Abstract Submitted
for the SHOCK09 Meeting of
The American Physical Society

Shock Wave-Induced Chemical Decomposition of RDX Crystals
ZBIGNIEW DREGER, JAMES PATTERSON, MAOSHENG MIAO, YOGENDRA GUPTA, Institute for Shock Physics, Washington State University — Time-resolved optical spectroscopy and quantum chemistry calculations were combined to gain insight into molecular processes in shock-induced decomposition of RDX. Crystals of [111] orientation were shocked to peak stresses between 7.0 and 20.0 GPa. Broadband light emission was observed over the range of 350 - 850 nm with a threshold in spectral behavior at about 10 GPa. Below this threshold, the spectral profile remained unchanged during the experiment. Above 10 GPa, the emission spectrum changed with time and shifted to longer wavelengths. Based on these observations and quantum calculations, the emission spectrum was assigned to NO_2 radicals and HONO intermediates. Unimolecular decomposition of RDX leads to the production of these species through multiple decomposition steps. The observed threshold behavior is proposed to be due to the onset of bimolecular reactions between radical decomposition products and unreacted RDX molecules. We put forward a full decomposition scheme consistent with the main observations from our spectroscopy experiments. This work demonstrates the value of combining spectroscopy experiments with first principles calculations to understand decomposition of HE crystals.

Zbigniew Dreger
Institute for Shock Physics, Washington State University

Date submitted: 17 Feb 2009 Electronic form version 1.4