ONR (351) Final Performance Report

Grant Number:	N00014-16-1-2088
Date Prepared:	September 27, 2019
Project Title:	Understanding Molecular and Crystalline Mechanisms that Govern Insensitivity in Shocked Energetic Crystals
Period of Performance:	December 1, 2015 – May 31, 2019
Principle Investigator:	Yogendra Gupta Institute for Shock Physics Washington State University ymgupta@wsu.edu; 509-335-7217

I. Overview of Project

Abstract

The research focus of this project was on a fundamental understanding of the intrinsic properties of energetic crystals (molecular and crystalline attributes/mechanisms) that govern their insensitivity at conditions relevant to shock wave induced chemical decomposition. Some aspects of this effort were also relevant to thermal loading. The combination of well-characterized shock wave and static compression experiments on insensitive energetic single crystals – and different types of measurements – were used to gain insight into the molecular and crystalline mechanisms of interest. To the best of our knowledge, the shock wave measurements carried out on insensitive high explosive (IHE) single crystals represent the first such measurements. Shock wave experimental capabilities – central to this research effort – were also utilized for developing a research collaboration with NSWC-IH.

Objective

- Understanding molecular/crystalline mechanisms governing the insensitivity of shock compressed insensitive high-explosive (IHE) single crystals
- Using FOX-7, a prototypical IHE crystal, combine static HP-HT measurements and first-principles calculations to provide the baseline information to guide shock experiments
- Develop experimental capabilities to examine molecular/crystalline changes in an IHE single crystal (FOX-7) subjected to planar shock compression
- Obtain time-resolved continuum and spectroscopic measurements in well characterized shock experiments on FOX-7 to understand shock-induced changes

Payoffs / Key Technologies

- Understanding shock sensitivity of HE and IHE crystals is essential to optimizing their performance and safe use under dynamic loading.
- Understanding the shock response of HE and IHE crystals at different length scales is valuable to gaining insight into the shock response of PBXs of interest to Navy applications.
- Understanding molecular/crystalline mechanisms governing insensitivity can help guide synthesis and development of novel IHEs.

Introduction

Naval platforms and ships have unique and special challenges regarding the storage of high explosives (HE) for extended periods. Even the transport (including handling) of HE to Naval vessels requires special protocols and procedures. As such, the Navy's need for insensitive munitions (which release energy only on demand) – but also possess the requisite chemical energy to provide the lethality for Naval missions – cannot be emphasized enough. Development and deployment of insensitive high explosives (IHE) for conventional munitions has been a long standing S&T objective for the Navy.

Despite the significant progress to date regarding different types of HEs, there is not yet a predictive capability to systematically and accurately provide the fundamental molecular/crystalline requirements for synthesizing and developing the HEs with the desired combination of performance and sensitivity. *Avoidance of unwanted and unforeseen detonations is a must.* Since shock wave initiation is a prerequisite to a detonation, a good understanding of the fundamental molecular and crystalline attributes/mechanisms under the conditions pertinent to shock wave initiation is both relevant and important for Navy's ordnance applications. Hence, this research effort was focused toward achieving this understanding and contributes to identifying the fundamental characteristics that govern insensitivity of HE crystals.

Background/Approach

Numerous efforts have been made to correlate shock sensitivity of HE formulations to both intrinsic properties of HE crystals (molecular and crystalline properties including crystal defects) and extrinsic parameters relevant to HE formulations (size and shape of HE crystals, void and inclusion shapes and concentrations, binder response, etc.). To date, considerable progress has been made in understanding the sensitivity of HE formulations under thermal and shock loading through a combination of synthesis and chemical insights, crystal packing analyses, a broad range of sensitivity tests, and recent advances in modeling and simulations. However, there is not yet a well-established, fundamental approach that can be implemented to develop a new HE crystal with the desired combination of high performance and sensitivity. Such a goal is extremely challenging due to the inherent scientific complexities at different length scales and due to the multidisciplinary nature of the problem. However, the programmatic payoff is enormous. We believe that separating the technical problem into two separate parts -- developing an understanding of the intrinsic and the extrinsic parameters that govern insensitivity -- is likely an efficient approach. To keep the scientific scope manageable and within academic bounds, our research effort focused on the following question: *What molecular and crystalline properties of HE crystals (intrinsic properties) influence/govern insensitivity under shock compression?*

A key element of our effort was to develop an in-depth understanding of the molecular and crystal attributes/mechanisms that govern the insensitivity of shocked HE crystals. This challenging, long-term objective was addressed as follows: focusing primarily on a representative insensitive HE (IHE) single crystal; pursuing a comprehensive approach that combines optical spectroscopy and X-ray diffraction measurements in static high pressure-high temperature (HP-HT) experiments; time-resolved continuum and optical spectroscopy measurements in well-characterized shock experiments; and partnering with other investigators/institutions, as needed, regarding theoretical support and material acquisition for our work.

A central, and likely unique, feature of our work was the use of single crystals in all of our experimental studies (both static and shock wave). This feature, though experimentally quite challenging and time-intensive, was important for the following reasons: to gain fundamental insight into molecular and crystalline mechanisms; to connect better with theoretical studies; and to understand the role of crystal anisotropy on the shock response of HE crystals.

II. Activities and Accomplishments

A. Determination of molecular and crystalline changes in FOX-7 under high pressure

A.1 Crystal structures of HP polymorphs

Synchrotron single-crystal x-ray diffraction measurements and analysis of these data were used to understand the link between high-pressure polymorphic phases and insensitivity/stability of FOX-7. The phase transitions, alpha-alpha' (2 GPa) and alpha'-epsilon (4.5 GPa), previously identified with Raman spectroscopy, were investigated and the structures of the alpha' and epsilon polymorphs were determined at 4.27 and 5.9 GPa, respectively. To obtain the refined position of hydrogen atoms, the experimental results were combined with dispersion-corrected density functional theory (DFT-D2) calculations. The results revealed that the alpha' phase – because it has the same space group and the same molecular arrangement as the ambient phase - is structurally indistinguishable from the alpha-FOX-7 phase. The only changes observed at the alpha-alpha' transition involved subtle changes in: the amino group angle with respect to the molecular plane and the distance of hydrogen bonds. These changes are unlikely to affect the insensitivity/stability of FOX-7.

In contrast to the alpha-alpha' transition, the alpha'-epsilon transition introduces significant changes to the FOX-7 structure. It transforms the monoclinic structure to a triclinic structure. Several structural factors were identified that may contribute to the enhancement of insensitivity/stability of FOX-7 in the epsilon phase. These are: (i) formation of planar layers of molecules, (ii) increase in molecule conjugation due to the "flattening" of molecules and shortening of intramolecular bonds, i.e., C−C and some C−N bonds, (iii) strengthening of hydrogen bonding network. Most importantly, the epsilon-FOX-7 crystal structure was found to be similar to the ambient structure of TATB – currently, the most insensitive HE crystal. This finding is significant for understanding the insensitivity of shocked IHE crystals.

A.2 High pressure structural changes and compression to 13 GPa

To provide a further understanding of the insensitivity/stability of IHE crystals, the structure of FOX-7 was investigated using synchrotron single-crystal x-ray diffraction measurements over a broad range of pressures. Pressure-induced changes in molecular and crystal structures were used to examine the stability of alpha' and epsilon phases and hydrogen bonding, and to determine the compressibility to 13 GPa. Over the entire pressure range, FOX-7 shows anisotropic compression, irrespective of the phase transitions at 2 and 4.5 GPa. This result is consistent with the anisotropic interactions in the layered structure due to differences between the interlayer (van der Waals) and in-layer (H-bonds) forces. A detailed examination of molecular and crystal structures indicated distinct behavior of some structural parameters below and above the alpha'-epsilon phase transition at 4.5 GPa. At the unit cell level, we found that all unit cell parameters show gradual decrease up to 4.5 GPa, without any discontinuity at 2 GPa. At the alpha'-epsilon transition, the transformation to triclinic crystal system (P1) reduces the c-axis dimension by ~ 38%, considerably increases all unit cell angles, but only slightly affects the dimensions of the a and b axes. As a result, the volume/molecule decreases by 1.1 % and the interlayer distance increases by 2.4%. Beyond the alpha'-epsilon phase transition, changes in unit cell parameters were gradual, and the epsilon phase structure was maintained to 13 GPa, the highest pressure applied. The 3rd-order Birch-Murnaghan equation parameters were used to fit the p-V data below and above the alpha'-epsilon transition. We have shown that changes in the unit cell parameters are well reproduced by dispersion-corrected density functional theory (DFT-D) calculations. At the molecular level, we identified significant changes in hydrogen bonds (H-bonds) distance. These changes include: (i) a considerable decrease in the intermolecular H-bonds distance below 4.5 GPa, (ii) significant decrease in the distance of most H-bonds at the alpha'-epsilon transition, and (iii) moderate changes in their distance above 4.5 GPa. The observed decrease in H-bonds distance implies that the crystal stability increases with pressure.

B. Determination of HP-HT phase diagram and decomposition of FOX-7

B.1 Completion of a comprehensive static high pressure-high temperature (HP-HT) study on FOX-7

With support from ONR and DOE/NNSA, we undertook – to the best of our knowledge – the first study on understanding the shock wave response of an IHE single crystal (FOX-7). Because of the lack of previous relevant data, we chose to focus our initial efforts on static HP-HT response of FOX-7. As noted in previous reports, many excellent and valuable scientific insights have been gained regarding the HP-HT response of FOX-7. The past year's effort was the culmination of a systematic, comprehensive study regarding the molecular and crystalline changes due to static HP-HT conditions. The static HP-HT effort undertaken on FOX-7 was essential to the proper design/conduct of shock wave experiments. The achievements of these efforts are best conveyed by reproducing the abstract of our paper[1]:

High-pressure structural response of an insensitive energetic crystal—1,1-diamino-2,2-dinitroethene (FOX-7)—was examined to gain insight into its structural and chemical stability and to obtain isothermal compression data. Using synchrotron single-crystal X-ray diffraction measurements, details of pressure-induced structural changes to 12.8 GPa were determined across three FOX-7 phases: α ($P2_1/n$), α′ ($P2_1/n$), and ε ($P1$). We found that the C–NO_2 bond is the most compressible chemical bond, and high pressure significantly reduces and homogenizes the length of H bonds in the hydrogen-bond network. The α′−ε phase transition, at 4.5 GPa, significantly affects all molecular and crystal properties, whereas the α–α′ transition, at 2 GPa, is associated with subtle molecular and intermolecular changes. Anisotropic compressibility was observed over the entire pressure range, consistent with the layered structure of the crystal. The equation-of-state parameters were obtained using the third-order Birch–Murnaghan equation below and above the α′−ε phase transition. It is shown that dispersion-corrected DFT-D calculations reproduce well pressure-induced changes in the unit cell parameters. The findings of this work provide new insights into the molecular and structural mechanisms governing the high-pressure stability/insensitivity of insensitive energetic crystals.

[1]Dreger, Z. A., A. I. Stash, Z.-G. Yu, Y.-S. Chen and Y. Tao (2017). "High-Pressure Structural Response of an Insensitive Energetic Crystal: Dihydroxylammonium 5,5′-Bistetrazole-1,1′-diolate (TKX-50)." The Journal of Physical Chemistry C 121(10): 5761-5767.

B.2 Thermal decomposition under high pressure

To gain insight into the decomposition of FOX-7, we carried out IR spectroscopy (FTIR) measurements to identify the decomposition products. Experiments were performed at several pressures from ambient to 3.5 GPa to examine the effect of pressure on decomposition. Analyses of HP-HT FTIR spectra revealed formation of various products, including gases, water, and a solid residue containing the C-N, C-H, N-H and C=O bonds. By identifying this broad set of products, we provide important information to evaluate the computational models used to gain insight into the thermal decomposition of FOX-7 crystal. More importantly, we found that the same products are observed at different pressures examined in this work (up to 3.5 GPa). This finding suggests similar decomposition pathways occur in FOX-7, irrespective of the pressure.

C. Investigating the static high pressure response of a novel insensitive high explosive crystal (TKX-50) to determine the similarities and differences between TKX-50 and FOX-7

Although the FOX-7 single crystal results have provided valuable and new insights into molecular/crystalline features governing the HP-HT response of an IHE crystal – essential for shock compression studies – it is important to determine/establish similarities and differences with another IHE crystal. Toward this objective, we chose to examine TKX-50 – a recently synthesized, novel IHE crystal. The scope of the TKX-50 was considerably smaller; below we reproduce an abstract from the TKX-50 paper just published:

The structural response of a novel, insensitive energetic crystal—dihydroxylammonium 5,5′-bistetrazole-1,1′-diolate (TKX-50)—was examined under high pressure. Using synchrotron single-crystal X-ray diffraction measurements, details of molecular, intermolecular, and crystal changes were determined to ~10 GPa to understand its structural stability. The experimental results showed that TKX-50 exhibits highly anisotropic compression and significantly lower volume compressibility than currently known energetic crystals. These results are found to be in general agreement with our previous predictions from the DFT calculations. Additionally, the experimental data revealed anomalous compression—an expansion of the unit cell along the *a* axis (negative linear compressibility, NLC) upon compression to ~3 GPa. The structural analyses demonstrated that this unusual effect, the first such observation in an energetic crystal, is a consequence of the highly anisotropic response of 3D motifs, comprised of two parallel anions $[(C_2N_8O_2)^{2-}]$ linked with two cations $[(NH_3OH)^+]$ through four strong hydrogen bonds. The present results demonstrate that the structural stability of TKX-50 is controlled by the strong and highly anisotropic intermolecular interactions, and these may contribute to its shock insensitivity.

D. Develop experimental techniques to undertake the first ever shock wave experiments on an IHE single crystal

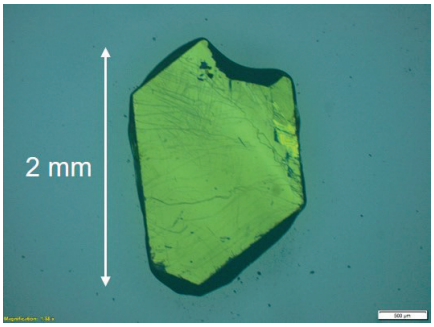

Figure 1. FOX-7 Single Crystal

As described above, the overall goal of this research project was to understand the molecular/crystalline mechanisms governing the insensitivity of shock compressed IHE single crystals. The challenging nature of this undertaking is best conveyed by the following statement: to the best of our knowledge, there exist no published shock wave data on IHE single crystals. The unavailability of even modestly sized single crystals (~1.5 mm, lateral dimensions) is a large factor in the paucity of such studies. A considerable effort was spent in growing such crystals (it takes 3-4 months to grow 1-1.5 mm crystals) and learning how to handle/prepare such small crystals for shock wave experiments.

In a parallel effort, the design/development of experimental techniques was undertaken to achieve both continuum measurements (laser interferometry) and vibrational/electronic spectroscopy under well characterized planar shock wave loading. The small size of the samples (~1.5 mm x 1.5 mm x 0.2 mm) and their extreme fragility constituted the primary challenges. After considerable effort and use of similar sized surrogates (more readily available materials), we were able to develop experimental methods to provide the desired high quality data: real-time continuum and spectroscopy measurements Because of the fragile nature of the FOX-7 crystals, each experiment required considerable effort/expertise and was quite time-intensive. Despite the successful development of the methods to undertake the desired shock experiments, two aspects of these experiments are emphasized: it is unreasonable to expect a graduate student and/or postdoc to fabricate and conduct these experiments; and even the highly experienced staff members had considerable difficulty in preparing the sample assemblies. *Hence, no graduate students or postdocs were involved in the shock wave experiments.*

E. Shock compression of FOX-7 single crystals

After the successful development of the experimental methods, indicated above, FOX-7 single crystals were shocked normal to the (101) plane to a range of peak stresses – up to ~20 GPa. Samples ranging from 140 – 260 µm in thickness were subjected to well characterized plane wave loading. Time-resolved, continuum measurements (using laser-interferometry) and molecular level measurements (using Raman spectroscopy) were successfully obtained. Because two journal manuscripts regarding this work are in preparation, only a very brief summary of this work is presented in this report. These manuscripts will be submitted to ONR at a later date.

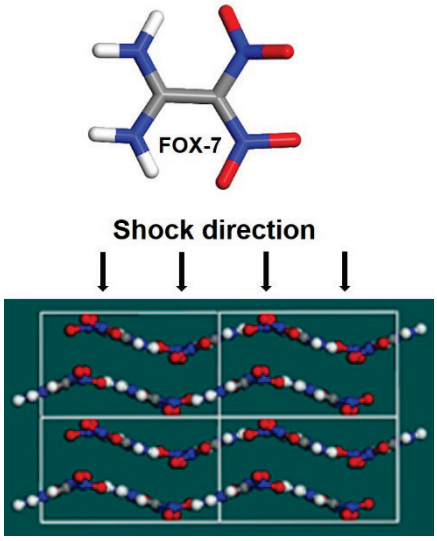

Figure 2. FOX-7 Sample Orientation

1. Continuum Measurements

A schematic view of the experimental configuration used for obtaining continuum response is shown in Figure 3. VISAR measurements, as shown, were used to determine the shock velocity (U_s) and the particle-velocity profile at the sample/LiF interface in each experiment. The main findings from these measurements are summarized below.

- Two-wave structure observed at low stresses, and the Hugoniot Elastic Limit was comparable to the [110] PETN results obtained at LANL.
- Above 4 GPa, only a single (overdriven) is observed.
- No wave profile features related to a phase transformation were observed – not surprising since the static HP data showed an extremely small volume change.
- No sign of chemical reaction to 21 GPa.

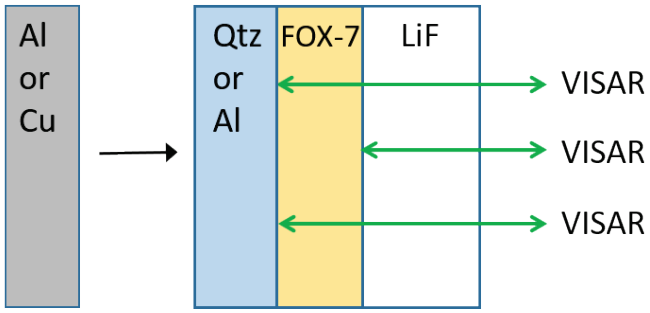

Figure 3. Schematic view of the experimental configuration used for obtaining continuum response.

The data obtained from these experiments were used to obtain the Hugoniot curve for FOX-7. The shock data and the static HP-HT data were used to develop a phenomenological material model for FOX-7. By incorporating this model into a wave propagation code, numerical simulations corresponding to the measured wave profiles were undertaken. The calculated wave profiles provide good agreement with the measured profiles.

2. Raman Spectroscopy

A schematic view of the experimental configuration used to obtain time-resolved Raman spectroscopy data is shown in Figure 4. The use of a gated intensifier provided 15 ns time resolution. Furthermore, the elimination of the streak camera (used in our previous time-resolved spectroscopy studies) from the experimental configuration increased the detection efficiency and resulted in a significantly improved signal-to-noise ratio. The stress history and intensifier gate times for a representative experiment are shown in Figure 5.

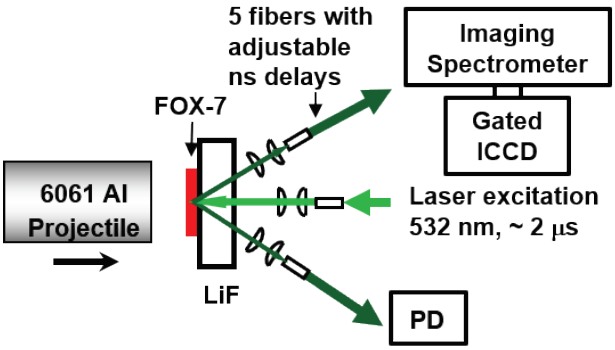

Figure 4. Schematic of experimental configuration for Raman

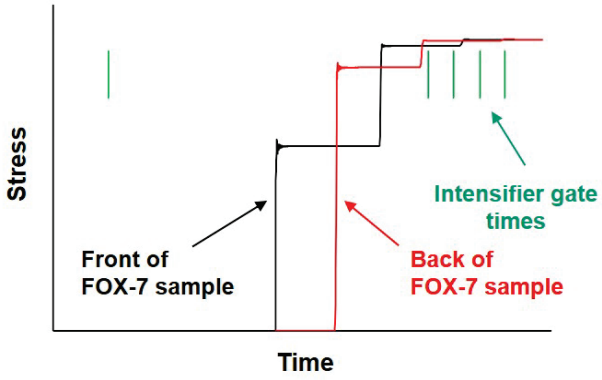

Figure 5. Stress history and intensifier gate times

Figure 6 shows the time-resolved Raman spectra – spectral coverage from 800 – 1500 cm^{-1} – for a peak stress of ~6 GPa. Of the five spectra, each with an integration time of 15 ns, one spectrum was obtained prior to impact and four spectra were obtained after impact to examine shock reverberation and the peak stress state.

To date, Raman measurements (comparable in quality to the data shown in Figure 6) have been obtained to 16 GPa peak stress. Overall, the shock data are showing results that are in reasonable agreement with the static results. Up to 16 GPa, the Raman data show no signs of a chemical reaction in shock compressed FOX-7. We will complete one experiment at ~20 GPa before submitting our manuscript – currently under preparation – for publication.

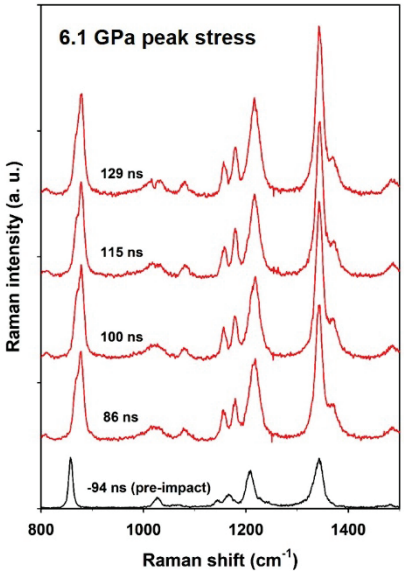

Figure 6. Time-resolved Raman spectra

F. NSWC IHEODTD Collaboration

During the final year of this project, and per discussions with Dr. Chad Stoltz (ONR Program Manager), a collaboration in energetic materials research was initiated between the Institute for Shock Physics (ISP) and NSWC IHEODTD (Drs. Zbigniew Dreger and Demitrios Stamatis are the scientific POCs at Indian Head). The goal of this collaboration is to utilize the ISP scientific expertise and experimental capabilities for studying the shock response of PBX compositions of interest to the Navy. Because Zbig Dreger had worked at the Institute for 19 years (before joining NSWC-IH), he is well suited for establishing a meaningful collaboration between the two organizations.

As noted in the previous parts of this report, the ISP effort to date has focused entirely on HE single crystals. The single crystal results provide an ideal scientific benchmark for examining and understanding the shock response of different PBX compositions.

To define the collaboration activities and to familiarize the NSWC researchers with the expertise/capabilities available at the ISP, a meeting was held on December 11, 2018. The agenda for this meeting is included in the Appendix. This meeting was very helpful in discussing and finalizing experimental design and related details. It was decided that emission experiments on four PBX samples, at 20 GPa peak stress, will be conducted. Relevant experimental drawings were provided to the NSWC scientists since NSWC was responsible for the sample preparation and target assembly. WSU was responsible for all other aspects associated with the conduct of the shock experiments to obtain time-resolved emission data. The experiments were successfully conducted in April 2019 and excellent emission results were obtained from all the samples.

Since all the PBX samples in these experiments consisted of RDX crystals, our previously published results on RDX single crystals have been valuable for interpreting the PBX data. Because this was a research collaboration with NSWC, we are not showing preliminary findings in this report. At a later date and, as appropriate, a brief joint report can be submitted to the ONR regarding the effort to date.

III. Findings and Conclusions

The research activities undertaken in this project provided new knowledge on the HP-HT behavior of FOX-7 crystal under well-controlled compression conditions that can be used for developing and evaluating theoretical models describing the structural stability and chemical reactivity of IHE crystals.

The comprehensive static HP-HT activities were essential to the development and conduct of the shock wave experiments. As a result, the first determination of continuum and molecular response of shocked insensitive high explosive single crystals was achieved. The findings and conclusions of shock wave studies may be summarized as follows:

- The FOX-7 wave profiles were measured to 21 GPa in plate impact experiments.
  - A two-wave structure to ~4 GPa was observed and the single (overdriven) waves were observed above 4 GPa.
  - The wave profiles and Hugoniot curve show no sign of chemical reaction to 21 GPa.
- A continuum model was developed for shocked FOX-7.
  - Numerical simulations provide a good match to measured profiles.
  - Strain-softening behavior is indicated at low stresses.
- Time-resolved Raman spectra were measured for FOX-7 shocked to 16 GPa.
  - Peak positions show reasonable agreement with static compression results.
  - Raman spectra show no indication of chemical reaction to 16 GPa.

IV. Project Metrics

A. Metrics for Period of Performance (December 1, 2015 – May 31, 2019)

Number of faculty supported under this project during this reporting period: 1 (through March 2017)

Number of post-doctoral researchers supported under this project during this period: NA

Number of graduate students supported under this project during this reporting period: NA

Number of undergraduate students supported under this project during this period: NA

Number of scientists / engineers / technicians supported under this project during this reporting period: 3

Number of refereed publications during this reporting period for which at least 1/3 of the work was done under this effort: 5

Number of publications (all) during this reporting period: 5

Number of patents during this reporting period: NA

Number of M.S. students graduated during this reporting period: NA

Number of Ph.D. students graduated during this reporting period: NA

Awards received during this reporting period: 1 (Y. M. Gupta, Recipient of the Army Research Laboratory Partnering Award, 2016)

Participants (December 1, 2015 – May 31, 2019)

Personnel	Nearest Person Month
Yogendra Gupta (Principal Investigator)	0
Zbigniew Dreger (Separated from WSU in March 2017)	5
Nathan Arganbright	4
Yoshimasa Toyoda	4
Kurt Zimmerman	8

As noted earlier, the involvement of graduate students and postdocs was not feasible in the shock experiments on FOX-7.

B. Products

B.1 Publications

Publications resulting from this project during the reporting period are listed below.

1. Dreger, Z. A., A. I. Stash, Z.-G. Yu, Y.-S. Chen, Y. Tao and Y. M. Gupta (2016). "High-Pressure Crystal Structures of an Insensitive Energetic Crystal: 1,1-Diamino-2,2-dinitroethene." The Journal of Physical Chemistry C 120(2): 1218-1224. https://doi.org/10.1021/acs.jpcc.5b10644
2. Dreger, Z. A., Y. Tao and Y. M. Gupta (2016). "Phase Diagram and Decomposition of 1,1-Diamino-2,2-dinitroethene Single Crystals at High Pressures and Temperatures." The Journal of Physical Chemistry C 120(20): 11092-11098. https://doi.org/10.1021/acs.jpcc.6b02360

3. Dreger, Z. A., A. I. Stash, Z.-G. Yu, Y.-S. Chen, Y. Tao and Y. M. Gupta (2016). "High-Pressure Structural Response of an Insensitive Energetic Crystal: 1,1-Diamino-2,2-dinitroethene (FOX-7)." The Journal of Physical Chemistry C 120(48): 27600-27607. https://doi.org/10.1021/acs.jpcc.6b10010
4. Dreger, Z. A., A. I. Stash, Z.-G. Yu, Y.-S. Chen and Y. Tao (2017). "High-Pressure Structural Response of an Insensitive Energetic Crystal: Dihydroxyl ammonium 5,5′-Bistetrazole-1,1′-diolate (TKX-50)." The Journal of Physical Chemistry C 121(10): 5761-5767. https://doi.org/10.1021/acs.jpcc.7b00867
5. Dreger, Z. A., C. J. Breshike and Y. M. Gupta. (2017). "High Pressure-high Temperature Phase Diagram of an Energetic crystal: Dihydroxylammonium 5,5′-bistetrazole-1,1′-diolate (TKX-50)." Chemical Physics Letters 679: 212-218. https://doi.org/10.1016/j.cplett.2017.05.019

Two manuscripts regarding the shock work on FOX-7 single crystals are currently under preparation.

B.2 Presentations

Presentations related to this project during the reporting period are listed below.

1. Gupta, Y. M. *The Institute for Shock Physics: Understanding Materials at Extreme Dynamic Compression.* SSAP Symposium. Bethesda, MD. Contributed Presentation. (February 2016).
2. Gupta, Y. M. *Understanding Shock Wave Induced Chemical Reactions in Energetic Crystals*. ONR Collaborative Exchange Meeting. Cambridge, MA. (March 2016).
3. Dreger, Z. A., Y. M. Gupta and K. Zimmerman. *Understanding Insensitivity of Shocked Energetic Crystals: Molecular and Crystal Mechanisms*. ONR Collaborative Exchange Meeting. Argonne, IL. (March 2017).
4. Gupta, Y. M. The Institute for Shock Physics: *Understanding Materials at Extreme Dynamic Compression. SSAP Symposium.* Naperville, IL. (April 2017).
5. Gupta, Y. M. The Institute for Shock Physics: Focus on Dynamic Compression of Materials. Dynamic Compression Summer School. Argonne, IL. (August 2017).
6. Gupta, Y., Z. Dreger, Y. Gruzdikov, and M. Winey. *Linking Chemical Decomposition to Physical Changes in Shocked HE Crystals: Real-time Multiscale Measurements*. ONR Advanced Energetic Materials Collaborative Workshop. West Lafayette, IN. (March 2018).
7. Gupta, Y. M. *Focus on Dynamic Compression of Materials*. Dynamic Compression Summer School. Lemont, IL. (August 2018)
8. Dreger, Z. and Y. M. Gupta. *Effect of Nonhydrostatic Compression on the Structural and Chemical Stability of FOX-7 Crystals*. 21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter (SCCM). Portland, OR. Contributed Presentation. (June 2019).
9. Winey, J. M., Y. Toyoda, and Y. M. Gupta. *Shock Wave Response of an Insensitive High Explosive: Wave Profiles and Continuum Model for FOX-7 Single Crystals*. 21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter (SCCM). Portland, OR. Contributed Presentation. (June 2019).

V. Points of Contact in Navy
Joel Carney, NSWC Indian Head
Gerry Pangilinan, NSWC Indian Head
Zbigniew Dreger, NSWC Indian Head

VI. Acknowledgement/Disclaimer

This work was sponsored by the Office of Naval Research (ONR) under grant number N00014-16-1-2088 and by the DOE/NNSA under grant number DE-NA0002007. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the Office of Naval Research, or the U.S. government.

APPENDIX

Meeting Agenda
NSWC IH Visit
December 11, 2018
ISP Seminar Room (201)

Attendees
WSU: Yogi Gupta, Jim Hawreliak, Stefan Turneaure, Mike Winey, Yoshi Toyoda, and Kurt Zimmerman

NSWC IH: Zbib Dreger, Demitrios Stamatis, Daniel Wilson, Sean Maharrey, and Eric Herrera

Tuesday, December 11

8:30 AM	Arrive at the Institute for Shock Physics (ISP) and Introductions
8:40 – 9:25	ISP Overview
9:30 – 10:30	Tour of the ISP Facilities
10:30 – 10:45	*Break*
10:45 – 11:15	Naval Surface Warfare Center IHEODTD Brief
11:15 – 12:00	Outline of Potential Collaboration Areas
12:00 – 1:00	Working Lunch
1:15 – 2:45	Discussion of Planned Experiments
2:45 – 3:00	*Break*
3:00 – TBD	Next Steps including Specific Action Items

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*Times indicated are approximate and can be adjusted as needed.

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27-09-2019	Final	12/01/2015 - 05/31/2019

4. TITLE AND SUBTITLE

Understanding Molecular and Crystalline Mechanisms that Govern Insensitivity in Shocked Energetic Crystals

5a. CONTRACT NUMBER

5b. GRANT NUMBER

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14. ABSTRACT

The research focus of this project was on a fundamental understanding of the intrinsic properties of energetic crystals (molecular and crystalline attributes/mechanisms) that govern their insensitivity at conditions relevant to shock wave induced chemical decomposition. Some aspects of this effort were also relevant to thermal loading. The combination of well-characterized shock wave and static compression experiments on insensitive energetic single crystals – and different types of measurements – were used to gain insight into the molecular and crystalline mechanisms of interest. To the best of our knowledge, the shock wave measurements carried out on insensitive high explosive (IHE) single crystals represent the first such measurements. Shock wave experimental capabilities – central to this research effort – were also utilized for developing a research collaboration with NSWC-IH.

15. SUBJECT TERMS

Energetic materials, shock wave experiments, insensitive energetic single crystals, static compression experiments, chemical changes

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