Atomistic Simulations of Dislocations and Grain Boundaries in Metallic Materials

Prof. Douglas E. Spearot
University of Florida

Abstract

The objective of this presentation is to provide an overview of select atomistic simulation studies in the Spearot research group aimed at the exploration of defect structure and behavior in metallic materials at the atomistic length scale. Following a brief introduction to atomistic simulation methods, two research problems will be highlighted. (1) An atomistic simulation framework to study dislocation – grain boundary interactions is developed that allows dislocation glide loops to be driven into grain boundaries at realistic stresses and velocities. Atomistic energy minimization methods are used to determine the stabilizing stress of dislocation glide loops as a function of loop radius and the Peierls stress for individual segments of the dislocation loop. The algorithm is extended to molecular dynamics simulations and used to determine the temperature dependence of the minimum shear stress required to expand dislocation loops. Combined, this atomistic information is targeted for mesoscale dislocation dynamics simulations. (2) A new approach is presented to select grain boundaries for atomistic analysis. Specifically, sets of grain boundaries will be analyzed whose lattice orientations traverse isocurves within a stereographic triangle associated with critical lattice properties (e.g., elastic stiffness, Schmid factor for primary slip). This provides a route to deconvolute the role of the grain boundary structure on decohesion from the influence of the surrounding lattices, which is a critical issue in the interpretation of atomistic simulations of grain boundary mechanical behavior. This approach is used to study decohesion of pristine Ni grain boundaries and Ni grain boundaries with segregated H. Decohesion behavior is assessed through extraction of traction-separation relationships, employing atomistic cohesive zone volume elements.

Biography

Dr. Spearot is an Associate Professor in the Department of Mechanical and Aerospace Engineering with an affiliate appointment in the Department of Materials Science & Engineering at the University of Florida. From 2005-2015, he was an Associate Professor in the Department of Mechanical Engineering and a member of the Institute for Nanoscience and Engineering at the University of Arkansas. His research centers on the use of atomistic and mesoscale simulation techniques to study the mechanical and thermodynamic properties of materials, with particular focus on the behavior of interfaces and the development of computational tools to extract experimentally relevant material metrics from simulation generated data. Dr. Spearot was awarded the 2010 NSF CAREER Award to elucidate the nanoscale mechanisms associated with phase nucleation during vapor deposition. While at the University of Arkansas, he received the 2014 College of Engineering Imhoff Outstanding Teaching Award and the 2014 Arkansas Alumni Association Rising Teaching Award for classroom excellence. Originally from Bloomfield Hills, Michigan (a suburb of Detroit), Dr. Spearot received his B.S. in Mechanical Engineering from the University of Michigan. He completed his M.S. and Ph.D. degrees in Mechanical Engineering from the Georgia Institute of Technology working with Dr. David McDowell and Dr. Karl Jacob.