

# Combined MD and continuum approaches towards modeling inter-granular failure using cohesive zone models<sup>1</sup>

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## ABSTRACT

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 (MD) is a valuable tool to understand GB response to loading conditions and hence, derive accurate cohesive laws for finite element simulations. In a MD study, we carried out a series of simulations on an arrangement of constrained atoms under loading in order to identify traction-separation laws in nanocrystalline GBs. Several dependencies were parametrically studied; these include dependence of grain boundary property on strain rate, mis-orientation, deformation modes (tension or shear), temperature etc. Modified cohesive laws which include thermal, rate dependence and deformation mode effects as provided by MD are presented and bicrystal simulations are initially carried out. These simulations employ a continuum slip theory based model for the interior of the grain. Extension from bicrystals to polycrystals with additional MD studies of cohesive response of tri- and quad- junctions to loading and subsequent incorporation of these effects in cohesive laws will be shown. In addition, we explore recently developed equivalent-continuum models as a framework for extending these laws to the micro- and meso- length scales. These tools employ information-passing schemes, in which the discrete scale is modeled and its gross response is infused into the continuum scale.

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