

Abstract

This thesis work utilizes the local near-tip stress field at the critical state, just before crack propagation initiation, to measure critical stress intensity factor in crystalline silicon and amorphous silica using atomistic simulations. Compared to the already utilized methods, which employ global overall/remote stress to find critical energy release rate and then relate it to critical SIF, the method used in the present work is more direct as it makes measurements in the near-tip region where crack propagation will indeed initiate.

Furthermore, the local near-tip stress field method is the only way to study crack propagation initiation under mixed-mode conditions in amorphous solids since any global measurement (like remote/overall stress) will be agnostic to individual mode contributions. A crack propagation initiation criteria has thus been derived in the present work by utilizing the near-tip measured stress intensity factors at the critical state. A rigorous validation has been conducted at all stages of this work.

Since the continuum concept of deformation gradient has been used, the methodology developed in the present work can be applied to any other kind of crystalline or amorphous solid. An atom has been considered as a continuum point, and hence, the method does not distinguish between the number or type of elements involved or their atomic structure as a solid.