Abstract Submitted
for the SHOCK19 Meeting of
The American Physical Society

Anisotropic Thermomechanical Response to Shock Wave Loading in TATB PUHAN ZHAO, University of Missouri, MATTHEW KROONBLAWD, Lawrence Livermore National Laboratory, NITHIN MATHEW, Los Alamos National Laboratory, TOMMY SEWELL, University of Missouri — Molecular dynamics simulations were used to study shock loading in oriented crystalline TATB. The crystal structure consists of planar hydrogen-bonded sheets of individually planar TATB molecules that stack into graphitic-like layers. Shocks were studied for seven crystal orientations, with limiting cases that correspond to propagation exactly perpendicular and exactly parallel to the molecular layers. The simulations were performed for initially pristine crystals using a reverse-ballistic configuration with an impact speed of 1 km/s. Orientation-dependent properties are reported including pressures, temperatures, compression ratios, shock speeds, and local strain rates. Analysis of temperature, stress, material flow, and molecular orientations reveal complicated processes that arise for specific shock directions. The shock response is highly sensitive to crystal orientation, with significant qualitative differences for the evolution of stress and temperature, elastic/inelastic compression response, defect formation and growth, and strain rates. Several inelastic deformation mechanisms are identified, ranging from twinning to dislocation-mediated plasticity to intense shear strain localization.

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Date submitted: 02 Mar 2019 Electronic form version 1.4