Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Thermal Decomposition of Plastic Bonded Explosives by Molecular Dynamic Simulations with the ReaxFF Force Field LUZHENG ZHANG, ADRI VAN DUIN, SIDDHARTH DASGUPTA, WILLIAM GODDARD III, California Institute of Technology — Plastic bonded explosives (PBX) are a type of composite energetic materials in which a high explosive is dispersed in a polymer matrix. The main purpose of making such high explosive polymer bound is to reduce their sensitivity to shock, friction, impact, etc. Thermal decomposition is an essential process to characterize an energetic material, because it is one of main causes of initiation of the explosives. In this work, we used MD simulations with the reactive force field (ReaxFF) to study the thermal decomposition of RDX crystal boned with polyurethane chains (Estane) and with nitrocellulose chains. The simulation results showed that RDX's thermal decomposition processing varies when a polymer binder was bonded to the crystal. With addition of polymer binders, RDX's sensitivity is reduced. In all cases studied, the products such as N_2, H_2O, CO, CO_2, OH, etc. can be identified. However, the contributions to these individual species are different: nitrocellulose has much more contributions to N_2, CO_2, and CO; but Estane has a little contributions to H_2O and almost no contributions to N_2, CO and CO_2. In addition, we found that the decomposition of RDX with Estane along the Y-direction is slower than that along the X-direction.

Luzheng Zhang
California Institute of Technology

Date submitted: 03 Dec 2004 Electronic form version 1.4