Abstract Submitted
for the SHOCK13 Meeting of
The American Physical Society

Reactive Molecular Dynamics Simulation of Hotspot Formation in Shock-Induced Void Collapse of Pentaerythritol Tetranitrate (PETN)
TZU-RAY SHAN, AIDAN THOMPSON, Sandia National Laboratories, New Mexico — We present results of molecular dynamics simulations of hotspot formation in shock-induced void collapse of pentaerythritol tetranitrate (PETN) with the ReaxFF reactive force field. A supported shockwave is driven through a PETN crystal along the [110] orientation; void size and piston velocity are varied to investigate their effects on hotspot formation and detonation initiation. Formation of hotspots during void collapse is characterized by hotspot extent and maximum temperature. Results show hotspot extent is directly related to void size, but maximum temperature is only slightly affected. On the other hand, both hotspot extent and maximum temperature are strongly dependent upon piston velocity. Hotter and larger hotspots facilitate detonation and subsequent chemical reactions. During void collapse, NO_X molecules are shown to be the dominant ejectile from the upstream void surface. Once the void is filled and the hotspot develops, formation of final products such as N_2 and H_2O become more dominant.

Tzu-Ray Shan
Sandia National Laboratories

Date submitted: 05 Feb 2013 Electronic form version 1.4