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Mesoscale simulations of shockwave energy dissipation via chemical reactions EDWIN ANTILLON, ALEJANDRO STRACHAN, Purdue University — We use a particle-based mesoscale model that incorporates chemical reactions at a coarse-grained level to study the response of materials under shockwave-loading conditions. An additional implicit variable (the particle size) is used to describe volume-reducing chemical reactions using an intra-molecular potential inspired by Transition State Theory, while the dynamics of the center-of-mass motion evolves according to inter-particle forces. The equations of motion are derived from a Hamiltonian and the model captures both: total energy conservation and Galilean invariance. We demonstrate that this model captures complex thermo-mechanical-chemical processes, and we use these features to explore materials with the capabilities to dissipate shocks-wave energy due to ballistic impacts. Our results characterize how the parameters of the chemical model affect shock-wave attenuation, and we elucidate on how the coupling between the different energy-transferring mechanisms influences nucleation of chemistry for conditions away from equilibrium.

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