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Application of Classical Nucleation Theory to Cavitation in Metallic Glass

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In order to predict the fracture toughness of amorphous solids such as metallic glasses it is necessary to understand the physics of the process zone. Theories of plastic deformation provide information about response to shear, but on their own these theories provide limited insight into the microscopic mechanisms that mediate the free surface generation critical to crack propagation. Previous molecular dynamics simulations indicate that cavitation likely plays this role. We have undertaken a series of molecular dynamics simulations of cavitation under hydrostatic tension in a binary metallic glass analog using pair-wise potentials. We compare the rate of cavity nucleation directly to homogeneous nucleation theory to examine the role of surface energy and irreversible deformation in the cavitation process. We find that both the reduction of the surface energy at small cavity size and the plastic deformation required for the cavity to grow play important roles in setting the strain-dependent free energy barrier to cavitation.

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