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Shock Propagation Modeling in Heterogeneous Materials[1]

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Shock compression of foams is an intriguing research area that challenges our abilities to model experiments using computer simulations that span 9 orders of magnitude in spatial scales from the atomistic scale through the mesoscale and up to the continuum levels. Experiments test shock compression of dense polymers, polymer foams, and high-Z doped foams. Random distributions of polymer fibers, variations in pore size, and non-uniformities in the bulk properties of the foam (such as mean density) lead to spread in the experimental data. Adding dopants to foams introduces new complexities and the effect of the distribution and sizes of dopant particles must be characterized and understood. Therefore we turn to computer simulation to illumine the intricacies of the experiments that cannot be directly measured. This paper overviews of our range of methods to model pure and platinum-doped poly-methyl-pentene (PMP) foams. At the nanometer scale, hydrodynamic simulations compare favorably to classical molecular dynamics (MD) simulations of porous foams, verifying models of foam vaporization under strong shock conditions. Inhomogeneous mesoscale and homogenized continuum simulations present contrasting pictures of shocked foams. Mesoscale simulations at the micron scale have diffuse shock widths that depend upon the pore size, and post-shock vorticity results in fluctuations about the mean post-shock state and lower mean pressures and temperatures. Homogenized simulations, in the limit of zero pore size, have narrow shock widths, steady post-shock states, and higher mean pressures and temperature that compare favorably with 1D analysis of experiments. We reconcile the contrasting mesoscale and continuum views using theoretical turbulent corrections to the Hugoniot jump condition to show a consistent picture of shocked foams over 9 orders of spatial scale.

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