Abstract

We conducted a series of experiments on the decompositions of the energetic materials: NaBH₄, NH₄BH₄, HMX, and RDX under different pressures using the x-ray diffraction (XRD) technique; we also studied the lesser known but high-pressure explosives using the infrared spectra (IR) technique. For the chemical decomposition of NaBH₄ and NH₄BH₄, we discovered two x-ray induced hydrogen gas generation; for the decomposition of HMX and RDX, we discovered that the decay rates of these two materials vary with pressure respectively, for the study of FOX-7's high pressure behaviors we discovered potential phase changes and pressure induced chemical reactions as pressure is increased.

X-Ray Induced Chemistry in Hydrogen Rich Materials: NaBH₄ and NH₄BH₄

Material Description

NaBH₄ (sodium borohydride) and NH₄BH₄ (ammonia borane) are potential hydrogen storage materials that are currently subjected to intensive research. Under the proper conditions, these materials can release hydrogen gas (2 mol equiv for NaBH₄ and 5 for NH₄BH₄). The current researches focus on heat or catalyst induced hydrogen generations, which proved to be too uncontrollable to be used in applications.

High Pressure Study of X-Ray-Induced Decay of HMX Using XRD

(HMX: Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine)

Material Description

HMX, also called octogen, is a powerful and relatively insensitive high explosive. It is a high melting, high-velocity military explosive.

The molecule of HMX is an eight-membered ring of alternating carbon and nitrogen atoms. Because of its high molecular weight, it is one of the most potent chemical explosives manufactured.

Figure 1: Integrated XRD spectra of HMX with respect to time. The pressures under which the sample was bombarded and labeled on the pictures.

Material Description

FOX-7 is an inexpensive high energy, high explosive compound. It has a two-carbon backbone, and the amine and nitro groups contribute to sensitivity and chemical decay processes of FOX-7, similar to most other nitrogen-containing explosives.

Figure 2: Line bond structure of RDX

Material Description

RDX is an abbreviation for Research Department Explosive. It is an explosive widely used in military and industrial applications. It is stable in storage and is considered one of the most brisant of the military high explosives.

Figure 3: FOX-7 crystal before and after x-ray bombardment respectively.

Results and Discussions

There are several indications of chemical reactions in both mixtures. In fig. 2, the relative change of the peak in the XRD spectra of the NaBH₄, changed as the x-ray bombardment proceed. In fig. 3, as indicated by the XRD spectra, the KClO₃ in the mixture is decomposed by the x-ray into KCl; and in fig. 4, we can observe the formation of water from the reaction in the NaBH₄ + KClO₃ mixture. In fig. 5, we integrated the XRD spectra of the sample over the course of the reaction and plotted their intensities as functions of time. We integrated the decay curves of the sample for three different pressure points (fig. 2). The integrated decay curve shows that the decay rate of HMX under x-ray bombardment drops as pressure increases. The reason of this effect would be the focus of our follow-up studies.

Figure 4: Photostimulated picture of NH₃BH₄+KClO₃ mixture. The liquid mixture are water formed in the reaction.

Peak 1

Peak 2

Figure 5: FOX-7 crystal before and after x-ray bombardment respectively. (X-ray used is synchrotron x-ray from the Argonne National Laboratory’s Advanced Photon Source).