Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

Atomistic Simulation of Initiation in Hexanitrostilbene[1] TZU-RAY SHAN, RYAN WIXOM, COLE YARRINGTON, AIDAN THOMPSON, Sandia National Laboratories — We report on the effect of cylindrical voids on hot spot formation, growth and chemical reaction initiation in hexanitrostilbene (HNS) crystals subjected to shock. Large-scale, reactive molecular dynamics simulations are performed using the reactive force field (ReaxFF) as implemented in the LAMMPS software. The ReaxFF force field description for HNS has been validated previously by comparing the isothermal equation of state to available diamond anvil cell (DAC) measurements and density function theory (DFT) calculations and by comparing the primary dissociation pathway to *ab initio* calculations. Micron-scale molecular dynamics simulations of a supported shockwave propagating through the HNS crystal along the [010] orientation are performed with an impact velocity (or particle velocity) of 1.25 km/s, resulting in shockwave propagation at 4.0 km/s in the bulk material and a bulk shock pressure of $\sim$ 11GPa. The effect of cylindrical void sizes varying from 0.02 to 0.1 μm on hot spot formation and growth rate has been studied. Interaction between multiple voids in the HNS crystal and its effect on hot spot formation will also be addressed. Results from the micron-scale atomistic simulations are compared with hydrodynamics simulations.

[1]Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DOE National Nuclear Security Administration under contract DE-AC04-94AL85000

Tzu-Ray Shan
Sandia National Laboratories

Date submitted: 28 Jan 2015 Electronic form version 1.4