Impact Sensitivity of RDX and HMX from ReaxFF MD Simulations

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Abstract

Detailed description of the chemical reaction mechanisms of condensed energetic materials at high densities and temperatures is essential for understanding events that occur at the reactive front of these materials under combustion or detonation conditions. Under shock conditions, for example, energetic materials undergo rapid heating to a few thousand degrees and are subjected to a compression of hundreds of kilobars, resulting in almost 30% volume reduction. Complex chemical reactions are thus initiated, in turn releasing large amounts of energy to sustain the detonation process. Therefore, understanding the various chemical events at these extreme conditions is essential to build predictive models of material properties that can be incorporated into full continuum approaches of describing the detonation process at the macroscopic level. Impact sensitivity of energy materials is an important property for the handling of explosive compounds. Determination, evaluation and prediction of impact sensitivity stimulated numerous studies in the last decade.

We demonstrated a molecular dynamic simulation approach to study the impact sensitivity of a RDX crystal and HMX crystals at different phases (α, β, and γ, and δ) under compression. The simulation results show that for the RDX crystals, at lower compression ratios only few RDX molecules are decomposed and primary reactions are found during this decomposition process, while at higher compression ratios (x>40%), all RDX molecules are decomposed very quickly and both primary and secondary reactions are found in the decomposition, which produces not only various intermediates NO₂, NO, HONO, OH, but also the final products H₂O, N₂, CO, CO₂. For the HMX at different phases, the simulation results show the impact sensitivity increases in this order: β < α < γ < δ. At the same compression ratio x=40%, all HMX molecules in δ-phase are decomposed and both primary and secondary reaction are found. However, only few HMX molecules in α-, β-, and γ-phases are decomposed. Generally the simulation results for both RDX and HMX crystals agree qualitatively with experiment observations. The simulation method is depicted in Figure 1. MD simulation results for RDX and HMX are shown in Figures 2 and 3, respectively.
Figure 1. Schematic simulation process of impact sensitivity for a HE crystal. Apply $V_0$ (100-$x$) % uniaxial compression (~0.15ps) followed by a 1.0 ps NVE, then Apply $V_0$ (100+$x$) % uniaxial expansion at the compressed state (~0.90 ps) followed by a 4.0 ps NVE.

Figure 2. System temperature (a) and fragments (b) for the RDX crystal at the compression ratios of $x$=30%, 40% and 50%.

Figure 3. System temperature (a) and fragments (b) for $\alpha$-HMX, $\beta$-HMX, $\gamma$-HMX, and $\delta$-HMX at the compression ratio of $x$=40%.