Multiscale Modeling of Dislocation/Grain Boundary Interactions

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The interaction of dislocations with grain boundaries (GBs) determines a number of important aspects of the mechanical performance of materials, including strengthening and fatigue resistance. Dislocations and GBs are both non-crystalline defects, and so their fundamental interactions must be studied at the atomistic level. However, dislocation pile-ups in the lattice or in the GB can exert significant additional stresses that could influence the local dislocation/GB interactions. Modeling methods for this problem must thus be multiscale in nature, both to remove the effect of artificial boundaries that usually arise in fully atomistic-scale models, such as molecular dynamics, and to handle the large-scale pile-up behavior. In this talk, we present a multiscale method, the coupled atomistic/discrete-dislocation method (CADD), to study dislocation/grain-boundary deformation, specifically the interaction of edge, screw, and mixed dislocations with Σ3, Σ11, and Σ9 symmetric tilt boundaries in Al [1,2,3]. The goals of the work are (i) to extend the scope of generic "rules" for dislocation transmission through boundaries and, moreover, (ii) to extract general trends and phenomena that can be incorporated into higher-scale models via appropriate constitutive models, both under applied load levels that would be typical in applications. Unfortunately, the complexity of the specific interactions of dislocations at the grain boundary can be staggering. Of general importance, however, is the overall stress state on the boundary - the resolved stresses along the GB plane also have an influence on the evolution of the system. For the low-energy Σ3 and Σ11 boundaries, lattice dislocations can be absorbed and the deformation accommodated by the creation of extrinsic grain boundary dislocations (GBDs). For the Σ9 grain boundary, which is composed of a more complex set of structural units, dislocations absorbed at the boundary remain localized without GBDs, and subsequent transmission and reflection are observed with increasing load and pile-up size. The overall outcomes of the work are an extended set of "rules" for transmission and a "yield surface" for transmission that depends on various components of the local stress tensor, GB step energies, residual Burgers vector, and other local measures at the GB/dislocation intersection region.

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2. M. P. Dewald and W. A. Curtin, "Multiscale Modeling of Dislocation/Grain-Boundary Interactions: II. Screw Dislocations Impinging on Tilt Boundaries in Al", Phil. Mag. 87, 4615-4641 (2007).
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