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Abstract

Alumina (Al_2O_3) and silica (SiO_2) are important network-forming components in many oxide glasses. It is therefore important to understand how these oxides respond structurally and mechanically to applied stresses and strains. Based on molecular dynamics simulations, we here reveal to which extent the propensity of glassy Al_2O_3 and SiO_2 to exhibit nanoscale ductility is encoded in their static structures. We address this by studying the fracture response of a series of glassy Al_2O_3 and SiO_2 systems quenched under varying pressures and cooling rates. We demonstrate that the degree of nanoductility is correlated with the number of bond switching events around Al and Si atoms, and in turn attempt to predict the tendency for bond switching based on classification-based machine learning and topological data analysis. These results are helpful for designing oxide glass formulations with improved resistance to fracture.

Sesssion: mechanical properties