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Particle Based Multi-Scale Modeling of the Dynamic Response of RDX JOSHUA D. MOORE, SERGEI IZVEKOV, JOHN K. BRENNAN, U.S. Army Research Laboratory, MARTIN LISAL, J.E. Purkinje University — Modeling the thermal and mechanical response of nanocomposites atomistically, despite growing computational power and resources, remains a challenge due to the length and time scales required. To overcome these challenges, we have used multiscale modeling to bridge the atomistic and microscale levels of description by coarse-graining RDX through force-matching, resulting in density-dependent potentials. The resulting model reproduces several atomistic properties within reasonable agreement from ambient to high pressures for the molecular crystal. Despite this, the model cannot account for accurate energy and momentum exchange due to mechanical stimulation via traditional molecular dynamics due to coarse-graining of the intramolecular degrees of freedom. To correct this, we account for momentum and energy transfer in mechanical shock treatments by utilizing the constant energy Dissipative Particle Dynamics method (DPD-E). In this talk, we will present results for mechanical and thermal shock loading of our MS-CG model of RDX using DPD-E. Various modeling parameters have been investigated for sensitivity. Results will be assessed by comparison to both atomistic simulation and experiment.

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