Grain boundary modeling using an elasto-plastic theory of dislocation and disclination fields

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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 0.1µm/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

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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

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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

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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 pattering 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

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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

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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.

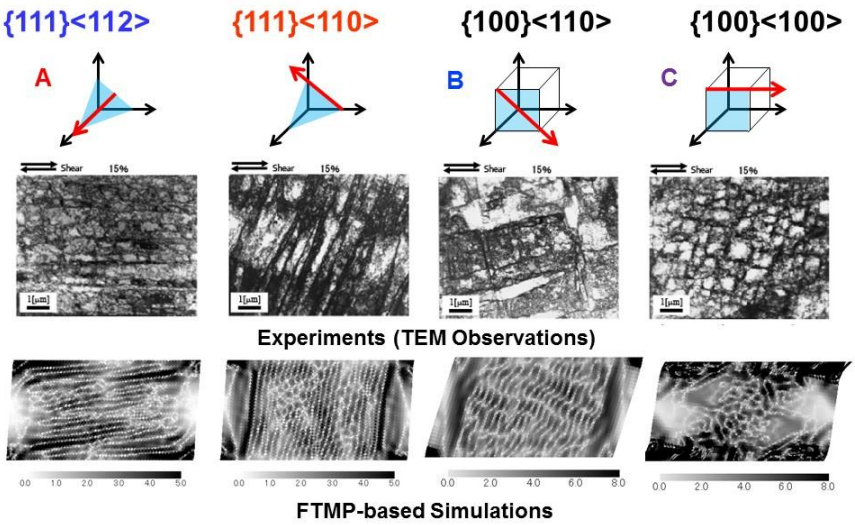

Figure 1: Simulated orientation-dependent dislocation substructures for Fe-Cr alloy single crystal under simple shear, comparing with transmission electron micrographs.

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A Continuum Approach Towards Formation of Persistent Slip Bands During Cyclic Deformation

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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

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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.