Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

**Reactive molecular dynamics simulations of shocked PETN**[1]
JOANNE BUDZIEN, AIDAN P. THOMPSON, Sandia National Laboratories, SERGEY V. ZYBIN, California Institute of Technology — We have performed molecular dynamics simulations of PETN crystals subjected to shock along the [100] direction. Using the reactive forcefield, ReaxFF, and the molecular dynamics code, GRASP, allows us to track the chemical reactions that occur as both a function of time and position. By simulating larger systems, we can observe the formation of both primary and secondary products to make comparisons with experiments. Composition profiles of these products will be shown along with profiles of stress, temperature, and potential energy.

[1]Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Date submitted: 19 Nov 2007 Electronic form version 1.4