A continuum theory for defect dynamics in metallic glasses

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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

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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

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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.

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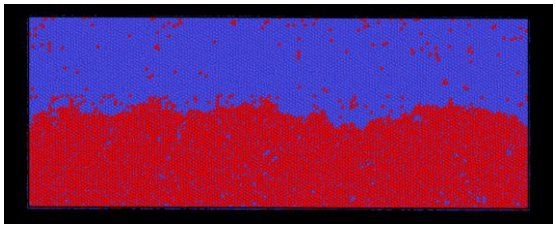

Figure 1: step configuration on a (111) surface of Copper. Red atoms are on the first layer (step).

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Anisotropic geometrical damage for dynamic processes

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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 tripole with standing acoustic wave

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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 tripoles 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 tripoles may be formed by impact of a single dislocation with an immobile dislocation dipole. The structure of the dislocation tripoles is very multiform. We have considered 15 different stable tripole 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 tripoles were found to be mobile under ultrasonic influence. The other dislocation tripoles were either immobile, or rearranged themself 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 tripole 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

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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.

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Atomistic Modeling on Elastic Heterogeneities Evolution and Elementary Activations in Metallic Glass

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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

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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

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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

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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, $Z \approx 10^{-7}$ m^2/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 μm $\leq d \leq$ 10 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

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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

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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**

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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.

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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

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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

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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.

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A mesoscopic stochastic model for micron-scale plasticity

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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

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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 8^{th} 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.

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A Continuum model for dislocation dynamics incorporating Frank-Read sources and Hall-Petch Relation in Two Dimensions

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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.

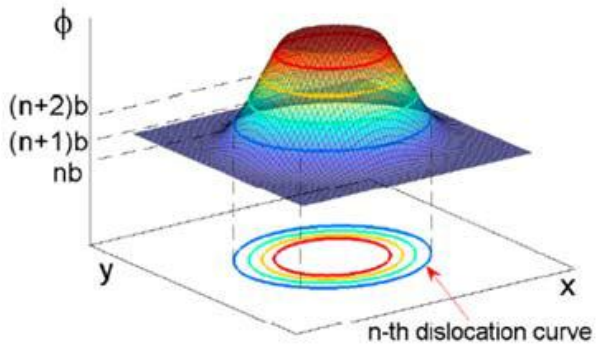

Figure 1: a smooth coarse-grained disregistry function whose contours describe dislocation curves

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 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.

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Modeling polycrystal plasticity using field disclination and dislocation mechanics

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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

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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

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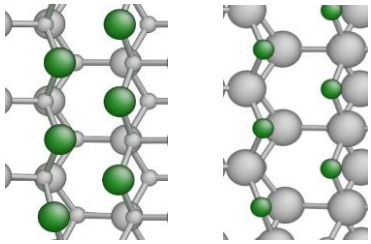
As the third generation core semiconductor material, silicon carbide is attracting more and more attention, for its excellent electricity performance in the high temperature due to the wide bond gap [1]. In device manufacture, one of the main difficulties for SiC devices to reach a larger production 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).



(a) (b)

Figure 1: (a) Si-core. (b) C-core. Stocking faults composed by Si atoms and carbon atoms.

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 Si-core can move easier than C-core [4].Furthermore, we attempt to explain this results though the structures' geometry characteristics.

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Solid phase recrystallization of Si and Ge nanowires

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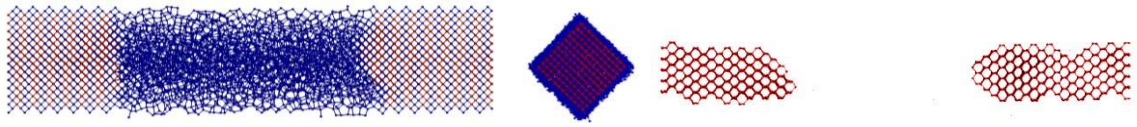
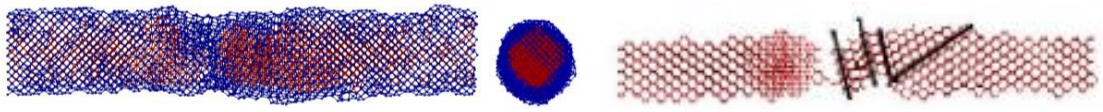
Advanced Si and Ge nanowire transistors can be produced by top-down or bottom-up approaches. In order to obtain the desired electrical properties doping of the nanowires is required. Ion implantation is one of the favored methods to introduce dopant atoms in a controlled manner. If relatively high ion 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].



(a)



(b)

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.

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Large-scale molecular dynamics simulation of microstructure formation during plasma spray process

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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