

# Assessing the fracture strength of geological and related materials via an atomistically based J-integral

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## Abstract

Predicting fracture initiation and propagation in low-permeability geomaterials is a critical yet unsolved problem crucial to assessing shale caprocks at carbon dioxide sequestration sites, and controlling fracturing for gas and oil extraction. Experiments indicate that chemical reactions at fluid-geomaterial interfaces play a major role in subcritical crack growth by weakening the material and altering crack nucleation and growth rates. Engineering the subsurface fracture environment, however, has been hindered by a lack of understanding of the mechanisms relating chemical environment to mechanical outcome, and a lack of capability directly linking atomistic insight to macroscale observables.

We have developed a fundamental atomic-level understanding of the chemical-mechanical mechanisms that control subcritical cracks through coarse-graining data from reactive molecular simulations. Previous studies of fracture at the atomic level have typically been limited to producing stress-strain curves, quantifying either the system-level stress or energy at which fracture propagation occurs. As such, these curves are neither characteristic of nor insightful regarding fracture features local to the crack tip. In contrast, configurational forces, such as the J-integral, are specific to the crack in that they measure the energy available to move the crack and truly quantify fracture resistance. By development and use of field estimators consistent with the continuum conservation properties we are able to connect the data produced by atomistic simulation to the continuum-level theory of fracture mechanics and thus inform engineering decisions. In order to trust this connection we have performed theoretical consistency tests and validation with experimental data. Although we have targeted geomaterials, this capability can have direct impact on other unsolved technological problems such as predicting the corrosion and embrittlement of metals and ceramics.

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