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Abstract

Heavy ion irradiation can modify the surface structure of glasses and consequently their mechanical properties. Here, we attempt to clarify structure-property relations in two families of irradiated glasses. First, in calcium aluminoborosilicate glasses, we use a combination of experiments and atomistic simulations and find that the ion irradiation reorganizes the borate subnetwork through a partial transformation of tetrahedral to trigonal boron units and a coarsening in the distribution of loop structures. This leads to an improvement in both the resistance to crack formation and crack growth as irradiation induces coordination defects that act as local reservoirs of plasticity by allowing more bond switching activities. Second, in organic-inorganic hybrid systems, we simulate irradiation of both zeolitic imidazolate framework crystals and glasses. We track the convergence of the two phases toward a new disordered state upon irradiation, with simultaneous evolution of both structure and mechanical properties. Both studies therefore help to establish structure-property relations in forbidden glass states that are not accessible through any thermal path.

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