# INFLUENCE OF GRAIN BOUNDARIES ON THE DEFORMATION OF POLYCRYSTALS IN A DISLOCATION DENSITY-BASED PLASTICITY FORMULATION

**A. Arsenlis[a†], V. V. Bulatov[a], R. Becker[a], and D. M. Parks[b]**

[a]University of California
Lawrence Livermore National Laboratory
P. O. Box 808
Livermore, CA 94551-0808

[b]Department of Mechanical Engineering
Massachusetts Institute of Technology
77 Massachusetts Avenue
Cambridge, MA 02139

The mechanical behavior of polycrystals is determined by the evolution of dislocation density and the interaction of that density with itself, grain boundaries, other microstructural features, under the applied stress. In large representative volume elements (RVE's), the evolution of the dislocation density is predominantly statistical in nature and governed by generation and annihilation processes. The plastic deformation characteristics of large RVE's result from the statistical interactions between the dislocation density that has evolved within the RVE over time and the microstructure of the polycrystal. In small RVE's, the evolution of the dislocation density in the volume not only depends on the statistical processes of generation and annihilation occurring within the volume, but also on the divergence of the dislocation density convecting through the volume. The plastic deformation characteristics of small RVE's result from interactions between the dislocation density currently in the volume that may have originated elsewhere in the crystal and the local microstructure in the RVE. The relative size of the RVE may be gauged by the relative contributions of the statistical processes and dislocation density flux divergence to the evolution of the dislocation density state within the volume.

A dislocation density-based crystal plasticity formulation intended to model the plastic behavior of small RVE's is developed that enables the dislocation density to convect across neighboring volumes elements. The finite element implementation of the formulation requires the introduction of additional nodal degrees of freedom associated with the dislocation density field variables and their fluxes. Along with the traction/displacement boundary conditions needed to solve the equilibrium equations in conventional plasticity models, this higher-order model introduces dislocation density/density flux boundary conditions that must also be specified to solve a general boundary value problem. A material-length scale dependence in the behavior of the model may be incorporated through the addition of configurational stresses that depend on spatial gradients of the dislocation density field, such as those proposed by Gurtin(2000) and Menzel and Steimann (2000). The absorption, transmission, and emission of dislocations at grain boundaries can be explicitly modeled in the formulation through a mixture of the dislocation density/density flux boundary conditions. The influence of grain boundaries on the mechanical behavior of polycrystals is investigated through a series of simulations on idealized two-dimensional crystals.

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[†]corresponding author: Email: arsenlis@llnl.gov FAX: (925) 424-5205