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Strain Energy Density Approach for Brittle Fracture: From the Nanoscale to the Macroscale and the Breakdown of Continuum Theory

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Objectives
This study proposes a novel strain energy density-based approach to describe brittle fracture in ideal materials from the macroscale down to the atomic scale. The primary goal is to understand the limitations of classical continuum fracture mechanics, which fails at sizes of a few nanometers due to atomic discreteness. Using numerical simulations, the study investigates the behavior of single-crack silicon specimens of varying sizes, assessing the transition from continuum-based to atomistic-based fracture descriptions.
Methodology
The study employs Molecular Statistics (MS) simulations on cracked silicon specimens subjected to Mode I loading. Strain energy density is defined as a function of interatomic potential and averaged over the fracture process zone (FPZ). A gradient attenuation function is used to homogenize atomic strain energy density, allowing comparison with continuum-based fracture mechanics models. The approach is validated through Finite Element Method (FEM) analyses on similar sample geometries.
Results
Results show that the fracture process zone (FPZ) is scale-independent, measuring approximately 0.4 nm. This confirms that brittle fracture is ultimately governed by atomic bond breaking, regardless of specimen size. However, continuum mechanics models fail when the singular stress field length falls below 4-5 times the FPZ. Classical linear elastic fracture mechanics (LEFM) underestimates the critical strain energy density at fracture for specimen widths smaller than 40-50 nm. The newly proposed model, however, remains valid even at the nanoscale.
Conclusions
This study demonstrates that the discrete strain energy density formulation is scale-independent and accurately describes fracture from the macroscale to the atomic level. Continuum-based fracture mechanics fail below a critical size linked to the FPZ, while the atomistic approach remains valid. These findings provide new insights for modeling fracture in nanomaterials and micro/nano-scale devices, emphasizing the importance of considering the discrete nature of matter when predicting mechanical behavior.

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