, Laurent Dupuy²

¹HiePACS team, Inria Bordeaux Sud-Ouest
²SRMA, CEA-Saclay, 91191, Gif-sur-Yvette, France

Dislocation dynamics simulation is a powerful and widely used tool to model the collective behavior of large dislocations ensemble in crystalline materials. Massively parallel codes, based on message passing paradigm (MPI) have been proposed [2], [3] , and are able to simulate millions of segments over thousand of cores. Nowadays, such approach are not well suited to take advantages of new multicore architectures. The goal of OptiDis project is to develop a new parallel code for such architectures. This code is based on the physics and algorithm of the Numodis code [1].

On the numerical side, we consider the non-singular force field formulation introduced by Cai et al. [4] and we use a fast multipole method based on Lagrange polynomials to compute the force with a linear complexity. This kernel was introduced inside our fast multipole library ScalFMM [5].

On the computer science side, we developed new data structures and algorithms to be more efficient with hierarchical architectures, both in term of memory and computing units. First of all, we introduced an adaptive cache-conscious data structure to manage large set of segments and nodes. It combines good computing performance and data management. Second of all, thanks to the octree used by the FMM, we split the domain on each processor, we use a message passing paradigm to communicate between sub-domains. Each sub-domain is mapped on one multicore machine. Moreover, inside a subdomain (i.e. one multicore architecture) we consider a task parallelism, based on the OpenMP standard to speed up computation inside a node. Thanks to the hybrid parallelism (MPI/OpenMP) we are able to improve computation efficiency, and to decrease the memory used for the parallelism.

On the physical side, particular attention was given to the junction formation algorithm that allows to explicitly treat the individual interactions between dislocations and radiation-induced loops. This approach was validated by carefully comparing individual interactions obtained with dislocation dynamics [6] and available molecular dynamics simulation results [7].

Finally, two kinds of results will be shown. The first one will validate our strategies in term of parallelism. Then, we will introduce a large scale simulation involving more than one million segments in order to study the clear band formation mechanism in irradiated zirconium.

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Fast Multipole Method with Application in Dislocation Dynamics

Chao Chen¹, Sylvie Aubry², Clif Dudley¹
Tom Arsenlis², Eric Darve¹

¹Stanford University, Stanford, California 94305, USA

²Lawrence Livermore National Laboratory, Livermore, California 94550, USA

In the dislocation dynamics (DD) code ParaDis [1], as in other DD codes, the exact computation of forces on the dislocation nodes using the anisotropic elasticity formalism [2] has a complexity of $O(N^2)$, where N is the number of segments. This calculation can be sped up to $O(N)$ using the fast multipole method (FMM). The black box FMM [3] using the Chebyshev interpolation requires a small pre-computation time. We combined it with the singular value decomposition to guarantee a minimal number of coefficients under the L^2 norm. In our tests, we considered both the isotropic as well as the recently implemented anisotropic version of the ParaDis. For DD, we found that a fifth order Chebyshev interpolation is sufficient and that it achieves an accuracy of three digits even for very anisotropic cases.

One special difficulty with DD is that, because of the tensorial nature of the interaction kernel in the FMM, the memory requirements of the method are very large. For that reason, we also implemented uniform grids with Lagrange interpolation which cuts the storage from $O(n^6)$ to $O(n^3)$, where n is the number of grid points in every dimension. In addition, the new scheme enables using the fast Fourier transform in the multipole-to-local operations, which is the most expensive step in the FMM. According to our experiments, the new scheme has a much lower increasing rate.

We have also developed a reference FMM implementation based on the Taylor expansion of the kernel. The Chebyshev FMM is a general purpose method that leads to $O(N)$ FMMs for any analytic kernel, while the Taylor expansion method was specially developed for DD. Having both methods fully implemented, we will present comparisons of both methods in terms of memory footprint, accuracy and computational cost.

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Mathematical Model of Anisotropic Surface Diffusion

Dieu Hung Hoang, Tomáš Oberhuber

Department of Mathematics, Faculty of Nuclear Sciences and Physical Engineering,
Czech Technical University in Prague, Trojanova 13, Prague, Czech Republic

We consider the heteroepitaxial growth where a lattice mismatch between the film and the substrate exists. Due to the effects of mismatch stress, a flat film surface is unstable to small perturbations and undergo the Asaro-Tiller-Grinfeld instability [1,2] that results into various self-organized nanostructures. In addition to the influence of stress, anisotropic surface energies play an important role as well.

In this contribution, we deal with the anisotropic surface diffusion in the context of heteroepitaxial growth in relative geometry, where quantities are referred to the given Finsler metric Φ exhibiting the desired anisotropy. The motion law reads as

$$v = \Delta_\Gamma(\kappa_\Phi + F) \text{ on } \Gamma, \quad (1)$$

where Γ is the surface in \mathbb{R}^3 , v is the normal velocity of Γ , Δ_Γ is the Laplace-Beltrami operator with respect to Γ , κ_Φ is the anisotropic mean curvature given by the prescribed anisotropy Φ , and F is the forcing term given by the elastic energy density depending only on the film height.

Treating Γ in the motion law (1) as a graph, we obtain a nonlinear parabolic PDE in the divergence form with several important energy equalities. For the purpose of numerical solution, we present the numerical scheme based on the method of lines with the finite differences in space [3] and prove the corresponding discrete energy equalities. Finally, we show experimental order of convergence of the scheme and results of numerical experiments with various anisotropy settings.

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Insights on micro-mechanisms of damage in a cement-based geomaterial under uniaxial compression from multiscale modelling

Duc-Phi Do¹, Truong-Son Bui¹, Dashnor Hoxha¹

¹PRISME Laboratory, Orleans University, Polytech'Oréans, 8 rue Léonard de Vinci, Orleans 45072, FRANCE

In order to elucidate the mechanisms of damage initiation and growth the evolution of mechanical properties of various specimens were monitored while under uniaxial compression conditions. For that a number of piezoelectric sensors (P-143.01 of PI Ceramic GmbH) with a central frequency of 150 kHz were used allow measuring simultaneously at chosen directions one P (compressive) and two S (shear) ultrasound waves polarized in two orthogonal directions. The experimental results showed that the parameters of ultrasounds are stable up to a stress about 40% of yield strength of materials. Then they decrease gradually before dropping sharply at a stress level ranges from 85% to 94% of pick stress. Anisotropy induced by uniaxial stress is also observed in these samples initially isotropic.

In this paper a micromechanical model was developed to simulate the process of damage of material. For this purpose a two-level microstructural conceptual model is adopted. Then some micro-mechanisms of damage such as the nucleation, growth of micro-cracks as well as the debonding effect of inhomogeneities' interface were taken into account through a two-step homogenization using the Eshelby's solution. The comparison between the numerical and experimental results permits to elucidate the influence of each mechanism of damage in this type of material.

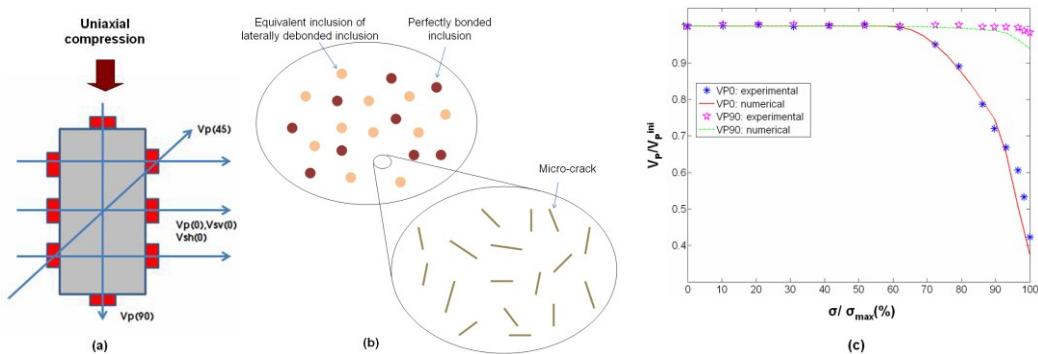


Figure 1: Disposition of ultrasonic measurement (a); two-level conceptual model of material (b); comparison of numerical and experimental results (c).

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A multiscale approach for 3D mixed mode crack propagation

Anthony Gravouil^{1,2}, Clément Roux¹, Julien Réthore¹, Marie-Christine Baietto¹

¹Université de Lyon, INSA-Lyon, LaMCoS, CNRS UMR5259, France

²University Institute of France

The question of the inclusion of a crack and its propagation in a finite element (FE) model initially not intended for this, is a question which is still today the subject of numerous studies. A special effort is dedicated to the development of tools increasingly generic, flexible and simple to implement and to use. In this sense, X-FEM has achieved a first step towards clearly less intrusive simulation of fracture problems. To reduce further this intrusiveness, a new family of non-intrusive coupling algorithms has recently been initiated by Gendre et al. [1]. The idea is to develop a local/global coupling algorithm while avoiding any modification of the industrial code used to simulate the global problem [2].

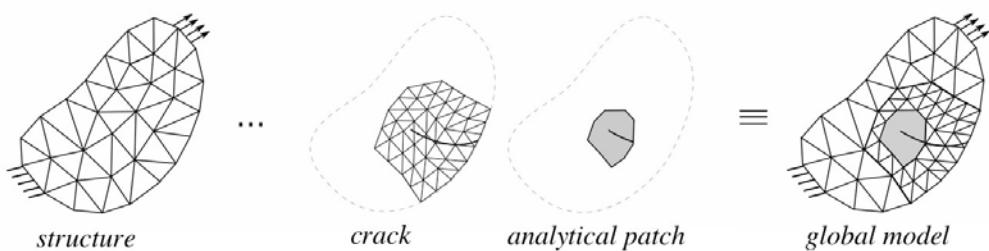


Figure 1: direct extraction of SIFs based on Williams series expansion in a 3D localized multigrid framework

These coupling algorithms have been originally based on domain decomposition (DD) solvers [1, 2]. Here an alternative algorithm based on a localised multigrid algorithm [3] is proposed for the simulation of mixed-mode crack propagation, while respecting the constraint of non-intrusiveness of the global problem [4]. For the global model, the contribution of the local patch consists in additional nodal efforts near the crack, which makes it compatible with most softwares. The shape of the local model is also adapted automatically during mixed mode propagation and it allows a direct extraction of fracture parameters from a truncated Williams serie. Extension to the three-dimensional case is in progress [5].

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Matched asymptotics of dislocation pile-ups against an interface in a coated solid.

Roman Voskoboinikov

Institute of Materials Engineering, Australian Nuclear Science and Technology Organisation, New Illawarra Road, Lucas Heights 2234 NSW, Australia

Multi-scale modelling implies a framework of complementary approaches at different length and time scales. Usually a modelling at a smaller scale is followed by modelling at a larger one and the output of preceding length-scale methods plays the role of the input parameters for consequent simulations. The approach breaks down if it is not possible to separate scales. This can happen, for example, when large a number of dislocations are considered.

An asymptotic technique for analyzing dislocation pile-ups has been suggested [1-3]. We provided robust systematic proof of the interconnection between continuum and discrete approaches to dislocation description. Taking the linear pile-up of n identical dislocations stressed by a constant loading against a lock as the archetypal dislocation agglomeration we derive equations for the leading order and first-order correction to the continuum dislocation number density. As $n \rightarrow \infty$, the dislocation density can be easily found whereas direct evaluation of the dislocation positions from the set of n force balance equations is not a simple task. In the framework of the proposed approach these positions can be easily established by reducing the infinite system of non-linear force balance equations to an ordinary differential equation.

The method has been developed further to find the equilibrium distribution of n dislocations in a pile-up stressed against an interface in a solid with coating or surface oxide layer. The stress at the interface is found as a prefactor of the singular part, which is mathematically analogous to a “stress intensity factor” in continuum fracture mechanics. It is determined to high accuracy from a lumped discretization of superdislocations away from the interface. We provide an example in which a hundred dislocations can be replaced by just four superdislocations with only 1 per cent error in the computation of the stress at the interface.

Partial support from the Russian Foundation for Basic Research under grant # RFBR-14-08-00859a is gratefully acknowledged.

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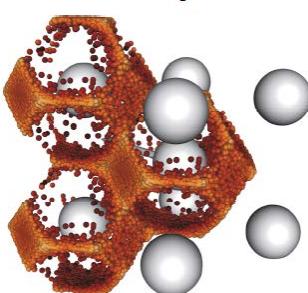
Hybrid continuum-atomistic simulations on the Bloch point dynamics in a single-crystalline ferromagnet

Christian Andreas^{1,2}, Attila Kákay¹, Riccardo Hertel²

¹Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, D-52428 Jülich,
Germany

²Institut de Physique et Chimie des Matériaux de Strasbourg, Université de Strasbourg,
CNRS UMR 7504, Strasbourg, France

Micromagnetic theory has been firmly established about 50 years ago [1] as the basis for the calculation of magnetic structures in ferromagnets, such as domain walls or vortices. Because it is a continuum theory, micromagnetism reaches its limits of validity when magnetic inhomogeneities develop on length scales comparable to the atomic lattice constant. Such situations are exceptions in homogeneous materials, but their occurrence under specific circumstances is undisputed. The most prominent example thereof is the magnetic structure around a Bloch point [2,3]. From a topological perspective the Bloch point represents a point defect in the vector field of the magnetization. Around this point the magnetization direction changes by 180°, and on each small sphere around this point any magnetization direction can be found. These defects occur, e.g., temporarily in the switching of vortex cores [4] or during the magnetization reversal of soft-magnetic cylinders [5], a process mediated by the nucleation and the propagation of Bloch points. We have developed a hybrid micromagnetic/Heisenberg model software package running on graphical processing units, which enables us to treat the core region of a moving Bloch point by means of an atomistic Heisenberg model and the surrounding, unproblematic part (where changes in the magnetic structure are smooth) within the standard continuum framework of micromagnetism [6]. Here we present multiscale-multimodel simulation studies on the field-driven vortex domain wall dynamics in a softmagnetic nanocylinder. These domain walls contain a Bloch point in their center. The simulations have been performed for fcc and for bcc lattice structures. The code enables us to determine precisely the position of the Bloch point in the atomic lattice during its motion – with a spatial resolution of a few picometers. By projecting the position of the Bloch point at different time steps into the primitive unit cell of the lattice, we show that its probability density is almost exclusively localized onto the surface of the Wigner-Seitz cell, as shown in the example of a bcc lattice displayed in Figure 1. By calculating the Bloch point position every few femtoseconds, we obtain detailed information on its pathway and velocity within the unit cell. We find that the pathways tend to avoid certain facets of the Wigner-Seitz cell due to variations in the exchange energy landscape. Our results demonstrate the impact of the crystal lattice on the mobility and on the pathways of Bloch points in crystalline ferromagnets.



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Figure 1: The set of positions of a Bloch point during its propagation in a bcc lattice, projected into a region of three adjacent primitive unit cells, shows that certain facets and edges of the Wigner-Seitz cell are preferential positions.

An efficient fast multipole evaluation of the elastic stress field and energy of a dislocation ensemble

Pierre Blanchard¹, Arnaud Etcheverry¹, Olivier Coulaud¹ and Laurent Dupuy²

¹HiePACS team, Inria Bordeaux Sud-Ouest

²SRMA, CEA-Saclay, 91191, Gif-sur-Yvette, France

Among all the steps involved in DD simulations, the computation of the isotropic elastic interaction forces and the global energy of the system are by far the most resources consuming. However hierarchical algorithms like the Fast Multipole Method (FMM) are intrinsically well suited for the fast evaluation of such long-ranged interactions. Our experimentations were performed on the core program OptiDis making use of the open source ScalFMM [1] library as a generic algorithm to balance near- and far-field computations. The development of dislocations-specific P2M/L2P operators was required as the continuum theory of dislocations involve interactions between segments in terms of double line integrals given by Mura's formula [2].

Difficulties implied by the evaluation of these interactions (e.g. tensorial structure, non-symmetry or even the non-homogeneity of the non-singular formulation introduced by Cai et al [3]) combined with a relatively low required accuracy brought us to develop specific approximation methods of the far-field. Namely, an approximation based on Lagrange polynomials of order p and an efficient application of the FMM operators in Fourier space ($O(p^3)$ in both memory and time) were developed in order to overcome the high computational cost of variants such as the Chebyshev-based FMM [4] ($O(p^6)$). This method was first suggested by Eric Darve in the context of a research collaboration. Since then much care has been taken toward maintaining the stability of the new method in a range of p suitable to DD simulations.

Meanwhile, the near-field is evaluated by means of analytical formulas provided by Arsenlis et al [5] and requires a rather performant implementation as it is the critical step of any FMM-accelerated DD simulation. Regarding parallelism, our code benefits from a hybrid OpenMP/MPI paradigm. Finally, an accurate handling of topological elements intersecting the structure of the octree was considered. The latter feature implied careful modifications of the P2M/L2P operators in order to deal with shared memory model of parallelism.

Numerical results will be presented to show the accuracy of this new approach and its parallel performances.

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Progresses towards coupling MD and FEM for the simulation of MEMS containing nanoelectromechanical components

Michel Devel¹, Laurent Hirsinger¹, Naoum Daher¹

¹FEMTO-ST institute, University of Franche-Comté, CNRS, ENSMM, UTBM, 32 avenue de l'observatoire, 25000 Besançon, France

The continuous increase of computer resources for simulation gives plenty of opportunities for the development of novel multiscale algorithms combining atomistic simulations with methods coming from Physics of the continuum. Recently, one of us co-authored a paper detailing a proof of concept for a method allowing the coupling of molecular dynamics (MD) and Finite Element Methods (FEM), in order to simulate the mechanical response of nanosystems submitted to an external, possibly non homogeneous, electric field [1]. In that paper, we considered a 1D system in which the total energy of the system per unit volume could be split into a "mechanical" atomistic part (responsible for the cohesion of the system in absence of an electric field) and an additional "electric" part due to the interaction of the system with an external electric field. This latter part was then restricted to the interaction energy between electric dipoles induced by the external electric field on each atom. To avoid any so-called "polarization catastrophe" we used a Gaussian Dipole Interaction model [2] in which traditional interaction tensors between point electric dipoles are convoluted with Gaussian functions in order to take into account the finite extension of the electron cloud of the atoms. The local Cauchy-Born approximation then allowed us to derive an analytical expression of the "electric" part of the first Piola-Kirchhoff tensors for the atoms belonging either to a finite element in the bulk or to the surface finite elements. Numerical comparison of this scheme with fully atomistic simulations allowed us to validate this method on the example of a carbon chain.

In this poster, we will show how this formalism can be extended to the analytic derivation of the "electric" part of the elasticity tensor and include the effect not only of effective dipoles but also of effective charges [3], [4].

This work was carried out within the framework of the ANR program Mat & Pro "MAFHENIX" (ANR 2011 RMNP 00502). The authors acknowledge useful discussions with Harold Park and Zhao Wang.

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Multi-scale quantum mechanical calculations of solute-grain boundary interaction

Liam Huber¹, Blazej Grabowski², Jörg Rottler¹, Matthias Miltitzer³

¹Department of Physics and Astronomy, The University of British Columbia, Vancouver, BC, V6T 1Z1, Canada

²Max-Planck-Institut für Eisenforschung, Düsseldorf, 40237, Germany

³Center for Metallurgical Process Engineering, The University of British Columbia, Vancouver, BC, V6T 1Z4, Canada

Many problems in computational materials science require the quantum mechanical (QM) accuracy of density functional theory (DFT) simulation, but have structural features which make simulation domains excessively large, e.g. solute interaction with general grain boundaries (GBs), dislocations, or crack propagation. Empirical embedded atom potentials in molecular mechanics (MM), allow much larger systems to be studied at the expense of reduced accuracy. Moreover, the development of new potentials for alloy systems is time consuming and thus not attractive for studies of solute behavior. In these cases quantum chemical accuracy in a local region is required while still being able to access the large-scale structures calculable in MM. While such methods are well established for quantum chemistry, methods for metals are still less mature.

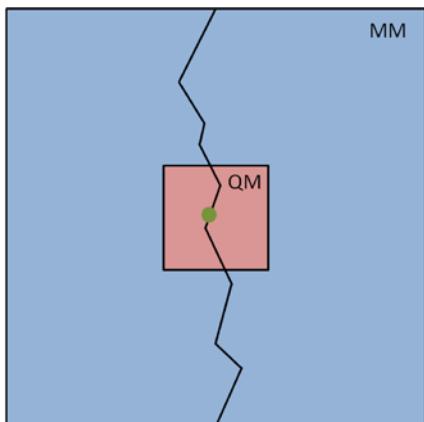


Figure 1: Schematic of embedding, with solute (green) evaluated in QM region (red) sitting at a GB which is only periodic on the scale of the MM region (blue).

To this end we develop a concurrent multiscale coupling method following the work of Lu *et al.* [1,2]. In the method we are building on, the system is decomposed into two regions: a small QM core region embedded within a much larger MM region, shown schematically in figure 1. In this way, interesting chemistry can be calculated with high accuracy in the QM region while still interacting elastically with a much larger structure—one that is not constrained to be periodic in the small QM region.

Since most common DFT codes for metals use a plane wave basis set with periodic boundary conditions (PBCs), isolation of the QM region in this method typically results in the formation of a vacuum interface. Without careful treatment, these surfaces can create very strong electronic perturbations penetrating deeply into the QM region and creating fictitious forces, damaging the perception of the QM region that it is embedded in a larger system. We present a strategy to mitigate this problem by replacing the vacuum interface with one that is electronically much less extreme.

As a test system we study the binding of solutes to a high symmetry boundary in Al which can be validated against periodic DFT calculations. Special attention is paid to the quality of the QM/MM coupling so that errors due to the treatment can be isolated and evaluated critically, allowing us to assess the efficacy and robustness of our improvements to this method. While results for GBs are presented, the model remains applicable to metallic systems in general.

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Computing traction force of dislocation stress field on free surfaces and grain boundaries in anisotropic crystals

B. Liu¹, S. Aubry¹, A. Arsenlis¹, S. Queyreau², G. Hommes¹

¹Lawrence Livermore National Laboratory, Livermore, CA 94550, USA

²LSPM – CNRS, Universite Paris XIII, 93430 Villetaneuse, France

The presence of dislocations in anisotropic elastic media not only exerts traction force on free surfaces, but also causes traction discontinuity across grain boundaries. To account for the elastic interaction between dislocations and interfaces, the traction force due to dislocation stress field has to be first evaluated before an image stress field in response can be determined to ensure the traction free boundary condition at surfaces and traction continuity at grain boundaries. For realistic microstructures, this problem of elastic interaction between dislocations and interfaces can only be solved through the coupling of dislocation dynamics code and finite element solver. The traction force is then calculated by integrating the dislocation stress field over a discretized interface area.

In anisotropic elasticity theory of dislocations, the analytic form of Green's function does not exist. Aubry and Arsenlis [1] have used spherical harmonic series to approximate the derivative of Green's function, and developed an accurate and efficient approach to calculate dislocation stress field and interaction force between dislocations via analytical integration of the spherical harmonic series. In this work, we will present an extension of this approach to calculate the traction force on a discretized interface area, which is also based on an earlier work of analytical surface traction integration in isotropic elastic media [2]. The accuracy and efficiency of the current implementation is evaluated by comparing with direct numerical integration of the derivative of Green's function and obtained dislocation stress field. How the traction force is affected by the anisotropic ratio will also be investigated.

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Accelerated molecular dynamics simulation of dislocation glide in magnesium

Peng Yi¹, Robert C. Cammarata¹, Michael L. Falk^{1,2,3}

¹Department of Materials Science and Engineering,

²Department of Mechanical Engineering,

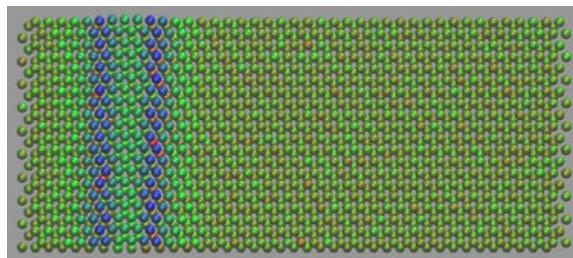
³Department of Physics and Astronomy, Johns Hopkins University, Baltimore, Maryland 21218, USA

Molecular dynamics (MD) simulation has become one of the most powerful tools to study dislocation processes. It enables an atomistic level of understanding of the mechanisms through which dislocations respond to stress and interact. However, computational limitations restrict MD investigations to very high strain rates (10^7 s^{-1} and above). Even high experimental strain rates are typically below 10^4 s^{-1} . To bridge this time scale gap, we use an acceleration method called hyperdynamics [1]. This method has the potential to speed up barrier crossing events by several orders of magnitude, and is well suited to study dislocation glide because dislocation motion is typically controlled by a series of barrier crossing events.

We apply this method to study the dislocation in magnesium crystals. Magnesium has an hcp crystal structure, a more complicated slip and twin system as compared to metals of fcc or bcc crystal structures, e.g., copper, aluminum and iron. For example, there are three slip planes in magnesium, basal, prismatic and pyramidal, all having significant contributions under stress. The interaction between these three slip planes is sensitive to the magnitude of the external stress field. It is therefore very desirable to have a method that allows study of dislocation dynamics over a wide range of strain rates.

The key to the hyperdynamics method is to choose a smart bias potential to facilitate barrier crossing events while keeping the potential landscape near energy barriers unchanged. The hyperdistance [2] method is used to detect transitions associated with atoms in the dislocation core, and a bias potential is designed based on this metric.

The embedded atom model developed by Liu et al.[3] is used in this study. The MD simulations are performed using LAMMPS package, modified in house for the implementation of hyperdynamics.



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A Scale-Bridging Elastoviscoplasticity Proxy Application for Exascale Co-design

Milo Dorr¹, Nathan Barton¹, James Belak¹, Timothy Germann², Jeffrey Keasler¹, Ricardo Lebensohn², Frankie Li¹

¹Lawrence Livermore National Laboratory, Livermore, CA 945550, USA

²Los Alamos National Laboratory, Los Alamos, NM 87545, USA

We describe our progress in the development of a new scale-bridging proxy application and its use in the ExMatEx exascale co-design center [1]. The proxy app combines the coarse-scale LULESH Lagrangian continuum mechanics proxy application with embedded plasticity models that provide the fine-scale constitutive material response. The fine-scale models include both simple flow-rule-based plasticity models and the spatially resolved viscoplastic, micro-structure-resolved polycrystal plasticity model implemented in the VPFFT proxy application also under development in ExMatEx.

The goal of this effort is to provide a flexible platform for investigating multiple questions related to the design of future exascale computing platforms and their associated software ecosystems. Based on the premise that a likely paradigm will consist of simulations of multiple scales running on different parts of the machine, many questions arise with respect to the algorithm and system software requirements of such heterogeneous approaches. Our starting point is the strategy developed in [2],[3] for similar purposes on petascale platforms, which also introduced the use of adaptive sampling as an effective method for allowing the simulation to dynamically learn the fine-scale response and apply it to reduce the cost of future constitutive model evaluations. An important component of ExMatEx is the characterization of the workflow for job schedulers and databases resulting from such multiscale, heterogeneous approaches. We expect the proxy application to also provide a useful tool in the development and analysis of new scale-bridging algorithms.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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Intersecting slip for dislocation dynamics in 2-dimensions

Wei Cai and William P. Kuykendall

Department of Mechanical Engineering, Stanford University, Stanford, CA 94305, USA

Dislocation dynamics (DD) simulations have been developed to advance the understanding of crystal plasticity in terms of the evolution of dislocation microstructures. In 2D DD models, dislocations are assumed to be infinitely long, parallel lines that are represented by a set of points on a 2D plane perpendicular to the lines. The simplicity of the 2D model (compared with the 3D line DD model) allows us to examine a number of important physical and computational issues that have been largely ignored to date.

For example, a group of dislocations on the same glide plane will end up on different (parallel) planes after the original planes are cut by dislocations moving on an intersecting glide plane. Similarly, dislocations on different (parallel) planes can also be brought to the same plane by intersecting slip. This has been suggested as a mechanism that promotes formation of persistent slip bands (see figure 1). However, this mechanism is automatically excluded in existing DD models because the glide planes of non-screw dislocations remain unchanged throughout the simulation. We developed a method to account for shifting of dislocation glide planes by intersecting slip. The method is combined with the non-singular formulation of dislocations, as well as the newly developed analytic solution to the conditional convergence problem in 2D DD models [2]. The predictions of this new model are compared with previous results in the literature to show the effect of slip plane cutting on dislocation microstructure evolution and crystal plasticity.

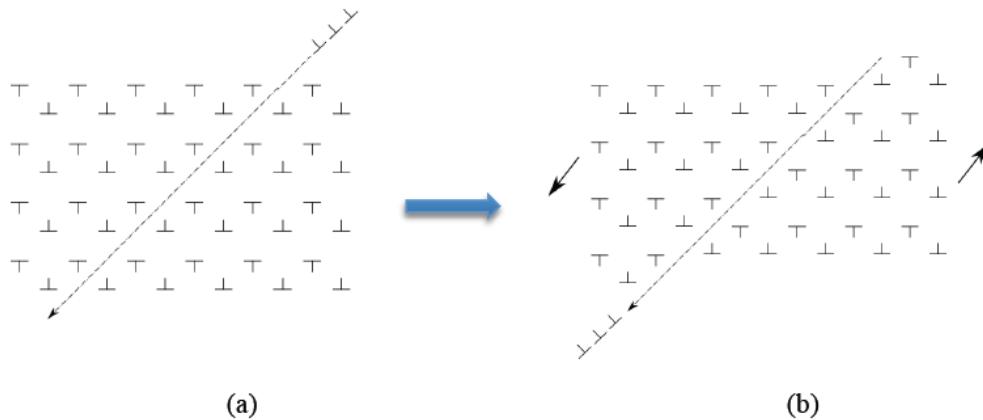


Figure 1. The process of intersecting slip proposed by Laird [1]. (a) A stable multipolar dislocation structure, before being cut by dislocations on intersecting slip planes. (b) After dislocations on intersecting slip plane have cut across the dislocation structure, the latter becomes unstable against massive annihilations.

This work was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-SC0010412.

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Polyethylene-based nanocomposites with carbon reinforcements: atomistic and coarse-grained approaches

Nikita Orekhov, Vladimir Stegailov

Joint Institute for High Temperatures of Russian Academy of Sciences

In the last few years, nanotube-polymer composites have become a subject of interest in the materials science due to their extraordinary mechanical properties in combination with low density and high resistance to corrosion. It is of great interest to establish the link between nanostructure and macroscopic mechanical properties of nanocomposite, i.e., between type and concentration of reinforcements and toughness of material. Molecular dynamics gives the opportunity to build such multi-level models with great predictive capabilities.

On the molecular level, nanoreinforcement-matrix interaction models predominantly use two different approaches: atomistic simulations and coarse-grained (CG) simulations. In this work we discuss and compare the results of atomistic and coarse-grained simulations of polyethylene matrix with multiwall carbon nanotube (MWCNT) nanoreinforcements under different loading conditions. Simulations are held within single model so that properties of intra - and intermolecular interactions are transferred from atomistic to CG level. Besides the mechanical properties of the material attention is given to the accuracy maintenance during coarse-graining and its benefits in the context of parallel efficiency on high-performance supercomputers.

Identification of dislocations by singular value decomposition of the Nye tensor

Fu-Zhi Dai, Wen-Zheng Zhang

School of Materials Science and Engineering, Tsinghua University, Beijing 100084, China

Nowadays, atomistic simulation has become a popular tool for gaining fundamental knowledge of materials. In making fast extraction of mechanistic information from simulation data, powerful analysis algorithms that can automatically identify the structural information play a key role. Though dislocations are important defects of materials, it is only until recently that the features of dislocations, including perfect, partial and secondary dislocations, can be automatically extracted from simulation datasets with a method developed by Stukowski et al [1]. However, this useful method is rather complicated. Extending from the pioneer work by Hartley and Mishin [2], we recently proposed a dislocation identification algorithm based on the singular value decomposition of the Nye tensor [3]. This method can directly extract atoms located at the dislocation cores and junctions respectively by non-trivial singular values, σ_1 and σ_2 . The Burgers vector direction and local line direction are defined by two singular vectors corresponding to σ_1 . Hence, dislocation type (edge, right-hand or left-hand screw) can be determined. The core structure of a dislocation is provided by the distribution of σ_1 , which is proportional to local Burgers vector content. This method is easy to follow and results provided by the method are simple to interpret. The method is also general, since it is applicable to perfect, partial and secondary dislocations. In the meanwhile, the method provides precise dislocation information reaching to an atomic level (Fig. 1). This method is also robust to thermal fluctuation and loss of atoms (even up to 40%!). This presentation will review this newly developed method and provide application examples.

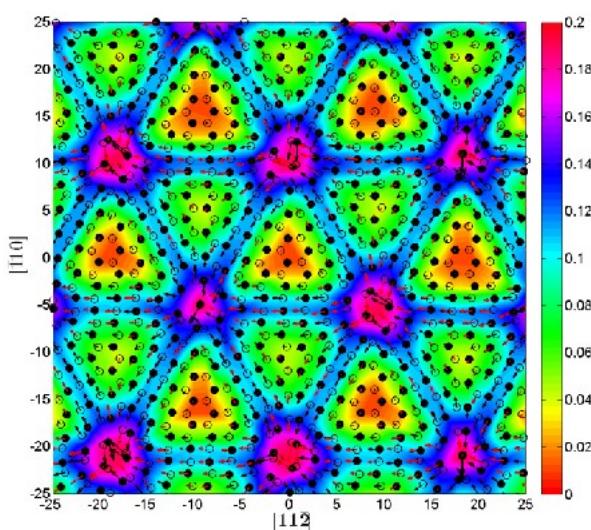


Figure 1. Dislocation features in an 8° [111] twist grain boundary identified by the present method. The filled and hollow circles are atoms in the top and the bottom crystal, respectively. The contour plot shows the distribution of σ_1 . Dislocation cores are in blue, while junctions are in purple. Arrows represent the local Burgers vectors (black) and local line directions (red). All dislocations are $<112>/6$ right-hand screw partial dislocations. The areas separated by dislocations consist of two types of triangular regions. The upright triangles represent the regions with normal stacking sequence, while the upside down ones represent the stacking fault regions.

This work is supported by National Nature Science Foundation of China (No. 51171088).

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First-principles study on the mechanical property of high-entropy alloys by MaxEnt modeling

S. Q. Wang, H. Q. Ye

Shenyang National Laboratory for Materials Science, Institute of Metal Research, CAS,
Shenyang 110016, P. R. China

The importance of entropy in the structure formation of condensed matters is convincingly exemplified by the discovery of high-entropy alloys (HEAs) [1]. The higher the temperature, the more important the entropy. The high configurational entropy acts as the decisive role in HEA phase solidification. The atomic structure model is usually created through finding the optimized configuration with the minimum system energy for the traditional alloys in a theoretical work. However, the maximum entropy configuration in line with the principle of maximum entropy (MaxEnt) should be the first consideration in HEAs model building. The HEAs bulk models were created by MaxEnt principle, and the paracrystalline lattice properties of these alloys were studied by molecular mechanics simulations [2,3]. In this work, the supercell models with periodic boundary condition are created for FCC CoCrFeMnNi and BCC AlCoCrFeNi HEAs by MaxEnt modeling. By means of the built models, the mechanical properties of the two HEA alloys are studied by first-principles calculation within the framework of the density-functional theory.

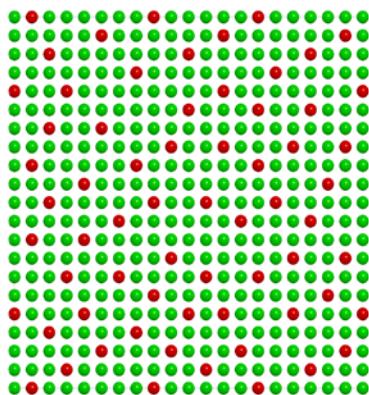


Figure 1: Periodic MaxEnt model of 2D A_xB_{1-x} ($x=0.15$) random-substitution alloy.

The procedure of the MaxEnt model building in this study is similar to our previous work [3], except that a periodic boundary condition is used to convenience for DFT calculation. Figure 1 shows the periodic MaxEnt model of 2D A_xB_{1-x} ($x=0.15$) random-substitution alloy in a 20×20 square lattice for an illustration of the technique. A series of $n \times n \times n$ MaxEnt models with $n=2, 3, 4$ and 5 are created for FCC CoCrFeMnNi and BCC AlCoCrFeNi HEAs. The elastic constants of these models are calculated by using the cell-volume-unrestricted energy-strain method [4]. The elastic constants of the two HEA phases are obtained from these theoretical results through numerical data interpolation. the synergistic effect in the elements

movement is observed during the structure deformation under strain in these HEA phases.

This work was supported by the National Basic Research Program of China (No. 2011CB606403).

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Quantum-Atomic-Continuum-Coupled Model for the Thermo-mechanical Behavior in Micro-nano Simulation

Tiansi HAN, Junzhi CUI

LSEC, ICMSEC, Academy of Mathematics and System Sciences, CAS, Beijing, 100190 China

In order to study the thermo-mechanical behavior of materials in micro-nano scale, a computational model which couples quantum-atomic-continuum natures together is presented in this paper (i.e. QACC model). Unlike traditional methods, the transition region is not needed since the nonlocal mechanical effects are naturally involved in this model. Some necessary assumptions are made when using first principle density functional calculations. Deformations based on Bravais lattice are explicitly derived.

The responses of 3-demensional 25313 copper atoms nanowires under different external loads are simulated in this paper. Stress and strain fields are calculated and dislocation distributions are predicted in the damage process (shown in Figure 1). Numerical results confirm the validity and transferability of this model.

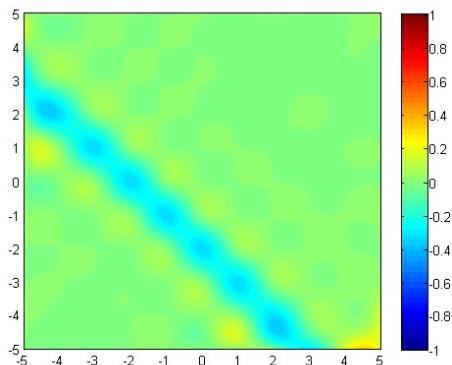


Figure 1 a)

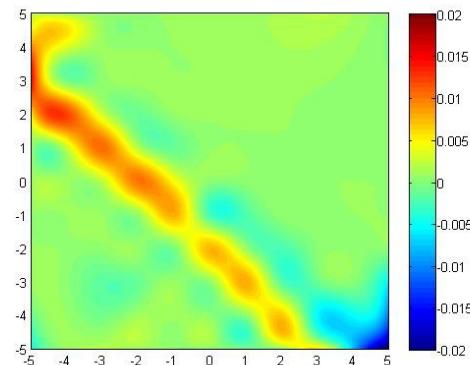


Figure 1 b)

Figure 1 a) xz component of the Cauchy-Green strain tensor and b) xz component of the first Piola-Kirchhoff stress tensor under tension on the middle plane.

This work is supported by the National Basic Research Program of China (973 Program No. 2012CB025904), and also supported by the State Key Laboratory of Science and Engineering Computing. The authors gratefully acknowledge help discussions with PhD. Bowen LI and PhD. Yuran ZHANG.

Numerical Simulation of Three-Dimensional Anisotropic Crystal Growth

Pavel Strachota¹, Michal Beneš¹

¹Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering,
Trojanova 13, 12 000 Praha, Czech Republic

The phase field formulation represents a versatile and widely used instrument for simulations of evolving phase interfaces in solidification and crystal formation. We consider the Stefan problem with surface tension for pure substance solidification and the corresponding phase field model [1]. Furthermore, we introduce a general description of three dimensional surface energy anisotropy by replacing the Euclidean spatial metric by a more general Finsler metric [2]. The model currently works with 4-fold, 6-fold, and 8-fold anisotropies.

The resulting problem is solved numerically by means of the method of lines, using our original multipoint flux approximation (MPFA) finite volume scheme [3,4] with low numerical diffusion for spatial discretization and the proven high order adaptive Runge-Kutta-Merson method for temporal integration. The parallel implementation of the numerical algorithm achieves very good scalability, allowing fully three dimensional simulations with very high resolution (Fig. 1).

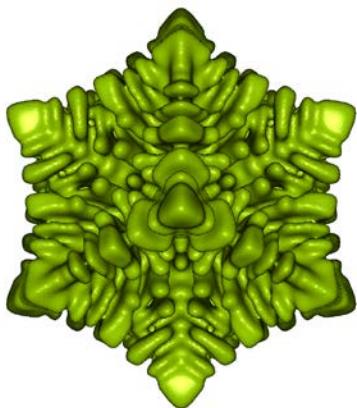


Figure 1: Sample simulation result of crystal growth with 6-fold anisotropy

The main part of the contribution is concerned with the validity of the numerical results, which is verified by experimental convergence analysis. In the isotropic case, an analytical solution of the sharp interface problem can be used for comparison, which provides simultaneous verification of both the phase field formulation and the numerical solution. In anisotropic cases, various comparisons indicate that the MPFA scheme opens up the possibility of using coarser meshes in contrast to standard finite volume schemes while still capturing the complex dendritic structure of the crystal. Further simulations cover the cases of Wulff shape formation in long term crystal evolution under adiabatic isolation and the transition from dendritic to seaweed structure with weakening anisotropy.

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Multiscale Dynamic Simulations and Microstructure of Dipole Colloid

Jianwei Zhang¹, Wenfeng Li¹, and Jiaxi Li¹

¹School of Physics, Tongji University, Shanghai, China 200092

The microscopic structures of dipole colloid are crucial for understanding dynamics behaviors of dipole colloid system. By adopting our multiscale continuum electrical-hydrodynamic model [1], we study microscopic structures and dynamics response of induced dipole colloid (i.e. Electro- rheological fluid). According to our numerical results, microscopic structure of dipole particle can be properly used to explain the shear thinning effect when applied electrical field is perpendicular to the shear direction. Deformation of dipole chains at high shear rate leads to reduction of dipole particle interaction and weak ER effect even in high electrical field region. In the dynamic response shear stress, we show that while our predicted results have features that resemble Bingham fluids, there can be important differences between our results and Bingham model, such as experimentally proved shear-thinning effect. In particular, we study dipole particle structures near maximum dynamics shear stress and found they have similar chains break as static yield stress region. The external field dependence relation of max dynamic stress and static stress also follow same energetic dominated rule. We also find one inter digit electrical field configuration which can avoid shear thinning effect by arrange microscope dipole structure to be partial parallel to shear stress[2]. From our results, we establish a connection relationship between micro-particles' structures and macro-dynamics properties in different conditions through our continuum study, which expose the physics inside of induced dipole fluid dynamics.

This work was performed under the auspices of the The National Natural Science Foundation of China (NSFC) under grant No.11274240. The authors acknowledge useful discussions with W. Wen.

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Adaptive Resolution Simulation of an Atomistic Protein in MARTINI Water

Julija Zavadlav¹, Manuel Nuno Melo², Siewert J. Marrink², Matej Praprotnik¹

¹Laboratory for Molecular Modeling, National Institute of Chemistry, Hajdrihova 19, SI-1001 Ljubljana, Slovenia

²Groningen Biomolecular Sciences and Biotechnology Institute and Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 7, 9747 AG Groningen, The Netherlands

We present an adaptive resolution simulation of protein G in multiscale water [1]. We couple atomistic water around the protein with mesoscopic water, where four water molecules are represented with one coarse-grained bead, farther away. We circumvent the difficulties that arise from coupling to the coarse-grained model via a 4-to-1 molecule coarse-grain mapping by using bundled water models, i.e., we restrict the relative movement of water molecules that are mapped to the same coarse-grained bead employing harmonic springs. The water molecules change their resolution from four molecules to one coarse-grained particle and vice versa adaptively on-the-fly. We observe within our error bars no differences between structural and dynamical properties of the protein in the adaptive resolution approach compared to the fully atomistically solvated model. Our multiscale model is compatible with the widely used MARTINI force field and will therefore significantly enhance the scope of biomolecular simulations.

This research was supported in part by the National Science Foundation under Grant No. NSF PHY11-25915. J.Z. and M.P. acknowledge financial support through Grant Nos. J1-4134 and P1-0002 from the Slovenian Research Agency. M.N.M. acknowledges funding (Veni Grant No. 722.013.010) from the Netherlands Organisation for Scientific Research (NWO).

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Multiscale simulation of atomic structure in the neighborhood of nanovoids

Irina V. Ershova¹, Andrei V. Nazarov^{1,2}, Alexander G. Zaluzhnyi^{1,2}

¹National research nuclear university (MEPhI), Moscow, Russia

²SSC RF Institute for Theoretical and Experimental Physics (ITEP), Moscow, Russia

The voids play a significant role in the processes of material structure forming, diffusion phase transformations, swelling, etc. Therefore it is necessary to develop the methods of determining the defects characteristics. Also it's obvious that defect characteristics are determined by the atomic structure. Atoms surrounding defect shift from the sites of ideal lattice, e.g. defect atomic structure changes with respect to an ideal one, that in turn leads to changes in interaction energy of neighbor atoms and results in modification of defect energy characteristics and other features. Generally displacement fields in the vicinity of point defects as well as nanovoids were determined by the solution of equations from the classical theory of elasticity. Such a description has its disadvantages as it doesn't take into account the discrete atomic structure of materials. Results of classical elasticity theory are expected to be valid at distances from a defect that are much larger than the lattice parameter which is a characteristic feature of discreteness, therefore the quantities of atom displacements in the vicinity of such defects as vacancies, vacancy complexes and nanovoids should significantly differ from the predictions of these displacements obtained by means of theory of elasticity. In our recent works a new approach was developed [1,2]. In particular in this approach an iterative procedure was used in which the atomic structure in the vicinity of point defect and constant, determining the displacement of atoms embedded into an elastic continuum with accordance with asymptotic solution of equations from the classical theory of elasticity, are obtained in a self-consistent manner. The vacancy features (including formation volumes and migration volumes) obtained for a number of cubic metals agreed well with experimental values. In this work we use our approach for direct investigation of the atomic structure in the vicinity of vacancy complexes and nanovoids in some fcc and bcc metals. The fields of displacements in the vicinity of nanovoids are significantly more complicated and with much bigger magnitudes of displacements than in the vicinity of vacancies. In addition, the displacement significantly different for variant crystallographic directions, and these differences are particularly large in metals with bcc structure.

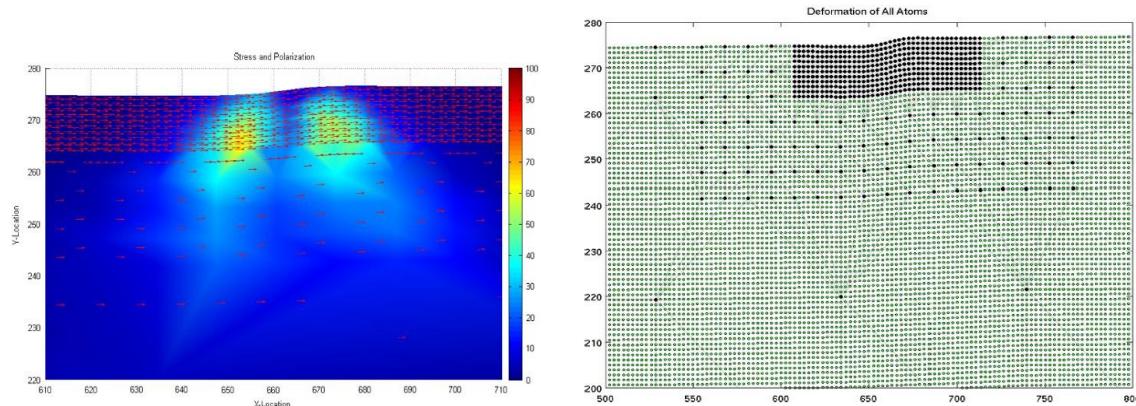
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A Multiscale Atomistic Method for Defects in Ionic Materials

Kaushik Dayal, Jason Marshall

Carnegie Mellon University, USA

Ionic solids are important for electronic and energy storage/conversion devices. Examples include ferroelectrics and solid oxides. Defects in these materials play a central role in enabling their properties: for example, the electromechanics of ferroelectrics occurs by the nucleation and growth of domain wall defects, and solid oxide ionic conduction is through the motion of point defects. I will talk about our efforts to develop multiscale atomistic methods to understand the structure of defects in these materials. These materials have long-range electrostatic interactions between charges, as well as electric fields that exist over all space outside the specimen. I will describe a multiscale methodology aimed at accurately and efficiently modeling defects in such materials in complex geometries. Our approach is based on a combination of Dirichlet-to-Neumann maps to consistently transform the problem from all-space to a finite domain; the quasicontinuum method to deal with short-range atomic interactions, and rigorous thermodynamic limits of dipole lattices from the literature.



The first figure shows an atomic-level stress measure and polarization vector field when a ferroelectric with a free surface is subject to a localized electric field just above the free surface, and the second figure shows the corresponding ionic displacements.

We thank ARO and AFOSR for support, and Richard D. James, Saurabh Puri, and Yu Xiao for useful discussions.

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Defect and surface properties of Multinary Alloys for Solar Energy Absorber

X. G. Gong

Key Lab for Computational Physical Sciences (MOE), Fudan University
Shanghai, 200433, China

Multinary alloys, such as Cu₂ZnSnS₄ and recently discovered ABX₃, are the most promising absorber materials for thin-film solar cells, since it is a low-cost material with the optimal band gap 1.5 eV for single-junction solar cells and a high adsorption coefficient. Although the synthesize of such compound could be long time ago, due to the complicity of these multinary compound, the properties are not well understood, which are crucial for improving the solar cell performance.

In this talk, I will focus on the defect properties of Cu₂ZnSnS₄ and ABX₃, the intrinsic point defects and also complex defects. The dominant defect in CZTS will be *p*-type Cu_{Zn} antisite, which has an acceptor level deeper than the Cu vacancy. We proposed that Cu_{Zn}+Sn_{Zn} and 2Cu_{Zn}+Sn_{Zn} defect complex could be detrimental to efficiency, with a small Voc. We predicted the possible reconstruction configurations of the frequently observed cation-terminated (112) and anion-terminated ($\overline{1}\overline{1}2$) surfaces, and found that the polar surfaces are stabilized by the charge-compensating defects, such as vacancies (V_{Cu}, V_{Zn}), antisites (Zn_{Cu}, Zn_{Sn}, Sn_{Zn}) and defect clusters (Cu_{Zn}+Cu_{Sn}, V_{Zn}+2V_{Cu}). I will also show the defect properties of the ABX₃, which is important to understand its high efficiency.

First-principles molecular dynamics of Li transport in Li_3InBr_6 : Tools for high-throughput screening

Nicole Adelstein¹, Boris Kozinsky², Brandon Wood¹

¹Lawrence Livermore National Laboratory, Livermore, California 94550, USA

²Bosch LLC, Cambridge, MA 02142, USA

All-solid-state batteries have the potential to dramatically improve the capacity and safety of high-density energy storage. Inorganic electrolytes with sufficiently high conductivity and mechanical and thermal stability are needed to develop these batteries.

Understanding the effect of ion correlation, lattice properties and disorder on Li conductivity will provide design rules to accelerate high-throughput screening of potential electrolytes.

Using a recently synthesized highly conductive electrolyte candidate [1], Li_3InBr_6 , we explore the role of phonon modes, 3D channels and lattice strain on Li diffusivity using first-principles molecular dynamics simulations. Molecular dynamics simulations allow us to discover new Li conduction pathways and mechanisms. Figure 1 shows the mean squared displacement of Li, projected along different directions in the lattice, which predicts a strong anisotropy of the diffusivity. In this work we will present some uncommon, though not entirely new[2], techniques for analyzing structural and electronic properties that could be predictors of high ionic conducting materials.

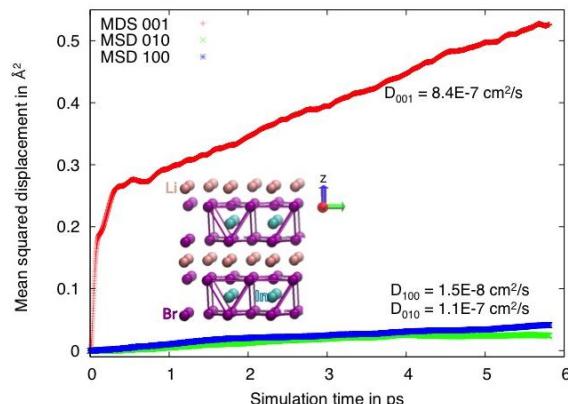


Figure 1: The mean squared displacement of Li in Li_3InBr_6 is projected into the three axes.

The insights gained from our in-depth character of the Li transport mechanisms in this promising material will aid the search for better inorganic solid-state batteries. Computer resources on Oak Ridge National Laboratory's TITAN supercomputer enable many different constraints to be placed on the system and run simultaneously using Quantum Espresso's Car-Parinello code. Our computer time is granted from an INCITE project, "Safety in numbers:

Discovery of new solid Li-ion electrolytes", to discover new battery materials using high-throughput screening. In-depth density functional theory simulations of a variety of Li-conducting electrolytes are an integral component of the project's Automated Infrastructure and Database for *Ab-Initio* design (AIDA).

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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Conductivity of doped ceria from non-equilibrium molecular dynamics

Johan O. Nilsson¹, Olle Hellman², Sergei I. Simak², Natalia V. Skorodumova¹

¹Dept of Materials Science and Engineering, Royal Institute of Technology
(KTH), ²Department of Physics, Chemistry and Biology (IFM), Linköping University

The color-diffusion algorithm is implemented in an *ab initio* molecular dynamics simulation of doped cerium oxide for calculating oxygen ion diffusion. The time scales needed to capture rare events such as ionic diffusion are typically too long to be simulated with conventional molecular dynamics. By assigning fictitious “color charges” to the oxygen ions and acting on them with a fictitious “color field”, it is possible to accelerate these rare events. In the limit of zero field this non-equilibrium algorithm gives the oxygen diffusion coefficient for the undisturbed system. We discuss some technical details of this approach and our results for ceria doped with rare-earth elements.

First-principles and molecular dynamics simulation for diffusion problem of YSZ and Ni/YSZ in solid oxide fuel cells

Yoshitaka Umeno, Albert M. Iskandarov, Atsushi Kubo

¹Institute of Industrial Science, The University of Tokyo, Tokyo 153-8505, Japan

The solid oxide fuel cell (SOFC) is one of the most promising energy sources due to its high efficiency in energy conversion and variety of fuel types. To achieve high performance and durability, diffusion problems must be addressed. For example, the mechanism of oxygen diffusion in electrolyte has to be revealed because lower diffusivity leads to lower electric current density. As sintering in anode materials, which can cause change in microstructures, has to be reduced for better reliability, the diffusion mechanism in anode cermet should be examined to find ways to suppress sintering.

In this study, we first develop a potential for yttria-stabilized zirconia (YSZ) and Ni/YSZ interface, which are typical electrolyte and anode materials in SOFCs. For better reliability and transferability, we adopt the Tangney-Scandolo (TS) dipole model [1], where electric polarization around each atom is represented by electric dipole. Potential parameters are fitted to first-principles density functional calculation results via the real-coded genetic algorithm and the force-matching method, so that the optimized potential can be applied to the cubic phase of YSZ for a reasonable range of yttria concentration. The optimized potential can reproduce YSZ surface energies, Ni/YSZ interface energies and energy barriers of oxygen vacancy migration.

We then perform nudged elastic band (NEB) calculations and molecular dynamics simulations of oxygen vacancy diffusion in YSZ, and discuss the effect of surfaces on ionic conductivity. We also examine Ni diffusion on YSZ surfaces by first-principles and molecular dynamics calculations to evaluate the effect of impurity segregation on Ni diffusion.

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Atomistic Simulations of Thermal Transport in Nanostructured Semiconductors

Yuping He¹, Giulia Galli²

¹Department of Chemistry, University of California, Davis, California 95616, USA

²The Institute for Molecular Engineering, the University of Chicago, Illinois 60637, USA

We present the results of atomistic simulations of heat transport in realistic models of ordered and disordered semiconductors. In particular we discuss the thermal properties of Si and SiGe at the nanoscale (with focus on nano-wires [1] and nanoporous materials [2,3]) as obtained from molecular dynamics simulations and Boltzmann transport equation calculations [4]. We also discuss recent ab initio results on Si based clathrates [5,6], e.g. the newly synthesized K₈Al₈Si₃₈.

These works were supported by the U.S. DOE/BES

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Stability and kinetics of Se overlayers on Mo(110) and the role of Na impurities: from ab initio data to thermodynamics and kinetics

Guido Roma^{1,2}, Elaheh Ghorbani², H. Mirhosseini², Janos Kiss^{2,3},
Thomas D. Kühne¹, Claudia Felser^{2,3}

¹CEA, DEN, Service de Recherches de Métallurgie Physique, Gif sur Yvette F-91191,
France

²Institute for Inorganic and Analytical Chemistry, Johannes Gutenberg Universität, Mainz
D-55128, Germany

³Max Planck Institute for Physical Chemistry of Solids, D-00187 Dresden, Germany

The selenization of molybdenum is nowadays technologically relevant for the production of thin film chalcopyrite solar cells based on CuIn_xGa_{1-x}Se₂ (CIGS) and might become an important step in the production of nanostructures based on the layered compound MoSe₂. However, the control of the process is still very poor, due to the lack of basic knowledge of the surface thermodynamics of the system. The kinetics, moreover, can become crucial to obtain preferred textures and, thus, electronic properties.

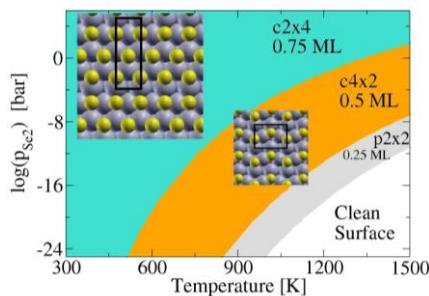


Figure 1: Surface phase diagram of Se adsorbed overlayer on the Mo(110) surface.

In the case of solar cells the role of sodium impurities, and maybe oxygen, has been invoked, claiming that it could help the formation of an Ohmic contact. Based on first principles calculations of adsorption energies [1,2] and migration energies of Se, Na, and O on the Mo(110) surface we predict stable patterns for adsorbed Selenium [3] -or surface selenides- for various ambient conditions. Our results show that the attainable Se coverages range from 1/4 to 3/4 of a monolayer, depending on the partial pressure and size of Se molecules composing the gas with which the surface is in equilibrium. We provide simulated scanning tunneling microscopy images to help the experimental characterization of adsorbed surface

patterns. We acknowledge financial support from the comCIGS II project of the Federal Ministry for the Environment, Nature Conservation and Nuclear Safety of Germany.

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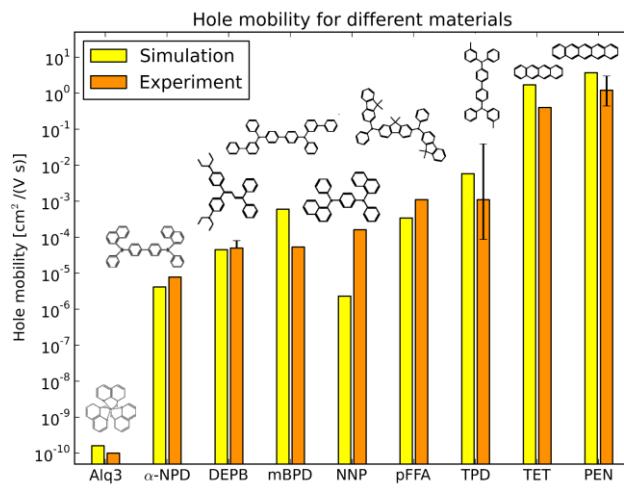
A self-consistent first-principles approach model carrier mobility in organic materials

Pascal Friedrich¹, Tobias Neumann¹, Franz Symalla¹, Angela Poschlad¹, Denis Danilov¹, Ivan Kondov², Velimir Meded^{1,2}, Wolfgang Wenzel¹

¹Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany

²Steinbuch Center for Computing, Karlsruhe Institute of Technology, Karlsruhe, Germany

Transport through thin organic amorphous films, such as those used in OLED and OPV devices, has been difficult to model on using first-principles methods. Nevertheless the carrier mobility depends strongly on the disorder strength and reorganization energy, both of which are significantly affected by the environment of each molecule. Here we present a multi-scale approach to model carrier mobility in which the morphology is generated using DEPOSIT, a Monte Carlo based atomistic simulation approach. From this morphology we extract the sample specific hopping rates, as well as the on-site energies using a fully self-consistent embedding approach to compute the electronic structure parameters which are then used in an analytic expression for the carrier mobility. We apply this strategy to compute the carrier mobility for a set of widely studied molecules and obtain good agreement between experiment and theory for over ten orders of magnitude in the mobility without any adjustable parameters.



Thermal Transport Modeling on Low-Dimensional Semiconducting Nanostructures

Yong-Wei Zhang, Gang Zhang, Qing-Xiang Pei, Xiang-Jun Liu, Yong-Qing Cai

Institute of High Performance Computing, A*Star, Singapore 138632

Low-dimensional semiconducting materials, such as one-dimensional and two-dimensional materials, have attracted extensive research interest recently due to their promising applications in electrical energy generation and thermal management. For low-dimensional semiconducting materials, controlling their size, shape, composition and surface chemical functionalization is of importance in controlling their thermal transport behavior since the characteristic lengths inherent to the phonon scattering are often strongly coupled with these extrinsic sizes of these materials.

In this talk, we present our recent works in using various modeling and simulation methods to study the thermal transport properties of several low-dimensional semiconducting nanostructures [1-6]. First, we report our work of using linearized Boltzmann transport equation by incorporating the phonon-surface coupling to the study the effects of the size, surface roughness and composition on the transport properties of $\text{Si}_{1-x}\text{Ge}_x$ nanowires. Next, we will report our work of using non-equilibrium molecular dynamics to study the thermal transport properties of (1) core-shell Si/amorphous Si nanowires focusing on the geometry factor and strain engineering; (2) MoS_2 sheet and nanoribbons focusing on the geometry effects; and (3) silicene focusing on the effect of isotopic doping and strain engineering. Then, we will report our work of using first-principles method based on density functional perturbation theory and non-equilibrium Green function method to study the phonon scattering and thermal transport behavior of MoS_2 nanoribbons focusing on the intrinsic umklapp scattering mechanism. Finally, we will discuss briefly on the basic principles of using phononic engineering to modulate the thermal transport properties of low-dimensional materials for thermoelectric applications.

This work was supported by the A*STAR Computational Resource Centre through the use of its high performance computing facilities.

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Understanding fracture in Si anodes: Experiments and Simulations

Katerina E. Aifantis

University of Arizona

Si is the most promising anode for next generation Li-ion batteries, as it can provide capacities that are 3-10 times greater than that of current graphitic anodes. The limiting factor in commercializing these promising anodes is the 300% volume expansion and subsequent fracture that they experience during Li-insertion. This talk will present new experiments and simulations that go hand-in-hand and allow the development of design criteria that predict the most promising configurations that will limit damage and allow for stable electrochemical cycling. It is noted that high resolution electron microscopy is used to obtain the fracture patterns after Li-insertion, while finite element simulations can simulate these patterns.

Exotic phase group IV nanoparticles and Si-ZnS nanocomposites: new paradigms to improve the efficiency of MEG solar cells

Gergely Zimanyi¹, Márton Vörös¹, Stefan Wippermann²,
Adam Gali^{3,4}, Francois Gygi⁵, Giulia Galli⁶

¹Department of Physics, University of California, Davis, 95616, Davis, CA, USA; ²Interface Chemistry and Surface Engineering Department, Max-Planck-Institute for Iron Research, 40237 Düsseldorf, Germany

³Department of Atomic Physics, Budapest University of Technology and Economics, H-1111, Budapest, Hungary

⁴Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, H-1525 Budapest

⁵Department of Computer Science, University of California, Davis, 95616, Davis, CA, USA

⁶Institute for Molecular Engineering, The University of Chicago, Chicago, IL 60637, USA

The efficiency of nanoparticle (NP) solar cells may substantially exceed the Shockley-Queisser limit by exploiting quantum confinement enhanced multi-exciton generation (MEG). However, (i) quantum confinement tends to increase the electronic gap and thus the MEG threshold beyond the solar spectrum and (ii) charge extraction through NP networks may be hindered by facile recombination. Using *ab initio* calculations we found that (i) Si and Ge NPs with exotic core structures such as BC8 or ST12 exhibit lower gaps and MEG thresholds than particles with diamond cores, and an order of magnitude higher MEG rates [1]. (ii) We also investigated Si NPs embedded in a ZnS host matrix and observed complementary charge transport networks, where electron transport occurs by hopping between NPs and hole transport through the ZnS-matrix (cf. Figure 1) [2]. Such complementary pathways may substantially reduce recombination, as was indeed observed in recent experiments. We employed several levels of theory, including DFT with hybrid functionals and GW calculations.

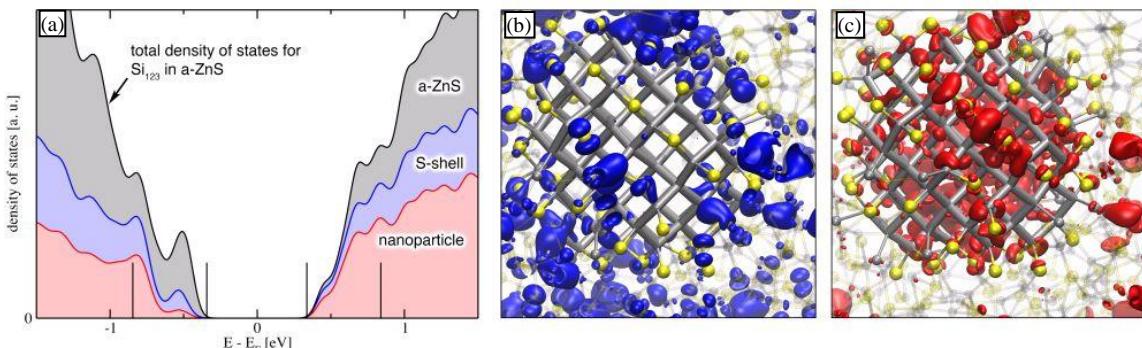


Figure 1: (a) Electronic density of states of the Si nanoparticle and host a-ZnS matrix for a sample of $\text{Si}_{123}\text{Zn}_{188}\text{S}_{201}$, partitioned into contributions from the nanoparticle, the surface shell (S-shell) and the host matrix (a-ZnS). Isodensity plots of the sum of square moduli of the states at the top of the valence band (blue) and bottom of the conduction band (red) are shown in (b) and (c), respectively. The sums were performed over an energy interval of 0.5 eV, as indicated by vertical bars in (a).

This research was supported by the NSF Solar Collaborative (No. DMR-1035468), DOE/BES (Contract No. DE-FG02-06ER46262), and the Deutsche Forschungsgemeinschaft (Grant No. WI3879/1), as well as by supercomputer time provided by NERSC (No. NISE-35687). G. G. acknowledges DOE/BES Grant No. DESC0008938. S.W. acknowledges BMBF Grant No. 13N12972.

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PEC H₂ production: is it PV + electrolysis or not?

Tadashi Ogitsu¹, Brandon Wood¹, Woon Ih Choi¹, Minoru Otani², Eric Schwegler¹

¹Lawrence Livermore National Laboratory, Livermore, California 94550, USA

²National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan

A photoelectrochemical (PEC) hydrogen production device converts solar energy into chemical energy as H₂ gas. Typically, photoelectrode surface is decorated with co-catalyst such as Pt nano particles since the surfaces of known efficient photo absorber materials, such as III-V semiconductors or CIGSe, do not exhibit good catalytic activity for hydrogen evolution reaction (HER). The photo absorber material will absorb photons and generate photo-excited electrons and holes, which, in turn, will drive HER where Pt co-catalyst plays a role of lowering the HER activation barrier. The observation that a high efficiency PEC device seems to require good co-catalyst implies that the underlying conversion mechanism may be a combination of photovoltaic and electrolysis, which will make a PEC device modeling as simple additive: an efficient and corrosion resistant photo absorber with the correct band alignment to H₂/O₂ redox potential combined with a good co-catalyst for HER.

In 2013, it was reported that addition of a disk shaped Pt co-catalyst on a silicon based Metal-Insulator-Semiconductor (MIS) PEC device significantly enhances HER not only on the Pt co-catalyst but also on its surrounding area of SiO_x surface [1]. Subsequently, based on ab-initio simulations of interfaces between water and III-V semiconductors, it was proposed [2] that certain types of semiconductor photo absorber surface, when it is in contact with electrolyte, might exhibit a good proton transport at the interface, and if, such a surface has a low activation barrier for Heyrovky step (the second step of HER), it will play a synergetic role with co-catalyst: a consistent picture with the aforementioned experimental observation [1]. Note that a catalyst such as Pt is known to have a low Volmer step (the first step of HER) activation barrier, while semiconductor (photo absorber) surfaces tend to have high Volmer step activation barriers.

In the presentation, we would like to discuss about a new design strategy, which will take advantage of the proposed synergetic effect between co-catalyst and photo-absorber surface.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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Efficiency assessment of novel materials based flexible thermoelectric devices

Malika Bella^{1,2,3}, Sylvain Blayac², Christian Rivero³, Valérie Serradeil³, Pascal Boulet¹

¹Aix Marseille Université, CNRS, MADIREL UMR 7246, 13397, Marseille, France

²Ecole Nationale Supérieure des Mines de Saint-Etienne, Centre Microélectronique de Provence

Georges, Charpak, 13541 Gardanne, France

³STMicroelectronics, ZI Rousset-Peynier, 13106 Rousset, France

In recent years, body heat energy scavenging has become a great source of interest as a power supply for autonomous systems, especially in the area of wearable electronics. The main issue regarding the materials currently used for room temperature thermoelectric applications is their reported health hazardousness [1]. The aim of this study is thus to propose a solution for flexible thermoelectric generators based on novel non health hazardous materials. For this purpose, we study the thermoelectric properties of the tetrahedrite group of materials (figure 1).

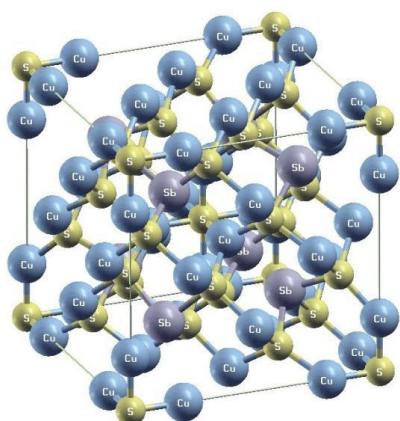


Figure 1: Crystal structure of $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$

A first step is to understand how doping helps improving the electrical properties of $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$ using an ab initio Density Functional Theory approach, with the open source code Quantum Espresso [2], through the analysis of the electronic structure (electronic band structure and density of states).

The Seebeck coefficient as well as the electrical conductivity as a function of temperature are calculated by solving the Boltzmann transport equation using the BoltzTrap code [3].

An interesting way of fabricating low cost flexible devices is by using printing techniques as it enables the processing of flexible substrates under standard temperature and pressure conditions. Besides the technological challenges (ink preparation, printing parameters control, post treatment...), it is necessary to evaluate the efficiency of an “ideal” printed device. In this context, a virtual prototype of a flexible thermoelectric device with an innovative design will be described and evaluated thanks to the COMSOL Multiphysics (Finite Elements Modeling) software. The impact of the electrical contact resistance will be taken into account in the model as it is a key parameter for device efficiency improvement.

The presented work will thus demonstrate a strategy for evaluating novel materials as potential replacements to bismuth telluride based alloys for room temperature thermoelectric applications and provide some insights into the development of flexible devices based on those materials.

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Better photovoltaic performance through randomized nanowires

Thomas Edwards

Imperial College London

Radial junction nanowires are expected to give a higher performance than planar solar cells. This is due to enhanced optical path length for absorption and shorter distance for excitons to travel to interfaces where they can dissociate. We have optimised, with respect to geometrical parameters, solar cells consisting of nanowires with TiO₂ cores and CdSe shells embedded in conducting polymer. Optical scattering and absorption is studied using Finite-Difference Time-Domain (FDTD) simulations. From this we obtain the generation rate of electron-hole pairs as a function of position, which is input into a charge transport model. We found that nanowires absorb more light when placed randomly rather than in a periodic array.

Synergistic Behavior of Tubes, Junctions and Sheets Imparts Mechano- and Thermo-Mutable Functionality in 3D Porous Multifunctional Boron Nitride Nanostructures

Navid Sakhavand¹, Rouzbeh Shahsavari^{1,2}

¹Department of Civil and Environmental Engineering, Rice University, Houston, TX 77005

²Department of Material Science and NanoEngineering, Rice University, Houston, TX 77005

One-dimensional (1D) Boron Nitride nanotube (BNNT) and 2D hexagonal BN (*h*-BN) are attractive for demonstrating fundamental physics and promising applications in nano/microscale devices. However, there is a high anisotropy associated with these BN allotropes as their excellent properties are either along the tube axis or in-plane directions, posing an obstacle in their widespread use in technological and industrial applications. Herein, we report a series of 3D BN prototypes, namely Pillared Boron Nitride (PBN), by fusing single wall BNNT and monolayer *h*-BN aimed at filling this gap. We use density functional theory and molecular dynamics simulations to probe the diverse mechano- and thermo-mutable properties of PBN prototypes, followed by tensile experiments on 3D printed thought-model specimens. Our results demonstrate that the synergistic effect of the tubes, junctions, and sheets imparts cooperative deformation mechanisms and phonon transport processes, which overcomes the intrinsic limitations of the PBN constituents, thus providing a number of superior characteristics including 3D balance of strength, toughness and thermal transport, emergence of negative Poisson's ratio, and elimination of strain softening along the armchair orientation (**Figure 1**). These features, combined with the ultrahigh surface area and lightweight structure, render PBN as a 3D multifunctional template for applications in graphene- based nanoelectronics, optoelectronics, gas storage and functional composites with fascinating in-plane and out-of-plane tailorable properties. Specifically, the ultrahigh surface area ($> 2200 \text{ m}^2/\text{g}$) could be a promising venue for energy storage and delivery.

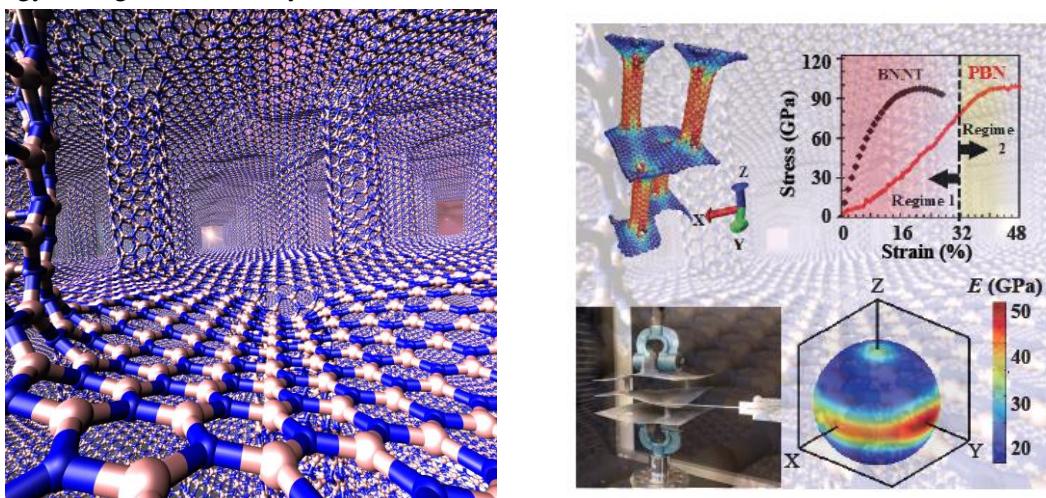


Figure 1. Pillared Boron nitride is a 3D porous multifunctional nanostructure exhibiting unique mechano- and thermo-mutable properties with ultra-high surface area.

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***Ab initio* lattice thermal conductivity in pure and doped half-Heusler thermoelectric materials**

Luc Andrea¹, Gilles Hug¹, Laurent Chaput²

¹Laboratory for the Study of Microstructures, LEM, CNRS/ONERA, France

²Material Physics Laboratory, University of Lorraine, CNRS, France

Half-Heusler phases are promising intermetallics for applications in thermoelectric generators. Optimization of their thermal transport properties is essential to improve their overall conversion efficiency [1]. Our goal is to perform a theoretical evaluation of thermal transport properties directly from first-principles calculations for various pure and doped half-Heusler compounds. The electronic structures are modeled in the framework of the density functional theory (DFT) [2]. The *ab initio* thermal properties are deduced from harmonic and anharmonic interatomic force constants calculations using finite size displacements method. Many-body perturbation theory is used for calculating the phonon-phonon interactions which yields the lifetime of phonons as function of momentum and band index [3]. Finally, thanks to a direct solution to the phonons Boltzmann transport equation [4] we computed the *ab initio* thermal conductivities, which are found in good agreement with the experimental data.

As a second step, we study specific localized impurities and size-controlled nanoparticles as they can lead to better thermal transport properties enhancing the thermoelectric efficiency [5,6,7,8]. In order to calculate the thermal conductivity in presence of localized defects, we developed a model to account for substitution defects and disorder in half-Heusler phases using perturbation theory and configurational analysis. Our results provide good insights for understanding the behavior of the thermal conductivity, which will be useful to guide experimental work to find pathways to improve the thermoelectric figure of merit of these materials.

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Large-Scale First-Principles Molecular Dynamics Simulations of Materials for Energy Conversion

Francois Gygi

University of California Davis, Davis, CA95616, USA

An accurate description of energy conversion mechanisms often requires atomic-scale models as well as the electronic structure of the materials under consideration. First-principles molecular dynamics (FPMD) provides a seamlessly coupled, consistent picture of both atomic structure and electronic structure. This approach is becoming increasingly popular for simulations of materials having complex structure, such as nanoparticles or interfaces. FPMD simulations are limited by the high computational cost of the underlying electronic structure computations, which are most often carried out using Density Functional Theory (DFT). In recent applications, the need for higher accuracy has motivated the use of hybrid-DFT approximations, which further increases the computational cost of simulations. We discuss the current limits and tradeoffs of feasible FPMD simulation, using examples of nanoparticles and solid-liquid interfaces relevant to solar energy conversion.

in situ Nanomechanics of Electrode Failure in Lithium-Ion Batteries

Ting Zhu, Shan Huang, Feifei Fan

Woodruff School of Mechanical Engineering Georgia Institute of Technology, Atlanta,
GA 30332

Lithium-ion batteries revolutionize portable electronics and are key to next-generation electric vehicles. However, they usually suffer from the electrochemically induced mechanical degradation in high-capacity electrodes, resulting in quick capacity fading and poor cyclability. Using a unique nanobattery cell inside a transmission electron microscope, we made the *in situ* observations of reaction, deformation and fracture in individual nanowire and nanoparticle electrodes. A wide range of novel phenomena were discovered, including the size dependent fracture in silicon nanoparticles, anisotropic swelling in silicon nanowires, two-phase lithiation in amorphous silicon, nanoporosity formation in germanium nanowires, and cracking in the coating of tin oxide nanowires. We developed the continuum and atomistic models to reveal the mechanistic origin of stress generation and mechanical failure in these high-capacity electrode materials. The results provide insights into the microstructural evolution and mechanical degradation in nanobatteries. Our work has broad implications for designing durable electrodes in lithium-ion batteries.

A Multiscale Analysis of Ion Conductivity in Non-Equilibrium Environment

Jan Hamaekers, Christian Neuen

Fraunhofer SCAI, Germany

Batteries and (super-)capacitors function on the basis of ion migration between electrodes. Even today our society can hardly function without batteries as they enable the use of a variety of mobile electronic devices.

Despite many different approaches, there is still no full understanding of the contribution of counterions to the conductivity and transference numbers within the batteries cell. In particular, the electric voltage along the cell and its respective fluctuation move the system to a non-steady state.

For the prediction of material properties, we use molecular dynamics where the ensemble specifically takes into account the non-equilibrium state of the system induced by the presence of outer forces and treat the corresponding energy flow.

Even with the ensemble being able to handle a non-equilibrium ensemble, the normal evaluation of macroscopic properties cannot be trivially transferred from the equilibrium case and need to be adapted to account for the flux introduced.

The extended measurement of macroscopic variables then allows us to evaluate the performance on the cell level with an adaptive finite element solver to the time dependent, fully coupled Poisson-Nernst Planck equations in 2/3D. In this context special challenges appear with the strong non-linear coupling via the ions' electric field and the boundary conditions of both equation types.

We demonstrate results achieved with this method by predicting the ionic current flow in an alternating voltage setting in order to compute transference numbers.

Composition and catalytic activity of Au/Cu electrocatalytic nanoalloys in solution: A combination of DFT and accurate neural network potentials

Nongnuch Artrith, Alexie M. Kolpak

Department of Mechanical Engineering, Massachusetts Institute of Technology, 77
Massachusetts Avenue, Cambridge, Massachusetts 02139, USA

Heterogeneous catalytic chemical reactions are at the core of many energy and environment related challenges. The shape, size, and composition of catalyst nanoparticles can have a significant influence on catalytic activity. Understanding structure-reactivity relationship is crucial for the optimization of industrial catalysts and the design of novel catalysts with enhanced properties. Recently, Shao-Horn, Hamand-Schifferli, et al. have shown that Au/Cu nanoparticles are stable and efficient electrocatalysts for the reduction of CO₂ [1]. We employ a combination of first-principles computations and large-scale Monte-Carlo simulations with highly accurate neural network (NN) potentials to study the equilibrium surface structure and composition of bimetallic Au/Cu nanoparticles (NPs), which have recently been of interest as stable and efficient CO₂ reduction catalysts. We demonstrate that the inclusion of explicit water molecules at a first-principles level of accuracy is necessary to predict experimentally observed trends in Au/Cu NP surface composition; in particular, we find that Au-coated core-shell NPs are thermodynamically favored in vacuum, independent of Au/Cu chemical potential and NP size, while NPs with mixed Au-Cu surfaces are preferred in aqueous solution. Furthermore, we show that both CO and O₂ adsorption energies differ significantly for NPs with the equilibrium surface composition found in water and those with the equilibrium surface composition found in vacuum, suggesting large changes in CO₂ reduction activity. Our results emphasize the importance of understanding and being able to predict the effects of catalytic environment on catalyst structure and activity. In addition, they demonstrate that first-principles-based NN potentials provide a promising approach for accurately investigating the relationships between solvent, surface composition and morphology, surface electronic structure, and catalytic activity in systems composed of thousands of atoms [2].

We thank the Schlumberger Foundation Faculty for the Future for financial support. Computing time at XSEDE and NERSC clusters are gratefully acknowledged

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A Multiscale Design Strategy for Advance Polymer Dielectrics

Ghanshyam Pilania¹, Chenchen Wang², R. Ramprasad²

¹Materials Science and Technology Division, Los Alamos National Laboratory, NM
87545 USA

²Department of Materials Science and Engineering, University of Connecticut, CT 06269
USA

High energy density capacitors are required for several pulsed power and energy storage applications, including food preservation, nuclear test simulations, electric propulsion of ships and hybrid electric vehicles. The maximum electrostatic energy that can be stored in a capacitor dielectric is proportional to its dielectric constant and the square of its breakdown field. The current standard material for capacitive energy storage is polypropylene which has a large breakdown field but low dielectric constant. We are involved in a search for new classes of polymers superior to polypropylene using first principles computations combined with coarse grain molecular dynamics, effective medium theory and machine learning methods [1]. Essential to this search are schemes to

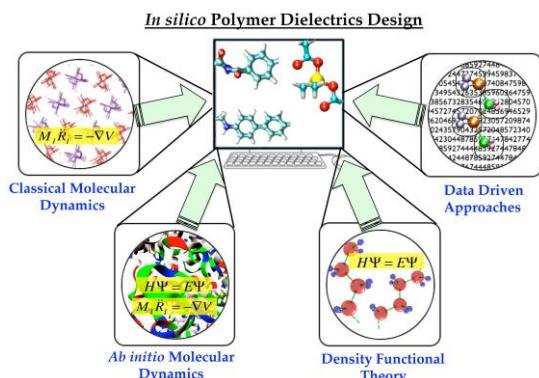


Figure 1: Various components that were used in our computational design strategy for advance polymer dielectrics.

conventional polymer dielectrics [2].

This work was performed under the auspices of Multidisciplinary University Research Initiative (MURI) grant from the Office of Naval Research.

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efficiently compute the dielectric constant of polymers and the intrinsic dielectric breakdown field, as well as methods to determine the stable structures of new classes of polymers and strategies to efficiently navigate through the polymer chemical space offered by the periodic table. These methodologies have been combined with statistical learning paradigms in order to make property predictions rapidly, and promising classes of polymeric systems for energy storage applications have been identified. Some of the polymer polymers predicted using our computational methodology have recently been synthesized and have been shown to have improved dielectric properties over

Unveiling role of salt in Li-ion transfer through boundary between SEI and liquid electrolyte in Li-ion battery: a multi-thousand-atom DFT study

Shuji Ogata,¹ Nobuko Ohba², Takahisa Kouno³

¹Graduate School of Engineering, Nagoya Institute of Technology, Japan

²Toyota Central Research & Development Laboratories, Inc., Japan

³Institute for Solid State Physics, The University of Tokyo, Japan

The solid-electrolytes interphase (SEI), formed on the graphite anode at the first charging, plays essential roles in currently used Li-ion batteries (LIBs). The SEI transfers Li-ions but blocks electron current, and works to prevent further decomposition of the electrolyte. The desolvation and solvation processes of the Li-ion at the interface between the SEI and liquid electrolyte are crucial to determine the throughput rate or power of the LIB. Large-scale, first-principles molecular dynamics (FPMD) simulation of the desolvation/solvation processes is therefore highly desired. The electronic density-functional theory (DFT) is suited well for the FPMD simulation of such dynamics due to its balance between physical accuracy and computation speed. The real-space grid based implementation of the DFT (RGDFT) that uses the finite difference method for derivatives of variables, has attractive features of parallelizability and applicability to various boundary conditions in addition to universality in target materials. Taking the divide-and-conquer strategy we have recently proposed the linear-scaling, divide-and-conquer-type real-space grid DFT code (DC-RGDFT) [1] to further speedup the FPMD simulation.

In this research, we apply the DC-RGDFT to investigate the microscopic mechanisms of the Li-ion transfer through the boundary between the SEI and liquid electrolyte in the LIB by the FPMD simulation [2]. A relatively large simulation system (about 2400 atoms) for the boundary is modeled using di-lithium ethylene di-carbonate (Li₂EDC), ethylene carbonate (EC), and LiPF₆ for the SEI, solvent, and salt, respectively. After inserting Li-ions in the Li₂EDC region, we perform the FPMD simulation for several ps using the DC-RGDFT. In the cases without salt, we find enhanced stability of the Li-ion at the EDC-EC boundary where both EDC and EC molecules bind to the Li-ion, which acts to impede the Li-ion transfer through the boundary. In regard to impedance for the Li-ions, the EDC-EC boundary, which is in reality only about 4 Å in depth, can be regarded as effectively 12-20 Å in depth of bulk EDC. In the case with 1.0 M LiPF₆ salt included in liquid EC, we find that the Li-ion transfer rate through the EDC-EC boundary becomes about twice as high as that in the case without salt. Separate DFT calculations about the reaction energy profiles of small model systems clarify that the energy required to detach a Li-ion from the boundary decreases to 0.9 eV from 1.7 eV if PF₆⁻ exists. The lowering in the detaching energy of the Li-ion results from weakening of the interaction between the Li-ion and EDC due to strong binding of PF₆⁻ to the Li-ion at the boundary. The temperature dependence of the Li-ion transfer rate is analyzed also.

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Unlocking the potential of cation-disordered oxides for lithium batteries

Alexander Urban, Jinyuk Lee, Xin Li, and Gerbrand Ceder

Department of Materials Science and Engineering,
Massachusetts Institute of technology, Cambridge, MA 02139, USA

Ordered lithium metal oxides, especially layered oxides such as lithium cobalt oxide, are the most important class of cathode materials for lithium-ion batteries in consumer electronics. The well-orderedness of these oxides, e.g., the segregation of lithium and metal cations into distinct layers, is commonly regarded as essential for sufficient lithium mobility, and cation mixing has been observed to result in deteriorating lithium extraction and re-intercalation capacity. During the past decades much scientific effort has therefore been geared towards the engineering of novel perfectly ordered cathode materials.

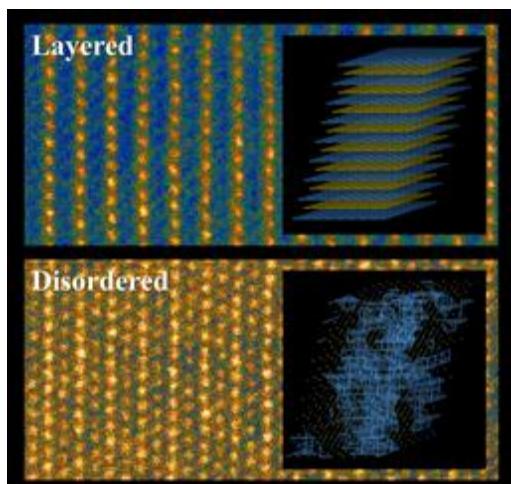


Figure 1: STEM image of layered (top) and cation-disordered (bottom) LMCO. The insets show the 3-d structure of the layered oxide (top) and the percolating network of lithium diffusion channels in the disordered oxide (bottom).

In contrast to these established beliefs we recently found that cation-disordered lithium-excess molybdenum chromium oxide (LMCO) provides a very high reversible electrochemical capacity. Using a combination of first-principles electronic structure calculations and large-scale Monte-Carlo simulations of lithium percolation we are not only able to explain the good performance of LMCO, we can also point out under which conditions cation-disordered lithium-excess materials are likely to exhibit high capacity. This fundamental understanding of lithium diffusion and percolation in lithium metal oxides will open up an entirely new compound space for the search for better lithium-ion battery materials.

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Ab-initio-based Cluster Expansion Study of the Phase Transformation and Voltage Fade of the Layered Li_xMnO_3

Eunseok Lee and Kristin A. Persson

Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

Li_2MnO_3 is believed to be a key material to determine the properties of the ‘Li-excess’ composite materials, which are attracting attention as promising cathode materials for Li-ion batteries. The material is intriguing as it shows electrochemical activity even though the oxidation state of Mn is already Mn⁴⁺. Although several previous studies point to oxygen release, conversion reactions and peroxide formation as possible oxidation mechanisms, none of them has been clarified. In addition, the material experiences the phase transformation from the layer structure to the spinel-like structure during the cycles of lithiation/delithiation. Despite the significant effects of phase transformation on the structural stability and electrochemical performance, the mechanism of the phase transformation has yet been revealed.

In this talk, we present our computational work on the electrochemical activity and structural stability of stoichiometric Li_xMnO_3 ($0 \leq x \leq 2$). The ternary cluster expansion method is used to describe the thermodynamic stability of Li_xMnO_3 and the elastic band method is used to calculate the activation energy barrier of electrochemical kinetics in Li_xMnO_3 . We observe that the Li_2MnO_3 structure is electrochemically active on delithiation and that charge neutrality during the delithiation is maintained by the oxidization of a fraction of the oxygen ions. Furthermore, we also observe that Mn-migration to the Li layer is thermodynamically and kinetically favorable at lower Li content, indicating a tendency towards the spinel structure transformation. Based on our observations, we propose a path of phase transformation from the layered structure to spinel-like structure and explain the mechanism of voltage fade. Oxygen stability is also discussed.

This work was supported by the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Vehicle Technologies of the U.S. Department of Energy, under Contract No. DE-AC02-05CH11231.

Defect substitution energies in cubic barium titanate

Juan J. Meléndez-Martínez¹, Y. A. Zulueta², Y. Leyet³

¹ Department of Physics, University of Extremadura. Badajoz (Spain)

² Departamento de Física. Universidad de Oriente. Santiago de Cuba (Cuba)

³ Instituto Federal de Educação Ciência e Tecnologia, Manaus (Brazil)

The interesting electrical properties of BaTiO₃, which is an electric insulator at room temperature, can be substantially changed by doping. Thus, doping donor impurities may yield semiconducting behavior at low concentrations (typically less than 0.5 at. %) or to improved resistance to dielectric breakdown at higher concentrations [1]. Doping has also been shown to modify the ferroelectric behavior of these ceramics under some conditions [2]. Several types of impurities may be accommodated at different sites in the BaTiO₃, and each substitution mode involves different energetics, structural modifications and changes in physical properties.

Some previous works have dealt with the defect structure of BaTiO₃ based ceramics [3-5]. Most of them are based in Molecular Dynamics (coupled with dipolar corrections for charged defects [6]), and have been able to give some insight into the favorable substitution modes under given conditions. However, *ab initio* calculations have been barely used to characterize defects in BaTiO₃ ceramics [7].

In this work, defect energetics and structure for several substitution modes in Fe-doped BaTiO₃ are studied by *ab initio* calculations performed by a DFT formalism within the Linear Density Approximation coupled with Hubbard-type corrections for strongly correlated electrons. The results are compared and critically analyzed in terms of literature data, and preliminary assessments about the physical behavior of these systems are made.

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Nanostructuring Bi_2Te_3 : influence on the phonon thermal conductivity

Natalia Bedoya, Adham Hashibon, Christian Elsässer

Fraunhofer-IWM, Wohlerstr 11, D-79108 Freiburg, Germany.

The use of thermoelectric materials to recover energy waste in form of heat has been limited so far by the low energy conversion efficiency. Recently, however, a renewed interest in these materials has arisen. An enhancement in their performance has been obtained mainly by lowering the phonon thermal conductivity due to nanostructuring, resulting in size confinement effects of the phonons and interface scattering [1]. The understanding of the vibrational properties of these materials, hence, is a key element to design and tailor their thermoelectrical properties. Here we study, by means of non-equilibrium molecular-dynamics simulations, the effects of dimensionality on the phonon thermal transport in Bi_2Te_3 , the best known thermoelectric material for room temperature applications. In a first stage we analyze the influence of point defects on the phonon thermal transport of bulk Bi_2Te_3 . Four types of defects at different concentrations are considered namely Bi and Te vacancies and antisites. A reduction of up to 50% of the bulk thermal conductivity is obtained, with a weak dependence on the nature of the point defects. The picture of dimensionality is then completed by studying the geometry dependence of the thermal conductivity in Bi_2Te_3 nanowires. All our results are analyzed in terms of the vibrational properties, providing a detailed atomistic study of the phonon thermal transport in the systems considered.

A study of iron impurities interacting with grain boundaries in photovoltaic silicon using density functional theory

Benedikt Ziebarth^{1,2}, Matous Mrovec¹, Christian Elsässer¹, Peter Gumbsch^{1,2}

¹Fraunhofer-Institut für Werkstoffmechanik IWM, 79108 Freiburg, Germany

²Karlsruher Institut für Technologie, Institut für Angewandte Materialien (IAM-ZBS), Engelbert-Arnold-Str. 4, 76131 Karlsruhe, Germany

Iron impurities have a negative effect on the efficiency of silicon-based solar cells because they act as trapping centers for charge carriers. Different processing techniques are applied to improve the efficiency by passivation of the iron contamination. For instance, internal gettering exploits the attractive interaction between the preexisting grain boundaries and the diffusing iron atoms. Therefore, it is interesting and important to build up a fundamental understanding of this interaction mechanism. To this end density functional theory is used to study the segregation mechanism for the impurity atoms at grain boundaries. The set of investigated symmetrical tilt grain boundaries in Si provides a variety of interface orientations and structures at the atomic scale. While some of the grain boundaries show very large segregation energies for interstitial Fe, most of these Si grain boundaries repel single interstitial Fe. Occasionally we find some grain boundaries to favor collective segregation of multiple Fe atoms, which may indicate a potential formation of Fe-Si precipitates at grain boundaries.

Passivation of silicon surfaces by aluminum oxide layers: a simulation study

Francesco Colonna^{1,2}, Christian Elsässer^{1,2}

¹ Freiburg Materials Research Center, University of Freiburg, Germany

² Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

By the Atomic Layer Deposition of Aluminum Oxide on a Silicon (100) surface, followed by a heat-treatment, it is possible to obtain an excellent surface passivation [1], which has the potential to enhance the efficiency of energy conversion in photovoltaic applications.

For a thorough understanding of the passivation process it is necessary to elucidate the interplay between physical properties at the electronic and atomistic scale. To this end we model the Silicon-Alumina interface by means of ab initio density functional theory (DFT) methods. Following experimental observations, we investigate the relation between chemical passivation and the local tetrahedral and octahedral environments in the alumina phase. To this end we simulate a number of stoichiometric and oxygen-rich models of interface between Silicon and α -Alumina, which entails both tetrahedrons and octahedrons as local environments at the interface. We also study the role played by the amount of Hydrogen at the interface, which is known to change during the heat treatment [2]. To obtain an accurate description of defect states in the band gap we refine our electronic structure simulations by applying a state-of-the-art DFT self-interaction-correction.

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A hybrid quantum classical simulation on the diffusivity of Li's in the graphite

Shuji Ogata,¹ Nobuko Ohba,², Takahisa Kouno³

¹Graduate School of Engineering, Nagoya Institute of Technology, Japan

²Toyota Central Research & Development Laboratories, Inc., Japan

³Institute for Solid State Physics, The University of Tokyo, Japan

The Li-graphite intercalation compound is put to practical use as the negative electrode of the Li-ion batteries (LIBs). The transport property of the Li-ion in the graphite is related to the output power of LIBs. We assumed the initial stage of the Li insertion into the graphite and applied the hybrid quantum (QM)-classical (CL) simulation for understandings of the thermal diffusion process of a single Li-ion in the graphite [1, 2]. In this study, the diffusion process of plural Li's in the graphite is analyzed with taking into account the interaction among the Li-ions.

In our hybrid QM-CL simulation, the number of atoms included in the QM-region is minimized within the physical accuracy tolerance, and the QM-region which consists of Li and the surrounding carbon atoms is selected adaptively following the migration of the Li-ion. The number of atoms (N) included in the QM-region increases in the case that plural Li's exist in graphite. Therefore the order-N type of divide-and-conquer-type real-space grid DFT code (DC-RGDFT) [3] is adopted for the QM calculation so as to reduce all calculation cost.

Firstly, seven Li's are placed near into the same layer of graphite. Then the Li's are scattered isotropically by the coulomb repulsion interaction. However, the expanse of the Li-ions is limited to the range of a radius of around 10 Å because of the cage effect. Figure 1 shows the distribution of the inter-layer distance (d) of the upper and lower graphite layers of Li's after 2.5ps hybrid simulation. The inter-layer distance of the graphite of the Li existing domain is longer than that of the domain where there is no Li, i.e., the cage effect is confirmed. An individual Li-ion diffuses well in the cage.

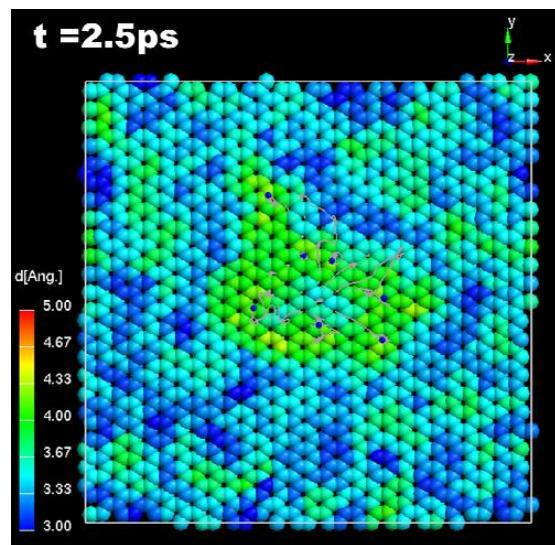


Figure 1: The distribution of the inter-layer distance of the upper and lower graphite layers of Li's after 2.5ps hybrid simulation. The small blue spheres denote Li-ions, the grey lines shows the trajectories of Li's.

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Abstracts