

Flaw Size Sensitivity of Amorphous Silica Nanostructures

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Abstract:

Silica is an abundant component in many porous materials such as concrete and rocks. A fundamental understanding of the fracturing behavior of Silica at molecular scales is crucial to explain failure mechanisms in these materials. Here we present an investigation into the flaw size sensitivity of amorphous Silica nanostructures, carried out via reactive molecular dynamics (RMD) analyses based on ReaxFFSiO¹, a bond order-based force field. First, an experimentally validated procedure is developed to build the amorphous Silica nanostructures via a melt, quench, and equilibration process to correctly reproduce the molecular structure and mechanical properties of Silica. The validated model is then used to analyze fracture propagation in amorphous Silica samples with varying flaw sizes under mode I tension. The analyses reveal that even at nanoscales, a marked transition from flaw sensitive behavior to flaw insensitive behavior can be observed. The transition flaw size is found to be roughly 25 Angstroms, comparable to prior estimates of the fracture process zone size. For flaw sizes longer than 25 Å, the signature inverse square root dependence of the nominal strength on the flaw size is observed, accompanied by a localized failure. On the other hand, for flaws shorter than 25 Å, damage is more distributed, and the nominal strength remains roughly constant with changing flaw size. In all cases fracture propagation is typically accompanied by the formation of several single atom thick strands near the crack tip, previously reported as “stress fibers”. This is proposed as the likely mechanism causing the transition from flaw sensitive to flaw insensitive behavior, analogous to blunting of macroscale cracks by inelastic damage zones.

¹ Van Duin Et Al (2003). *ReaxFFSiO reactive force field for silicon and silicon oxide systems*, Journal of Physical Chemistry A, 107 (19), 3803-3811