Probing Deformation on the Mesoscale Using Submicron-Resolution 3D X-Ray Microscopy and Dislocation Dynamics Simulations

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Formulating a predictive understanding of deformation in ductile materials represents a scientific grand challenge involving the statistical dynamics of interacting dislocations and dislocation densities as they evolve through complex, heterogeneous microstructures on mesoscopic length scales. We have investigated the initial stages of deformation in uniaxially compressed Cu through combined 3-dimensional x-ray microscopy (3DXM) experimental measurements and dislocation dynamics (DD) computational simulations. 3DXM with submicron resolution has been used to make high spatial (0.5 μm) and angular (0.005 degrees) resolution measurements of local lattice rotations in 1% compression-deformed single-crystal Cu over a ~25μm x 25μm x 10μm volume on Sector 34-ID-E of the Advanced Photon Source. To test our ability to predict initial-stage ductile deformation in Cu on an absolute basis, these measurements have been compared quantitatively with DD simulations of compression for a nominally 10μm x 10μm x 10μm volume of Cu using the microMegas discrete dynamics code and coarse-graining the simulations to the 0.5 μm three-dimensional spatial resolution of the 3DXM experimental measurements. Absolute comparisons between experimental measurements and DD simulations of local lattice rotations, spatially resolved geometrically necessary dislocation densities, and spatial correlations of the geometrically necessary dislocation densities will be presented. Good quantitative agreement (on a statistical basis) observed between the 3DXM measurements of these quantities in Cu and the DD simulations, without adjustable parameters, will be discussed along with the outlook for future directions.

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Multiplication mechanisms and topology changes of interacting dislocation densities investigated by Discrete Dislocation Dynamics

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The plastic deformation of crystalline structures such as metals is based on the movement of individual dislocations and during the process complex networks evolve. The further deformability of the specimen depends on the mobile dislocation density which is either produced by artificially introduced Frank-Read sources in the beginning or by naturally formed dislocation sources as a result of glissile reactions [1].

In Discrete Dislocation Dynamics (DDD) simulations [2], most of the time the influence of these natural sources is neglected or negligible [3], although their contribution to the accumulated dislocation density as well as overall plastic deformation is approx. 15% (Fig. 1, green), suggesting that they are rather active sources.

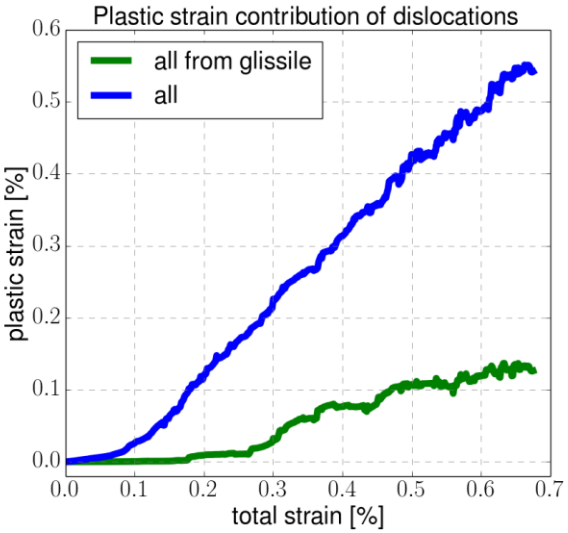

Figure 1: Plastic strain contribution from all dislocation resulting from glissile reactions (green) and total plastic strain produced by dislocations (blue) in tensile direction.

We track the activity of these sources during various loading conditions, different initial configurations (e.g. artificial and relaxed) and with different specimen sizes by DDD simulations and map their occurrence accordingly. An in-depth analysis of the resulting microstructures and their influence on plastic deformation of different specimen configurations as well as the dependency on sample dimensions is presented.

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[1] D. Weygand et al., Mat. Sci. Eng. A **400-401**, 158 (2005)
[2] D. Weygand et al., Model. Simul. Mater. Sci. Eng. **10**, 437 (2002)
[3] C. Motz et al., Acta Mat. **57**, 1744 (2007).

The Discrete-Continuum Model: An important breakthrough to simulate the mechanical properties of dislocated crystals with complex boundary conditions

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Plastic deformation of crystalline materials is the result of the collective movement of dislocations, in response of their mutual interactions, external applied loading and interactions with boundaries such as free surfaces, interfaces or grain boundaries. The dislocation microstructures emerging from such dynamics are intrinsically heterogeneous and the way they affect the mechanical properties is a puzzling problem. Therefore, the development of effective models for the study of this multiscale problem is a challenge in materials science.

A reliable tool to simulate crystal plasticity at the mesoscopic scale is the Discrete-Continuum Model (DCM). The DCM is based on a coupling between 3D Dislocation Dynamics (DD) simulations and Finite Element (FE) method. In particular, the DD simulation code is in charge of the dislocation microstructure evolution and dislocation short-range interactions, while long-range internal stress, displacement field, and boundary conditions (including surface and interface effects) are handled by the FE simulation code.

The DCM, which was proposed first in 1999 [1], has been significantly improved during the last two years [2]. It is now possible to handle problems with very large number of dislocations (the performances of the DCM algorithm overcome the multipole algorithm gain with large number of segments), to use non-regular FE meshes, to precisely take into account the influence of finite or periodic boundary conditions and consider isotropic and anisotropic elasticity.

Here, the new capabilities of the DCM are presented and illustrated with recent calculations made for Cu micro-samples and a SiGe nanostructure. With these examples, we show how the DCM is suitable to study plastic deformation in micro- and nano-objects. In particular, the calculation performed for the SiGe nanostructure highlights the attractive capability of running DD simulation in a full FE framework, using anisotropic elasticity.

[1] C. Lemarchand, B. Devincre, L. Kubin, and J.-L. Chaboche. In « Multiscale Modelling of Materials », vol. 538, pp. 63–68. MRS, Warrendale, Pennsylvania, 1999.
[2] A. Vattré, B. Devincre, F. Feyel, R. Gatti, S. Groh, O. Jamond, and A. Roos. Journal of the Mechanics and Physics of Solids, vol. 63, pp. 491–505, 2014.

Numerical Simulation of Glide Dislocations in Persistent Slip Band

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This contribution deals with the material imperfections in nanoscale having the line character, i.e. the crystallographic arrangement of atoms is disturbed along the dislocation line. Dislocations are modeled as smooth closed or open planar curves evolving in time and space [1]. Their motion is driven by the mean curvature flow

$$Bv = T\kappa + F ,$$

where v denotes the normal velocity, κ is the mean curvature and F is the sum of all force terms acting on the dislocation curve in the normal direction. In this model B denotes the drag coefficient and T stands for the line tension.

In this work two unlike dislocations gliding in parallel slip planes in the channel of the persistent slip band are considered. The interaction between the dislocation and the channel wall is represented by elastic field of rigid dipoles, which act as potential wells. As the dislocations are pushed by the applied stress between two walls in the opposite directions, they bow out and attract each other forming a dipole. With the increasing stress the dislocations become more and more curved, until they separate. The objective is to determine the passing stress in the channel needed for the dislocations to escape one another and compare the generated stress field in the stress and strain controlled regimes. In the stress controlled regime the stress in the channel induced by boundary conditions is assumed to be uniform. In the strain controlled regime the sum of elastic and plastic strain is taken to be uniform. The stress control provides an upper estimate of the passing stress, whereas the strain control yields a lower estimate.

For numerical simulations we explore the parametric approach and semi-implicit flowing finite volume method [2]. However, the parametric approach itself exhibits unintended behavior, since during the time evolution, the grid points tend to accumulate in certain segments of the curve and can be sparse in some other segments. We overcome this problem by adding the tangential velocity to the parametric equations, which moves the grid points along the dislocation curve. Since the tangential terms do not affect the shape of the evolved curve, we can achieve better numerical stability.

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[1] P. Pauš and M. Beneš, *Direct Approach to Mean Curvature Flow with Topological Changes*, Kybernetika, Vol. 45, No. 4 (2009).
[2] M. Beneš, J. Kratochvíl, J. Křišťan, V. Minárik and P. Pauš, *A Parametric Simulation Method for Discrete Dislocation Dynamics,* European Physical Journal ST, 177 (2009).

Dislocation-Dynamics based constitutive equations for crystalline plasticity of BCC metals at low temperature

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Based on recent Dislocation Dynamics (DD) simulations, we propose a set of constitutive equations for crystalline plasticity in iron at low temperature. Assuming that the flow stress is controlled by the mobility of screw dislocations, the equations account for the strain rate sensitivity to the applied stress, temperature and microstructure parameters, such as the dislocation density and the average length of screw dislocation segments. The model differs from the Kocks-Mecking formalism in the sense that strengthening is not always conditioned by the dislocation line tension. It is shown that the difference in mobility between screw and non-screw dislocations impacts the average spacing and the strength of obstacles, which become a function of the temperature. This crystalline law is used in homogenization computation and in Finite-Element simulations to predict the mechanical response to tensile load of iron polycrystals and single crystals as a function of temperature. The predicted temperature dependency of the yield stress of polycrystals and of the critical stress of single crystals is in close agreement with experimental results. Furthermore, the model offers a smooth transition towards the Kocks-Mecking formalism known to capture the main physical features of plastic deformation in the athermal regime.

Discrete dislocation analysis of dislocation interactions with voids and precipitates

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Material defects alter the evolution of dislocations by directly impeding their motion and perturbing the homogenous elastic fields of the bulk crystal. The small scale plasticity occurring in the vicinity of crystal defects is dependent on the motion of individual dislocations and is therefore well suited to models where plasticity is explicitly captured by the motion of discrete dislocations. In this work we study small scale plasticity near micron sized voids and impenetrable precipitates using the discrete dislocation approach of van der Geissen and Needleman[1] where the linear elastic fields due to dislocations in an infinite bulk crystal are superimposed onto the linear elastic fields produced by an auxiliary boundary value problem (BVP) containing the corrective image tractions on free surfaces and polarization stress due to the difference in material properties. The dislocation dynamics (DD) are simulated with ParaDiS from Lawrence Livermore National Lab [2], and the corrective BVP is solved using a parallel finite element (FE) code developed at ARL [3]. Both codes execute independently while a two-way parallel communication of elastic fields is performed through a distributed shared memory based virtual file driver. This allows ParaDis to perform dynamic load balancing to address the heterogeneous nature of dislocation motion and multiplication while the FE BVP solver utilizes a static domain decomposition strategy. In this presentation, we will discuss details of the DD-FE simulator and timings for the various components of the coupled DD-FE simulator including the FE linear solver.

We will use the FE-DD code to simulate dislocations interacting with inhomogeneities in three dimensions. Paradis allows us to model high dislocation densities in 3D and the parallel FE code will allow us to simulate large domains with finely resolved inhomogeneities. These simulations will be used to determine strain hardening mechanisms in crystal plasticity associated with Orowan strengthening and forest hardening. The role of inhomogeneity shape, size and density on the strain hardening mechanisms will also be studied. We would also like to study the effect of dislocation nucleation from the void or precipitate and its role in forest hardening.

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[1] E. van der Giessen and A. Needleman, Model. Simul. Mater. Sci. Eng. **3**, 689 (1995).
[2] A. Arsenlis *et al.*, Model. Simul. Mater. Sci. Eng. **15**, 553 (2007).
[3] J.C. Crone *et al*., Model. Simul. Mater. Sci. Eng. (Accepted 2014).

Anisotropic elasticity in dislocation dynamics

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The dislocation dynamics (DD) method models dislocations behavior, interactions and evolution in BCC and FCC materials. It is used to predict the strength of a material that varies with pressure, strain rate, temperature and evolving dislocation density by providing input parameters to continuum based approaches. Continuum models based on constitutive equations built using dislocation dynamics and molecular dynamics data have been successfully compared to high energy physics experiments in BCC tantalum and vanadium.

Large scale dislocation dynamics simulations usually involve several millions of interacting dislocation segments. The stress at a point and interaction force between two segments need to be computed many times during simulations. Up to now, DD simulations were restricted to isotropic elasticity calculations because using anisotropic elasticity was perceived as too expensive. We evaluate the cost versus accuracy of using spherical harmonics series to approximate the anisotropic elastic Green's function in calculating stresses and forces between segments. The stress at a point is obtained by analytically integrating the spherical harmonics series once and the forces by integrating it analytically twice. We analyze the convergence and cost of using this approach and describe the elements of a fast implementation.

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Discrete dislocation dynamics with anisotropic elasticity

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Discrete dislocation dynamics simulations have been generally limited to modeling systems described by isotropic elasticity. Effects of anisotropy on dislocation interactions, which can be quite large, have been ignored because of the computational expense involved when including anisotropic elasticity. We present a different formalism of dislocation dynamics in which the dislocations are represented by steps in the deformation tensor. The deformation tensor is a direct measure of the slip in the lattice caused by the dislocations and can be considered as an eigenstrain.[1] The stresses arising from the dislocations are calculated with a fast-Fourier transform method,[2,3] from which the forces are determined and the equations of motion are solved. Because FFTs are calculated on a grid, there are some uncertainties that will be discussed. A notable advantage of this approach is that there is no computational penalty for including anisotropic elasticity. We will review the method and discuss applications.

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[1] T. Mura. *Micromechanics of Defects in Solids* (Martinus Nijhoff, Boston, MA, USA, 1987).
[2] J. C. Michel, H. Moulinec, and P. Suquet. "A computational scheme for linear and non-linear composites with arbitrary phase contrast," International Journal for Numerical Methods in Engineering, 52:139–160, 2001.
[3] R. A. Lebensohn, K. Kanjarla, A, and P. Eisenlohr. An elasto-viscoplastic formulation based on fast fourier transforms for the prediction of micromechanical fields in polycrystalline materials. International Journal of Plasticity, 32-33:59–69, 2012.

Statistical properties of the velocity of dislocations

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In phenomenological theory of the evolution equation of dislocations quantities like mobile/immobile dislocations are often introduced. This quantities, however, are difficult to define on a quantitative manner. Since they are closely related to the velocity distribution of dislocations for a deeper understanding of the physical origin of the phenomenological dislocation theories it is of key importance to study the statistical properties of the velocity of dislocations.

In the first part of the presentation some analytical properties of the probability distribution of the velocity of dislocations are discussed. It is shown that the distribution has an inverse cubic tail. The theoretical result is verified by discrete dislocation dynamics simulations and experimental results on 2D crystals.

In the second part the time evolution of the velocity distributions obtained by 2D and 3D discrete dislocation dynamics simulations are analyzed during the relaxation of an initially random dislocation system [2] and under monotonic loading [1]. It is demonstrated that the velocity distribution exhibits power law type of scaling properties with a cut of depending on the system size.

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[1] Ispanovity PD, Groma I, Gyorgyi G, Csikor FF, Weygand D, Phy. Rev. Letters, **105**, 085503 (2010)
[2] Ispanovity PD, Groma I, Gyorgyi G, Szabo P, Hoffelner W, Phys. Rev. Letters **107**, 085506 (2011)