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Multiscale Modeling of Fracture

W. A. CURTIN, Brown University

Fracture in non-brittle crystalline materials involves material separation at the atomistic scale and dislocation plasticity, with its associated dissipation, occurring over much larger scales. Small-scale plasticity effects associated with dislocation interactions and ordering preclude the application of standard continuum plasticity models. Thus, multiscale models are required to handle the atomistic and mesoscale aspects of the deformation and fracture. Here, we first present the Coupled Atomistic Discrete Dislocation (CADD) model, which is a seamless method for addressing fracture while including the multiscale phenomena, and its extension to finite temperature dynamic modeling. The method is applied to investigate finite-temperature rate-dependent crack growth and dislocation emission in Al, Ni, and Fe. We then present a purely discrete dislocation model, wherein the atomistic region is replaced by a cohesive surface representation, to predict bimaterial interface fracture nucleation and propagation in a variety of geometries.