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Compression and Decompression of RDX [100] via Large-scale Simulation BRIAN BARNES, SERGEI IZVEKOV, N. SCOTT WEINGARTEN, US Army Research Laboratory — Response of single-crystal cyclotrimethylene trinitramine (RDX) to insult in the [100] direction has been a lively topic of investigation due to the shock sensitivity of RDX in that direction. Simulations of [100] shock response have yet to reproduce an experimentally observed phase transition, and experiments have yet to observe shear bands predicted by simulation. It remains an open question as to whether the shear bands are artifacts of the computational model/method, with reality corresponding to another relaxation mechanism such as dislocation-mediated plasticity. RDX response to uniaxial compression is expected to have a transition from brittle failure to plastic response at strain rates approaching shock compression, but this transition has not been identified in molecular simulation. Prediction of explosive initiation is challenging, and “unraveling this unpredictability starts with knowing about plasticity and failure in these materials.” We attempt to make progress toward understanding those observations through large-scale classical atomistic molecular dynamics simulations of RDX. We investigate effects of time scale, boundary conditions, system size, and strain rate on RDX response. We discuss possible comparisons of simulation to experiment.

Brian Barnes
US Army Research Laboratory

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