Abstract Submitted
for the SHOCK13 Meeting of
The American Physical Society

Modeling the Shock Compression of Coarse-Grained RDX using Constant Energy Dissipative Particle Dynamics JOSHUA D. MOORE, SERGEI IZVEKOV, JOHN K. BRENNAN, U.S. Army Research Laboratory, MARTIN LISAL, Institute of Chemical Process Fundamentals of the ASCR, v. v. i. — Mechanical stimulation of energetic materials often incites responses over a wide range of spatial and temporal scales, with a strong dependence upon micron-scale defects. Modeling these materials atomistically remains a challenge due to the length and time scales required, as billions of molecules would be necessary to model micron-size defects. To overcome these challenges, we have implemented multiscale techniques to bridge the atomistic and mesoscale descriptions by coarse-graining RDX through a multiscale coarse-grain force-matching technique, resulting in a density-dependent potential. The resulting model reproduces several atomistic properties, but only those properties which depend on intermolecular interactions. Properties that depend on the coarse-grained intramolecular degrees-of-freedom (d.o.f.) are underestimated. Implementing traditional molecular dynamics to simulate the mechanical response of such models inevitably results in inaccurate energy and momentum exchange due to these unaccounted d.o.f. To correct this, we utilize the constant-energy Dissipative Particle Dynamics method (DPD-E), which provides a mechanism to account for all coarsened d.o.f. through the inclusion of a coarse-grain particle internal energy. This work presents results for shock simulations of RDX using DPD-E with results assessed by direct comparison to fully atomistic simulations.

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Date submitted: 21 Feb 2013 Electronic form version 1.4