Mesoscale Investigation of Dislocation-Grain Boundary Interactions in Metals and Alloys

Abigail Hunter[a]

[a]*Los Alamos National Laboratory*

[a]*ahunter@lanl.gov*

"Microstructure" refers to the large number of crystal grains and their corresponding boundaries that make up metals and alloys. A material's ability to accommodate stress induced through mechanical loads is dependent on the ease with which dislocations can move through the microstructure to relieve accumulated stress. Grain boundaries (GBs) are the largest impediment to this motion – this is true to some extent regardless of the grain size. The GB structure defines whether a dislocation can transmit across a GB, be partially absorbed at the GB, or glide along the GB and re-emit, altering the GB structure. For poor alignment between grains, dislocations can pile-up against GBs, building localized internal stress regions that work harden the material. This preferential localization of strains and plastic deformation at specific microstructural sites are precursors to damage nucleation. Thus, understanding and predicting dislocation-grain boundary interactions are key for capturing mechanical response, but they are also incredibly complex in part due to the vast number of possible grain boundaries and corresponding dislocation interactions. This talk will focus on recent multiscale modeling efforts addressing dislocation-grain boundary interactions, with particular focus on a mesoscale approach called phase field dislocation dynamics. Connections to both experimental and atomistic efforts will also be discussed, along with methods/approaches that can be used to scale information.

Keywords: Phase Field Modeling, Dislocations, Grain Boundaries, Metals and Alloys, Polycrystal.

Acknowledgment: A. Hunter gratefully acknowledges support from support from the Laboratory Directed Research and Development (LDRD) program of Los Alamos National Laboratory (LANL) under project number 20210036DR.