Society of Engineering Science 51st Annual Technical Meeting

1–3 October 2014

Purdue University, West Lafayette, Indiana, USA

Investigation of deformation twins using a DFT-informed 3D phase field dislocation dynamics model

Hunter, Abigail, ahunter@lanl.gov; Beyerlein, Irene, Los Alamos National Laboratory, United States

ABSTRACT

Deformation twinning is a well-known deformation phenomenon in many nanoscale fcc metals. In addition, it is well established that partial dislocations are the basic defect responsible for deformation twins; however, the material parameters that control the inclination to twin and the mechanisms that control twin formation are not well understood. Using a density functional theory (DFT). phase field dislocation dynamics (PFDD) model, we present an unconventional kinetic pathway for twin formation in nanoscale fcc metals that involves two grain boundaries and is active at room temperature and at low strain rates. This work also relates the associated kinetics of nucleation and propagation to intrinsic material defect formation energies.

As mentioned, this research uses a 3D PFDD model informed by DFT to investigate the nucleation and propagation of deformation twins at grain boundaries and interfaces in various fcc metals at ambient conditions. The phase field approach is centered on energy minimization and, hence, evolution of the phase field variables and plastic deformation has a direct dependence on system energetics. This is advantageous for investigating extended dislocations and stacking faults because the PFDD model describes these defects using a parameterized surface (ag material dependent energy landscape that describes the energy maxima and minima that atoms must overcome as they shear pass one another on {111} planes) that surface as simulgis developed for specific materials using points from a ated by ab initio DFT. This incorporates a dependence on unstable SFEs in addition to the commonly used intrinsic SFE. In addition, this establishes a link between atomic-scale numerical methods and the DFT–PFDD model that enables us to follow the dynamics of several nucleating and interacting dislocations based on appropriate calculation of their stacking fault widths and accurately probe the physics that underlies plastic deformation of even the smallest volumes.