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Large-Scale Reactive Atomistic Simulation of Shock-induced Initiation Processes in Energetic Materials[1]

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Initiation in energetic materials is fundamentally dependent on the interaction between a host of complex chemical and mechanical processes, occurring on scales ranging from intramolecular vibrations through molecular crystal plasticity up to hydrodynamic phenomena at the mesoscale. A variety of methods (e.g. quantum electronic structure methods (QM), non-reactive classical molecular dynamics (MD), mesoscopic continuum mechanics) exist to study processes occurring on each of these scales in isolation, but cannot describe how these processes interact with each other. In contrast, the ReaxFF reactive force field, implemented in the LAMMPS parallel MD code, allows us to routinely perform multimillion-atom reactive MD simulations of shock-induced initiation in a variety of energetic materials. This is done either by explicitly driving a shock-wave through the structure (NEMD) or by imposing thermodynamic constraints on the collective dynamics of the simulation cell e.g. using the Multiscale Shock Technique (MSST). These MD simulations allow us to directly observe how energy is transferred from the shockwave into other processes, including intramolecular vibrational modes, plastic deformation of the crystal, and hydrodynamic jetting at interfaces. These processes in turn cause thermal excitation of chemical bonds leading to initial chemical reactions, and ultimately to exothermic formation of product species. Results will be presented on the application of this approach to several important energetic materials, including pentaerythritol tetranitrate (PETN) and ammonium nitrate/fuel oil (ANFO). In both cases, we validate the ReaxFF parameterizations against QM and experimental data. For PETN, we observe initiation occurring via different chemical pathways, depending on the shock direction. For PETN containing spherical voids, we observe enhanced sensitivity due to jetting, void collapse, and hotspot formation, with sensitivity increasing with void size. For ANFO, we examine the effect of reaction rates on shock direction, fuel oil fraction, and crystal/fuel oil/void microstructural arrangement.

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