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Towards Understanding the Role of Microstructure in Energetic Material Response: Coarse-Grain Modeling and Simulation JOHN BRENNAN, SERGEI IZVEKOV, U.S. Army Research Laboratory, MARTIN LISAL, Institute of Chemical Process Fundamentals of the ASCR, JAMES LARENTZOS, U.S. Army Research Laboratory — Mechanical and thermal loading of energetic material (EM) composites can incite responses over a wide range of spatial and temporal scales due to inherent microscale features. Many energy transfer processes within these materials are atomistically governed, yet the overall material response is manifested at the micro- and mesoscale – scales beyond those amenable to atomistic simulation techniques. Moreover, continuum level approaches rely on field-based formulations that are empirically based, which lack sufficient fidelity to capture microstructure effects. Particle-based microscale simulation methods that utilize coarse-grain models offer a promising route for extending the attributes of atomistic modeling toward the mesoscale. We have developed such microscale methods based upon the constant-energy dissipative particle dynamics method that includes chemical reactions. Coarse-grain models of EMs have been built using the Multiscale Coarse-Graining approach. Time-resolved depictions of an EM responding to insult has been simulated for a variety of microstructures, including samples with intra- and inter-granular voids of varying shape, size and relative orientation, varying grain shapes and sizes, and polymer binder. A sampling of these results will be presented.

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