High-Pressure Behaviour of Energetic Materials-Ammonium Nitrate

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Abstract

Although high pressure has been used extensively to study polymorphism, phase transitions and changes in physical properties in a wide range of materials (i.e., metals, minerals, ices), one class of material that have received less attention is that of energetic materials (EMs- explosives, propellants). Work is thus presented on the high pressure behavior of Ammonium Nitrate (AN). A novel high pressure phase of AN has been identified above 15 GPa using a combination of Raman spectroscopy and powder X-ray diffraction.

The knowledge gained thought this work, and though the ongoing study of energetic materials under pressure could lead to:

•Identifying new phases of EMs
•Enhancing the properties and sensitivities of EMs
•Greater understanding of detonation mechanisms
•Safer use and handling of EMs
•Improved ways of detecting these materials

Relevance

Ammonium Nitrate (AN)
•Used in Explosive mixtures
•Also used as a fertilizer
•AN explosives used in Oklahoma City Bombings
•AN used in Improvised explosive devices (IED)in Iraq and Afghanistan
•AN fertilizers currently banned in Afghanistan

Figure1:Improvised explosive devices containing Ammonium Nitrate

Figure2: Soldier dismantling improvised explosive device

This work could lead to
•Increased understanding of AN explosive capabilities
•Increased ability to safely dismantle AN IEDs
•Decreased threat of AN containing IEDs
•New high pressure forms of AN with new properties

Technical Approach

•Polymorphism and solid-solid phase transitions are crucial to the scientific study and applications of energetic materials [1].
•Can change sensitivity to shock, detonation velocity, and other performance characteristics of EMs.
•Phase transitions can be induced under the an explosion or detonation (Figure 3)
•Knowledge gained through studying the response of energetic materials to pressure may lead to better prediction/control of polymorphism in such materials, and provides valuable information for modelling of energetic materials under extreme conditions.

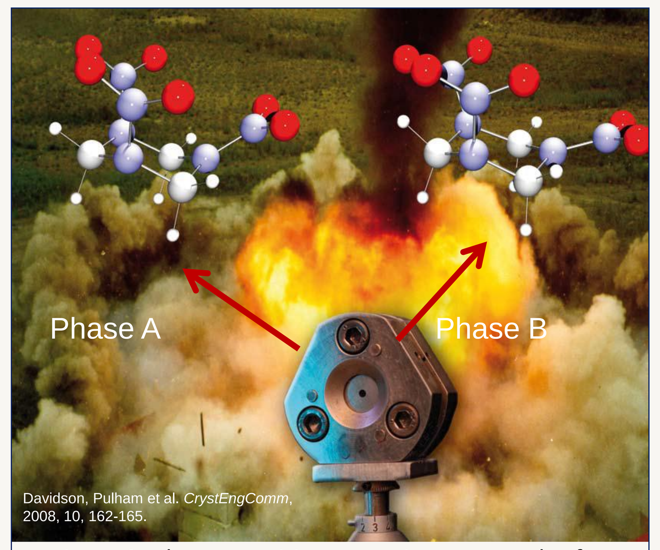

Figure 3: Phase transition occurring as a result of an explosion

Ammonium Nitrate (Figure 4)
•5 known phases at ambient pressure [2].
•Several previous high pressure studies conducted on AN
•Studied under static and dynamic pressure
•Results contradictory and not conclusive [3,4,5]
•Most recent study reported no high pressure phases up to 7.5 GPa [6]

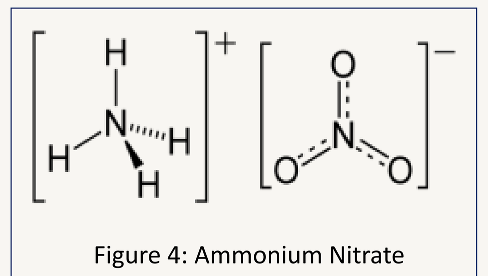

Figure 4: Ammonium Nitrate

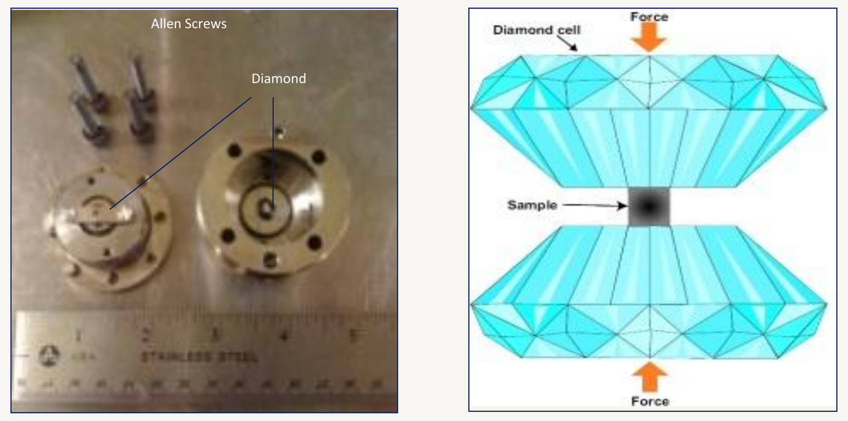

Figure 5: Diamond Anvil Cell.

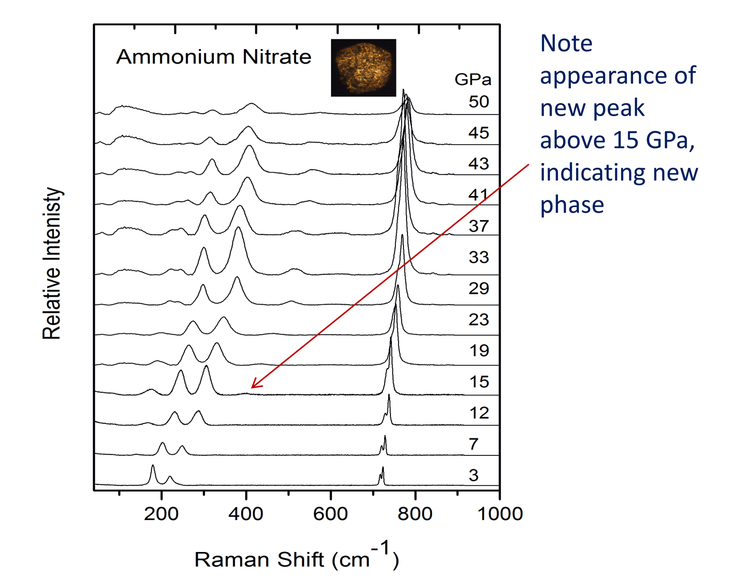

Figure 6: Raman spectra as a function of increasing pressure

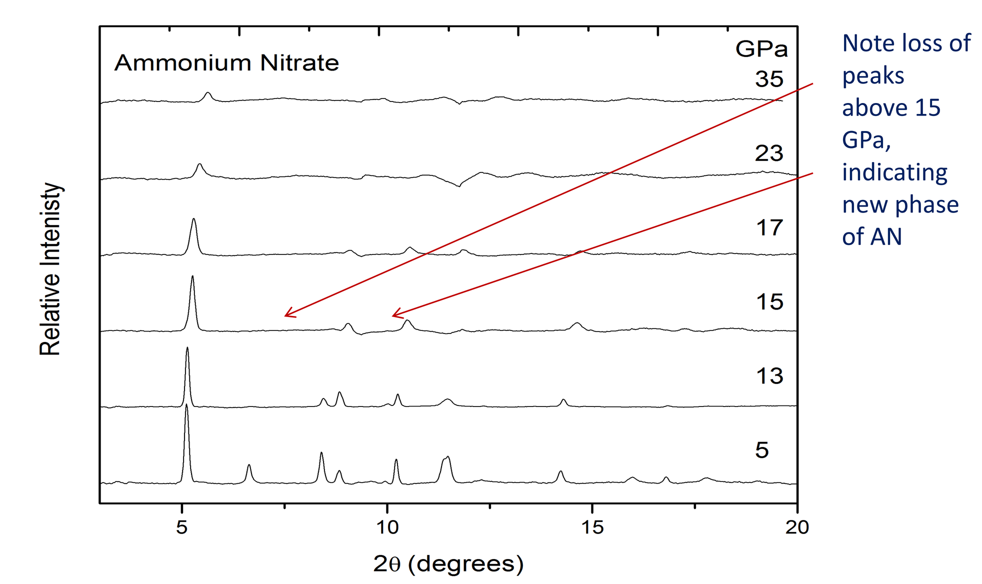

Figure 7: X-ray powder diffraction patters as a function of increasing pressure. Data collected on beamline 16 BM-D at the APS

High-pressure studies have been performed
•Diamond-Anvil cell (DAC) used to generate high pressures (Figure 5)
•**Evidence for a new high pressure of AN at 15.0 GPa**
•Raman Spectroscopy (Figures 6)
•X-ray powder diffraction (Figure 7)
•Refinement of powder data of new phase underway

Accomplishments Through Current Year

Investigated the phase stability and chemical decomposition of AN using micro-Raman spectroscopy and third-generation synchrotron x-ray at the APS:

•Phase transition at 15 GPa in static conditions

•No chemical changes under shock conditions (collaboration with Drs. Dattelbaum and Sheffield in the DX-group at LANL).

Presently investigating the stability in different chemicals of He, n-hexane, CO_2, carbonates, etc

Future Work

•Single crystal X-ray diffraction will be conducted to try and obtain structural information on the new high pressure phase of AN

•Shock wave studies will be undertaken to asses whether the transition occurs under dynamic pressure conditions

•Investigate the melting point behavior AN under different conditions of temperature and pressure

Opportunities for Transition to Customer

The work presented illustrates that the techniques utilized in these experiments are an excellent way of studying energetic materials under high pressure. The recent developments in the field of high pressure (data collection and analysis, high resolution) enable us to perform high quality experiments on a range of energetic materials. This work is at the forefront of the high pressure field, and has wide ranging applications, most notably in the use and study of explosives and propellants.

Publications Acknowledging DHS Support

- Alistair Davidson and Choong-Shik Yoo, Phase Transitions in Ammonium Nitrate under High Pressures, (2011) in preparation
- Alistair Davidson and Choong-Shik Yoo, Pressure Transitions and Amorphization of Formic Acid under High Pressures, (2011) in preparation

Other References

[1] T.B. Brill, "Polymorphism and Phase Transformations in Energetic Materials," 35th Course, International School of Crystallography, Erice, Italy, 2004. [2] C. S. Choi and H. J. Prask, J. Appl. Cryst., 1980, 13, 403-409. [3] P. W. Bridgman, Proc. Amer. Acad. Arts Sci., 1937, 71, 387. [4] D. M. Adams and S. K. Sharma, J. Chem. Soc., Faraday Trans 2., 1976, 72, 2069. [5] F. W. Sandstrom, P. A. Persson and B. Olinger, AIP Conference Proceedings, 1994, 309. 1409. [6]. A.J. Davidson, W.G. Marshall, C.R. Pullham, 38th International Annual Conference of ICT, 2007.

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