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Grain Boundary Cohesive Laws as a Function of Geometry VALERIE COFFMAN, Cornell University, JAMES SETHNA, Cornell University — Cohesive laws are stress-strain curves used in finite element calculations to describe the debonding of interfaces such as grain boundaries. It would be convenient to describe cohesive laws as a function of the parameters needed to describe the grain boundary geometry; two parameters in 2D and 5 parameters in 3D. However, we find that the cohesive law is not a smooth function of these parameters. In fact, it is discontinuous at all geometries for which the two grains have repeat distances that are rational with respect to one another. Using atomistic simulations, we extract cohesive laws of grain boundary fracture in 2D with a Lennard-Jones potential for all possible geometries which can be simulated within periodic boundary conditions with a maximum box size. We connect the atomistic result to analytic calculations of fracture toughness as a function of dislocation density.

Valerie Coffman
Cornell University

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