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Role of Corners in Fracture of Polymeric Adhesives

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Understanding the molecular mechanisms of deformation and failure in structural polymer adhesives is a challenging problem. About a decade ago, we performed MD simulations on coarse-grained models of epoxies or highly crosslinked polymer networks between solid adherends finding very large failure strains in contrast to experimental data. We now have performed similar tensile simulations except with open ends between two solid adherends. The open boundary and the presence of corners dramatically alters the fracture behavior. In contrast to systems with periodic boundaries, the failure strain decreases with increasing system size. This decrease greatly reduces the difference between simulation and experiment. In the open geometry, the sides of the polymer network contract inward forming wedge shaped corners where the crack initiation occurs. The deformation of the open ends is constrained by the minimal paths in the network connecting the two adherends, but the initiation of frature is not related to the minimal paths. The crack initiation in the corners is consistent with a diverging stress in the corners according to fracture mechanics. The local stress in the corners becomes large well before failure, but in the direction parallel to the interface due to the deformation of the corners into the wedge shape.