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Properties of Shocked Polymers: Mbar experiments on Z and multi-scale simulations[1]

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Significant progress has been made over the last few years in understanding properties of matter subject to strong shocks and other extreme conditions. High-accuracy multi-Mbar experiments and first-principles theoretical studies together provide detailed insights into the physics and chemistry of high energy-density matter. While comprehensive advances have been made for pure elements like deuterium, helium, and carbon, progress has been slower for equally important, albeit more challenging, materials like molecular crystals, polymers, and foams. Hydrocarbon based polymer foams are common materials and in particular they are used in designing shock- and inertial confinement fusion experiments. Depending on their initial density, foams shock to relatively higher pressure and temperature compared to shocked dense polymers/plastics. As foams and polymers are shocked, they exhibit both structural and chemical transitions. We will present experimental and theoretical results for shocked polymers in the Mbar regime. By shock impact of magnetically launched flyer plates on poly(4-methyl-1-pentene) foams, we create multi-Mbar pressures in a dense plasma mixture of hydrogen, carbon, at temperatures of several eV. Concurrently with executing experiments, we analyze the system by multi-scale simulations, from density functional theory to continuum magneto-hydrodynamics simulations. In particular, density functional theory (DFT) molecular dynamics (MD) and classical MD simulations of the principal shock Hugoniot will be presented in detail for two hydrocarbon polymers: polyethylene (PE) and poly(4-methyl-1-pentene) (PMP).

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