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Molecular dynamics simulations of uniaxial shock compression of RDX crystals DMITRY BEDROV, JUSTIN HOOPER, GRANT SMITH, University of Utah — Using the Hugoniostat methodology atomistic molecular dynamics simulations of uniaxial shock compressions along [001], [100], and [010] directions of RDX crystal have been conducted over a wide range of shock pressures. The Hugoniostat simulations allow modeling of shocked material without the necessity to have extremely large simulation cell required to explicitly resolve the shock wave propagation. Hugoniostat simulations on systems containing only few thousand molecules allowed us to determine Hugoniot elastic limit and to investigate shock-induced shear banding and phase transition in RDX crystal.

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