Cavitation in Amorphous Solids

MICHAEL FALK, PENGFEI GUAN,
Johns Hopkins University, SHUO LU, Beijing University of Aeronautics and Astronautics, MICHAEL SPECTOR, PAVAN VALAVALA, Johns Hopkins University —

Molecular dynamics simulations of cavitation in a Zr50Cu50 metallic glass exhibit a waiting time dependent cavitation rate. On short time scales nucleation rates and critical cavity sizes are commensurate with a classical theory of nucleation that accounts for both the plastic dissipation during cavitation and the cavity size dependence of the surface energy. All but one parameter, the Tolman length, can be extracted directly from independent calculations or estimated from physical principles. On longer time scales aging in the form of shear relaxations results in a systematic decrease of cavitation rate. The high cavitation rates that arise due to the suppression of the surface energy in small cavities provide a possible explanation for the quasi-brittle fracture observed in metallic glasses. Analogous simulations of Fe80P20 reveal that segregation of P on the nanoscale leads to qualitatively different behavior that may be attributable to the idiosyncrasies of the interatomic potential.