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Structure and Dynamics of Shock-Induced Nanobubble Collapse in Water MOHAMMAD VEDADI, AMIT CHOUBEY, KEN-ICHI NOMURA, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, University of Southern California, ADRI VAN DUIN, Pennsylvania State University — Structure of water under shock and shock-induced collapse of nanobubbles in water are investigated with molecular dynamics simulations based on a reactive force field. Shock induces dramatic structural changes, including an ice-VII-like structural motif at a particle velocity of 1 km/s. The incipient ice VII formation and the calculated Hugoniot curve are in good agreement with experimental results. In the presence of a nanobubble, we observe a focused nanojet at the onset of nanobubble shrinkage and a secondary shock wave upon nanobubble collapse. The secondary shock wave propagates spherically backwards and induces high pressure as it propagates. Both the propagation velocity and the induced pressure are larger than those of the primary shock. We explored effects of nanobubble radius and shock amplitude on nanojet formation. The nanojet size increases by increasing particle velocity but the effect of increasing radius is more significant. The jet length scales linearly with the nanobubble radius, as observed in experiments on micron-to-millimeter size bubbles. Shock-induced collapse of a nanobubble in the vicinity of a cell membrane creates a transient nanopore when the nanojet impacts the membrane. Transient cell poration has potential applications in drug delivery.

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