Fracture of sodium-silicate glasses: Insights from atomistic computer simulations

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Abstract

Understanding the fracture behavior of glasses at the atomic scale is of fundamental importance for improving the mechanical properties of these materials. Using an interaction potential that has been parametrized via *ab initio* calculations [1,2], we have carried out molecular dynamics simulations in order to investigate the influences of system size, sample geometry, and strain rate on the fracture behavior of sodium silicate glasses. In contrast to earlier simulation studies on fracture, in which the bulk glass sample has often been put directly under stress, we have applied here uniaxial tension to a glass sample that has stress-free surfaces, i.e. we adopt a setup that is close to the one used in experiments on fracture studies. Our results show that the used interatomic potential captures reasonably well the brittle fracture on the nanoscale of silica glass and the enhanced ductility when sodium oxide is added to the glass network. We have found that below a critical strain rate of around 0.5/ns the stress-strain curve remains basically unchanged. By investigating the formation, growth and coalescence of cavities in the strained glass samples we find that in sodium silicate glasses the formation of cavities is being more pronounced than in silica glass. The analysis of atomic energy, local stress and strain, and atomic displacements have confirmed the presence and the development of mechanically weak zones in the glass network, resulting in paths along which the cracks advance.

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