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Multi million-to-Billion Atom Molecular Dynamics Simulations of Cavitation-Induced Damage on a Silica Slab ADARSH SHEKHAR, KEN-ICHI NOMURA, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, Collaboratory for Advanced Computing and Simulations, University of Southern California — Cavitation bubble collapse causes severe damage to materials. For example, cavitation erosion is a major threat to the safety of nuclear power plants. The cavitation bubbles may also be utilized for preventing stress corrosion cracking with water jet peening technology. We have performed multi million-to-billion atoms molecular dynamics simulations to investigate the shock-induced cavitation damage mechanism on an amorphous silica slab in water. The system consists of a 60nm thick silica slab immersed in water in an MD box of dimension 285 x 200 x 200 nm3. A nanobubble is created by removing water molecules within a sphere of radius 100 nm. To apply a planar shock, we assign a uniform particle velocity vp on the entire system towards a planar momentum mirror. We have performed the simulation with two kinds of bubbles, an empty bubble and a bubble filled with inert gas. The simulation results reveal nanojet formation during bubble collapse causing damage on the silica surface; however, the damage was significantly reduced in the case of the filled bubble. We will discuss the effect of the presence of inter gas inside the nanobubble on the pressure distribution, the extent of damage, and collapse behavior corresponding the shock front.

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