Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Atomistic Simulations of Orientation and Shock Velocity Dependences on Pentaerythritol Tetranitrate Detonation TZU-RAY SHAN, AIDAN THOMPSON, RYAN WIXOM, ANN MATTSSON, Sandia National Laboratories, Albuquerque, NM 87185, SANDIA TEAM — Predicting the behavior of energetic materials requires a detailed description of how chemical reaction, energy and pressure fronts propagate during initial stages of detonation. In this talk, classical molecular dynamics (MD) simulations are used to examine orientation and shock velocity dependences in single crystal pentaerythritol tetranitrate (PETN). This work utilizes an empirical, variable charge reactive force field (ReaxFF) that is implemented in the LAMMPS package with a time-averaged bond-order method for on-the-fly chemical species identification. The accuracy of ReaxFF is validated by comparisons of activation barriers for dissociation of a single PETN molecule along various dissociation channels with higher-fidelity, but more expensive, density functional theory (DFT) calculations. The response of single-crystal PETN to shock compression is simulated using the multi-scale shock technique (MSST) along the insensitive (100) directions, as well as the sensitive (001) and (110) directions, at steady shock velocities ranging from 6-10 km/s. Hugoniot curves, particle velocities of shocked molecules, and evolution of reaction products with time from MD simulations with ReaxFF will be discussed and compared to that from DFT calculations.

Tzu-Ray Shan
Sandia National Laboratories, Albuquerque, NM 87185

Date submitted: 08 Nov 2011 Electronic form version 1.4