Society of Engineering Science 51st Annual Technical Meeting

1–3 October 2014

Purdue University, West Lafayette, Indiana, USA

The relationship between core structure of dislocation and material defect energies in fcc metals

Hunter, Abigail, ahunter@lanl.gov; Beyerlein, Irene, Los Alamos National Laboratory, United States; Zhang, Ruifeng, Iowa State University, United States

ABSTRACT

This research uses an ab initio density functional theory (DFT) informed phase field dislocation dynamics (PFDD) model to investigate the relationship between the dislocation equilibrium core width and the material surface for nine fcc metals. Furthermore, we show that due to an anomalous feature in its -surface, platinum has a fundamentally different core structure than other fcc metals and a much wider equilibrium core width than expected. Based on ab initio valence charge density difference calculations, we attribute this anomaly to distinct differences in the directionality of charge transfer in platinum.

Advantageously, the DFT–PFDD model can account for the entire surface (a material dependent energy landscape that describes the energy maxima and minima that atoms must overcome as they shear pass one another on {111} planes) developed for specific materials through direct connections to 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.