

## **Molecular dynamics approach for investigation of grain boundary response with applications to continuum simulation of failure in nano-crystalline materials**

Baskar Ganapathysubramanian, Veera Sundararaghavan and Nicholas Zabaras  
Materials Process Design and Control Laboratory  
Sibley School of Mechanical and Aerospace Engineering  
188 Frank H. T. Rhodes Hall  
Cornell University  
Ithaca, NY 14853-3801  
bg74@cornell.edu, vs85@cornell.edu, zabaras@cornell.edu

Finite element models of nanocrystalline microstructures reveal a highly non-linear response dominated by grain boundary accommodation mechanisms. Cohesive interface constitutive laws have been proposed to model the constitutive response of grain boundaries (GBs) and predict failure at grain boundaries. Although these models are inspired by the atomistic mechanics of grain boundaries, the parameters involved in the traction separation laws are often arbitrary. Molecular dynamics is a valuable tool to understand GB response to loading conditions and hence, derive accurate cohesive laws for finite element simulations. This presentation would discuss enhanced models of GB separation and sliding mechanisms based on quasi-static MD simulations in a bicrystal. In the present study, we carried out a series of molecular simulations on an arrangement of constrained atoms in nano-sized bicrystals under loading in order to shed light onto fundamental deformation mechanisms in nanocrystalline GBs, when no thermally activated mechanisms operate. From these models, stress-strain laws of GBs can be extracted. The motivation is to gain understanding of the constitutive response of a GB at the nanoscale and feed cohesive laws to FEM simulations. Simulations of response of nanocrystalline materials under quasi-static loads using the newly developed cohesive laws will be shown.