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

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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

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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

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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].

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

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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.

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

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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 <a>, <c> and <c+a> 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 <c> and <a> dislocations is very weak due to the exceptionally low Poisson's ratio. Experimental evidence reported in the literature suggests that the <c+a> dislocations in pyramidal planes can be easily dissociated into <c> and <a> dislocations. We enabled the mechanism of decomposition of pyramidal <c+a> dislocations into prismatic <c> and basal <a> 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], $[\bar{1}\bar{1}20]$ 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.

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

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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.

[1] F. Körmann, A. Dick, B. Grabowski, T. Hickel, and J. Neugebauer, Phys. Rev. B 85, 125104 (2012).

Uncertainty Analysis of Materials Phase Diagrams

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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.

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

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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.

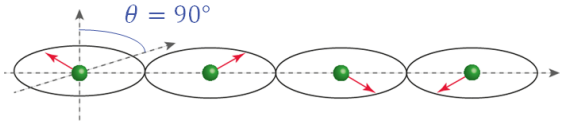

Figure 1: Planar spin spiral. Arrows represent schematic orientation of magnetic moments on atoms (green circles)

[1] A. V. Ruban, V. I. Razumovskiy, Physical Review B 85 (2012) 174407.

Multiscale Modeling of Heat Transport in Glassy and Amorphous Materials

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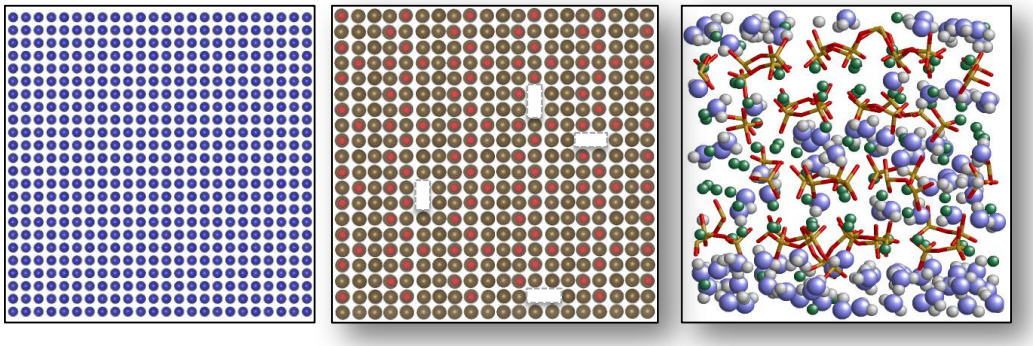
This work presents a bottom-up approach to study heat diffusivity of amorphous and glassy materials from the nano-scale, to the engineering scale. The thermal conductivity of materials originates from the propagation of phonons at the nano-scale and depends strongly on the molecular structure and the 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-hydrae (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.



Solid Argon Defective MgO Amorphous C-S-H

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

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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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