Abstract Submitted
for the SHOCK19 Meeting of
The American Physical Society

Shock Hugoniot Relationships for Crystalline and Amorphous HNAB: Insights from Atomistic Simulations and Virtual Diffraction Calculations JAMES A. STEWART, JOSEPH D. OLLES, RYAN R. WIXOM, REMI DINGREVILLE, SNL — The equation-of-state (EOS) for energetic materials characterizes the physical state of a system, e.g., temperature, pressure, and volume, when the material is subjected to sufficient shock conditions. The exact configuration of the microstructure (crystalline vs. polycrystalline vs. amorphous) further complicates the realized shock properties. This is especially the case in a model energetic system such as hexanitroazobenzene (HNAB), which can exist in crystalline or amorphous states. However, a fundamental understanding of the shock Hugoniot relationship as a function of crystalline structure, or lack thereof, is not well studied. As such, the goal of this work is to utilize molecular dynamics (MD) simulations and virtual diffraction calculations to elucidate the complex interplay between microstructural configurations, atomic-level processes, and the shock Hugoniot EOS in HNAB. First, we calculate the Hugoniot EOS for both the crystalline and amorphous HNAB polymorphs to compare the Hugoniot relationships between different crystal structures of the same material. These simulations systematically provide insight into the role of atomic structure on the resulting shock properties. Second, we perform virtual diffraction calculations on these atomistic data sets to identify possible structural changes occurring during the simulated shock compression. Taken together, these simulations bring a new understanding to the complex relationship between microstructure and shock properties in molecular crystals.

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Date submitted: 05 Jun 2019 Electronic form version 1.4