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Molecular dynamics and continuum studies of shock-induced pore collapse in TATB TOMMY SEWELL, PUHAN ZHAO, University of Missouri, S. LEE, H.S. UDAYKUMAR, University of Iowa — Molecular dynamics (MD) and continuum simulations, performed using LAMMPS and SCIMITAR3D, respectively, were used to study thermo-mechanical aspects of shock-induced pore collapse in oriented single crystals of TATB. The simulations were performed using (almost) the same system dimensions, and exactly the same pore size/location and impact speeds, to enable close comparisons between the atomistic and continuum predictions. Two impact speeds, 1 km/s and 2 km/s, were used to generate the shocks; these yield predominantly visco-plastic and hydrodynamic-like collapse, respectively. The initial pore, with a diameter of 50 nm, was located at the center of a sample that was 150 nm 150 nm along two edges. The MD simulations were "quasi-2D" with a length of ≈4 nm in the third direction (≈300,000 fully flexible molecules) whereas the continnum simulations were 2D. For the MD studies, three crystal orientations (i.e., shock-propagation directions) were studied that span the limiting cases with respect to the crystal anisotropy. For the continuum simulations an isotropic constitutive model was used, thereby requiring only two simulations per impact strength (two different specific heat models were used). The evolution of spatio-temporally resolved properties during collapse will be reported including local stress tensors, temperatures, pore size and shape, and velocity fields.

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