
Identification of Phase-Field Fracture Models from Molecular Simulations on Silicon

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Abstract

Understanding fracture behavior in silicon is crucial for the development of reliable semiconductor devices. This work aims to identify parameters for different phase-field fracture models using molecular simulations. We conducted molecular static and dynamics simulations to observe fracture processes at the atomic level, focusing on crack initiation and propagation in silicon. The simulation data is then used to calibrate the phase-field fracture model parameters, ensuring accurate representation of fracture mechanics. Our results demonstrate that the calibrated model can predict the fracture path and energy release rates for different crystal orientations. This approach bridges the gap between atomic-scale simulations and continuum-scale modeling, providing a robust framework for predicting fracture behavior in silicon-based materials.

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