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FFT-based phase-field modeling of fracture: Structure-property linkages in brittle heterogeneous microstructures

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Abstract

Designing materials with targeted failure properties requires understanding the interaction between microstructure and fracture resistance, referred to as structure-property linkage. This talk employs a recently developed FFT-based phase-field fracture [1] model to analyze the fracture resistance of statistically heterogeneous microstructures. In the initial step, we focus on brittle materials. Ensembles of two-phase microstructures are reconstructed from statistical descriptors via MCRpy [2] and embedded in virtual specimens to achieve near-stable mode-I crack propagation despite periodic boundary conditions. Far-field J-integral evaluation quantifies the impact of heterogeneities on fracture toughness. Statistical analysis reveals significant correlations between microstructural anisotropy and fracture resistance. Material parameter studies demonstrate that stiffness and toughness contrasts between phases critically influence both the magnitude and variability of fracture resistance. The results provide quantitative structure-property linkages for fracture toughness of heterogeneous microstructures and establish a computational framework for data-efficient fracture property prediction. This approach may guide the design of microstructures with enhanced fracture resistance and enables uncertainty-aware inverse design strategies.

Keywords:

phase-field fracture modeling fracture resistance heterogeneous microstructures structure-property linkages

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