Modeling the anisotropic shock response of single-crystal RDX

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Explosives initiate under impacts whose energy, if distributed homogeneously throughout the material, translates to temperature increases that are insufficient to drive the rapid chemistry observed. Heterogeneous thermomechanical interactions at the meso-scale (i.e. between single-crystal and macroscale) leads to the formation of localized hot spots. Direct numerical simulations of mesoscale response can contribute to our understanding of hot spots if they include the relevant deformation mechanisms that are essential to the nonlinear thermomechanical response of explosive molecular crystals. Analysis of X-ray diffraction is also useful for discerning crystal-scale deformation occurring during the transient high-pressure phase of shock loading.

We have developed a single-crystal model for the finite deformation thermomechanical response of cyclotrimethylene trinitramine (RDX). Because of the low symmetry of RDX, a complete description of nonlinear thermoelasticity requires a careful decomposition of free energy into components that represent the pressure-volume-temperature (PVT) response, and the coupling between isochoric deformation and both deviatoric and hydrostatic stresses. An equation-of-state (EOS) based on Debye theory that defines the PVT response was constructed using experimental data and density functional theory calculations. This EOS replicates the equilibrium states of phase transformation from alpha to gamma polymorphs observed in static high-pressure experiments. Lattice thermoelastic parameters defining the coupled isochoric free energy were obtained from molecular dynamics calculations and previous experimental data. Anisotropic crystal plasticity is modeled using Orowan's expression relating slip rate to dislocation density and velocity.

Details of the theory are presented along with simulations of flyer plate impact experiments, including recent experiments diagnosed with *in situ* X-ray diffraction at the Advanced Photon Source. Impact conditions explored within the experimental effort have spanned shock pressures ranging from 1-10 GPa for several crystallographic orientations. Bragg diffraction patterns are also simulated from the internal state of the material reported by the thermomechanical simulation. These simulation results assist in forming conclusions about the nature of dislocation-mediated plasticity in RDX, as well as, future directions to improve these models and quantitatively compare them to the average lattice response recorded with *in situ* X-ray diffraction.