Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Surface-induced effect on sensitivity of beta and delta HMX crystals ONISE SHARIA, MAIJA KUKLJA, Department of Materials Science and Engineering, University of Maryland, College Park — It is accepted that sensitivity of energetic materials depends on many factors, including presence of defects, surfaces, interfaces, or voids. However, details of atomistic mechanisms that govern sensitivity to initiation of detonation and correlations between structure, morphology, and degradation of chemical bonds are far from being understood. In this talk, we present quantum chemical calculations combined with transition state theory to analyze chemical decomposition reactions in beta and delta HMX crystals. We calculate the activation barriers and reaction rates in the ideal crystals and materials containing internal surfaces, vacancies, and voids. We show that N-NO_2 homolysis is the most favorable decomposition reaction in all cases. We discuss whether a large space available in the vicinity of voids facilitates the N-NO_2 break in comparisons to an ideal crystal, and if this effect is enhanced in the delta phase in comparison to beta phase. The conclusions and revealed trends are presented in the context of experimental data.

Onise Sharia
Department of Materials Science and Engineering,
University of Maryland, College Park

Date submitted: 12 Dec 2011 Electronic form version 1.4