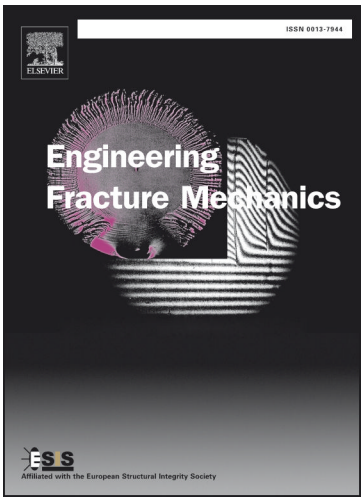

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Atomistic Modelling of Crack-Inclusion Interaction in Graphene

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Abstract

In continuum fracture mechanics, it is well established that the presence of crack near an inclusion leads to a significant change in the crack-tip stress field. However, it is unclear how atomistic crack-inclusion interaction manifests itself at the nanoscale where the continuum description of matter breaks down. In this work, we conducted molecular dynamics simulations to investigate the interactions of an atomic-scale boron nitride inclusion with an edge crack in a graphene sheet. Numerical simulations of nanoscale tensile tests were obtained for graphene samples containing an edge crack and a circular inclusion. Stress analysis of the samples show the complex nature of the stress state at the crack-tip due to the crack-inclusion interaction. Results reveal that the inclusion results in an increase (amplification) or a decrease (shielding) of the crack-tip stress field depending on the location of the inclusion relative to the crack-tip. Our numerical experiments unveil that inclusions of specific locations could lead to a reduction in the fracture resistance of graphene. Results of the crack-inclusion interaction study were compared with the corresponding results of crack-hole interaction problem. The study also provides an insight into the applicability of well-established continuum crack-microdefect interaction models for the corresponding atomic scale problems.

Keywords: Graphene; fracture; inclusion; nanomechanics; crack-tip stress field; molecular dynamics.