Materials Aging at Mesoscale: Activated Kinetics and Self-Organized Criticality

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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

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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

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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 $MgSiO_3$ 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 $MgSiO_3$ 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

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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

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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.

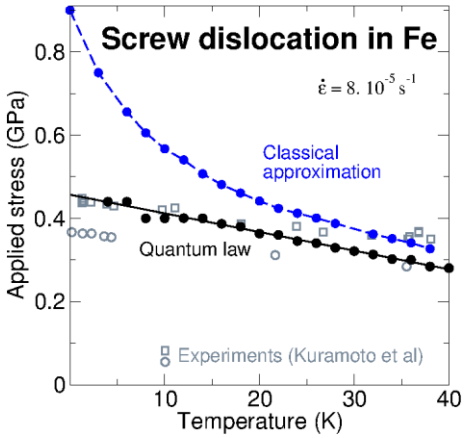

Figure 1: Critical shear stress versus temperature in α-Fe: experimental data from [1], and computed data from classical Orowan law and quantum Orowan law [2].

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

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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

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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 ½ 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 ½ 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 ½ 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 ol LiF [111] single crystals

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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 250ºC, 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 ($\approx 2.5 \cdot 10^{13}$ 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 250ºC. 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

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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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