INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

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High Explosives Science and Technology

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Mesoscale Mechanics of Energetic Materials: A coordinated experiment-theory effort using new *in situ* probes

Weak impacts on high explosives (HE) can give rise to either violent reactions or harmless fracture and material dispersal. Predicting this response or the state of damage in the material remains an unsolved technical challenge. *In situ* mesoscale insights to anisotropic dislocation-mediated plasticity, phase transitions, and damage are needed to quantify fundamental structure-property relationships, inform theory, and enable high fidelity simulations.[1] We have attempted such an effort and will present an overview of our progress so far.

Time-resolved, *in situ* X-ray diffraction (XRD) and phase contrast imaging (PCI) during dynamic loading has been performed for single crystal and plastic bonded formulations of cyclotrimethylene trinitramine (RDX), cyclotetramethylene tetranitramine (HMX), and pentaerythritol tetranitrate (PETN). Laser-driven shock, gas gun, and Split Hopkison Pressure Bar (SHPB) experiments have been performed to span multiple orders of strain rate, using synchrotron (Advanced Photon Source) and X-ray free electron laser (Linac Coherent Light Source) radiation to measure XRD and PCI *in situ*. This range of strain rates enables an investigation of the coupling between crystal mechanics, thermal softening, and microstructure that governs different explosive response in the different regimes from weak shock to subshock impact.

Multiphase single crystal plasticity models for the HE constituents have been developed. They consist of non-linear thermo-elasticity with the purely volumetric portion replaced with a Helmholtz free energy equation-of-state (EOS) based on a sum of Debye models for the inter- and intramolecular vibrational modes.[2, 3] Mobile and immobile dislocation density kinetics are described by the Orowan expression for slip rate using the Austin-McDowell model for dislocation velocity.[4] Multiphase EOS were constructed from pressure-density isotherms while imposing the temperature-presssure dependence of the transition through Gibbs free-energy.[2, 5] Constititutive equations were parameterized with: *i)* pressure-dependent vibrational modes computed from dispersion corrected density functional theory, *ii)* experimental elastic constants and their temperature derivatives, *iii)* pressure derivatives of elastic constants from atomistic calculations, *iv)* all slip systems identified from experiments, and *v)* the plasticity models were fit to velocimetry data from a small subset of available plate impact experiments. These multiphase, single crystal plasticity models are capable of predicting anisotropy, thickness, and pressure dependent effects remarkably well, as illustrated in Fig. 1 by the predicted and measured interface velocimetry for (100) and (210) oriented RDX single crystals as a function of pressure and crystal thickness.[4, 5]

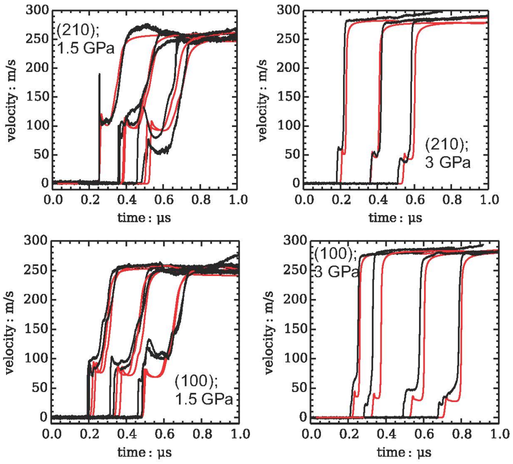

Fig. 1. Measured (black) and predicted (red) interface velocimetry for (100) and (210) oriented RDX single crystals under shock compression.[4]

Combining the new experimental and theoretical capabilities, mesoscale mechanics can be investigated from the average lattice response up in scale toward microstructures of plastic bonded explosives. For the first time, diffraction patterns, such as those presented in Fig. 2, quantify the average lattice response during elastic-plastic and phase transition and allow for direct comparison of experiments and simulations through measured and computed diagnostics. Using the experimentally validated constitutive models, simulation of strain and resulting temperature localization can also be performed and compared to PCI of heterogeneous micorstructure effects such as void collapse and grain boundaries.

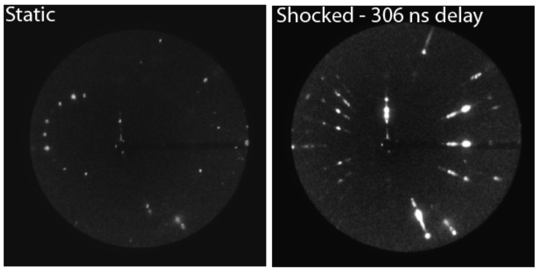

Fig. 2 Single pulse XRD from an RDX single crystal at the APS. The pattern on the right was obtained during shock compression and reveals peak motion, broadening, and additional peaks.

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