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A finite atomistic J-integral and the limits of continuum fracture mechanics

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The extension of fracture mechanics concepts to the atomic scale raises fundamental questions on the validity of continuum-based parameters. In particular, the J-integral relies on assumptions such as infinitesimal crack advance and scale separation, which become questionable when dealing with discrete atomic systems. This work aims to provide a physically consistent formulation of the J-integral at the atomic scale and to identify the conditions under which the continuum description ceases to be applicable.

An energy-based finite formulation is introduced, where the J-integral is evaluated as the potential energy difference between two configurations with slightly different crack lengths under the same critical deformation. The crack increment is defined as the smallest physically admissible advance, corresponding to a single bond-breaking event. Molecular statistics simulations are carried out on single-edge cracked single-crystal silicon specimens, considering geometrically scaled models from the macroscale down to nanometric dimensions. The results are compared with finite element analyses based on the conventional formulation.

The atomistic J-integral is found to be nearly constant across all considered sizes, with a value of about 2.5 J/m², indicating that fracture is governed by a localized bond-breaking mechanism independent of structural scale. Consistently, the fracture process zone exhibits a characteristic size of approximately 0.5 nm, which does not vary with specimen dimensions. In contrast, the continuum J-integral progressively departs from this behavior as the size decreases, with noticeable deviations when the structural dimensions approach the intrinsic length associated with fracture.

These results show that the loss of validity of continuum fracture mechanics originates from the disappearance of scale separation rather than from the inadequacy of a specific fracture parameter. The proposed formulation provides a simple and robust way to evaluate fracture at the atomic scale, without relying on stress or displacement field reconstruction, and establishes a direct link between fracture energy and atomic bond breaking.

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