Overview of recent results in simulation of dislocation nucleation

Introduction
As material microstructure progresses towards nanometer scale dimensions to achieve enhanced functional properties, understanding the mechanical behavior of materials at these scales (Fig. 2) makes atomistic simulations a very attractive tool for examining the inelastic deformation mechanisms in this regime (Fig. 3). Of particular interest is the heterogeneous dislocation nucleation from grain boundaries in nanocrystalline materials (Ref. 1, 2). Additionally, homogeneous dislocation nucleation in single crystals can also provide insight into plasticity at atomic-level length scales.

Simulation Methodology
Grain Boundary (GB) Dislocation Nucleation
In the research, atomistic simulations for dislocation nucleation in grain boundaries are performed in the following steps:
1. Generate the 3D periodic configuration by specifying lattice orientations and dimensions (Fig. 5).
2. Obtain the grain boundary structure using molecular statics calculations. Over 2,500 configurations are sampled to find the minimum energy structure (Ref. 3.4).
3. Equilibrate the configuration for 10,000 fs at temperature of interest (10 K or 300 K).
4. Deform under a uniaxial tensile load applied perpendicular to the boundary at a strain rate of 10^-2/s. Dimensions in the boundary plane are controlled via NPT boundary conditions (stress-free).

Grain Boundary Structure Results
The structure (Fig. 8), energy (Fig. 9) and free volume (Fig. 10) of symmetric and asymmetric tilt grain boundaries can provide insight into interfacial properties, such as dislocation nucleation.

SC Dislocation Nucleation Results
Simulations of homogeneous dislocation nucleation in single crystals (Fig. 11) indicates the importance of active slip system and conditions (Fig. 12) as well as providing insight into the combined behavior of orientation and heterogeneities at the nanoscale.

Temperature dependence
We have used activation energy and activation volume to account for the temperature dependence of dislocation nucleation (Ref. 1.8).

GB Dislocation Nucleation Results
The mechanisms of dislocation nucleation in grain boundaries depends greatly on the boundary structure and facing (Figs. 13, 14). The stress required for dislocation nucleation depends on both the boundary character and adjoining lattice orientation.

References

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