Simulations of Fracture at the Atomistic and Nano-Scales.

Diana Farkas [1]

Diana@vt.edu

[1] Department of Materials Science and Engineering

Virginia Tech, Blacksburg, VA 24061, USA

Abstract

We report atomistic simulation studies of crack propagation in various metallic materials with nano-scale features. The simulations are based on empirical interatomic potentials and use massively parallel molecular dynamics techniques at the atomistic level to study the local response of the crack tip. We analyze the results using various models and visualization techniques analyzing the plasticity mechanisms in the crack tip region. A main focus is the competition among the various plastic deformation mechanisms and crack advance and the role played by various nano-scale features.