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The project focuses on understanding the initial steps of energetic material ignition at the molecular level, with the long-range goal of understanding the fundamental mechanisms of the sensitivity of energetic materials. The effort involves three distinct, but ultimately related projects: (1) understanding the detailed behavior of solid-state molecules immediately behind a shock front; (2) developing new diagnostic techniques and using them to investigate the picosecond time scale behavior of insensitive energetic materials under shock loading conditions; and (3) studying molecular mechanical energy transfer in condensed energetic materials. In the past three years, new methods were developed for reproducibly shocking energetic materials and probing the result using vibrational spectroscopy with extremely high time resolution. A new vibrational spectroscopy technique was developed and used to study vibrational energy transfer in a condensed high explosive, nitromethane. Besides providing the first ever view into vibrational energy transfer in a condensed high explosive, some intriguing results were obtained involving the channeling of vibrational energy into the ubiquitous nitro group.

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Authors: Lee, I-Y Sandy., Hill, Jeffrey R., Dlott, Dana D.

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2. Name of Journal: Applied Physics Letters

Title of Article: Dynamics of a polymer shock optical microgauge studied by picosecond coherent Raman spectroscopy

Authors: David E. Hare, Jens Franken, Dana D. Dlott, Eric L. Chronister and James Flores

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3. Name of Journal: Journal of Physical Chemistry

Title of Article: Ultrafast energy transfer in high explosives: vibrational cooling

Authors: Sheah Chen, Xiaoyu Hong, Jeffrey R. Hill and Dana D. Dlott

Volume 99 Pages 4525-4530 Month Published: March Year: 1995

4. Name of Journal: Journal of Applied Physics

Title of Article: Coherent Raman measurements of polymer thin film pressure and temperature during picosecond laser ablation

Authors: David E. Hare, Jens Franken and Dana D. Dlott

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5. Name of Journal: Journal of Physique C

Title of Article: Picosecond dynamics behind the shock front

Authors: Dana D. Dlott

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6. Name of Journal: Journal of Physical Chemistry

Title of Article: Ultrafast mode-specific intermolecular vibrational energy transfer to liquid nitromethane

Authors: Xiaoyu Hong, Sheah Chen, and Dana D. Dlott

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7. Name of Journal: Journal of Chemical Physics

Title of Article: Molecular dynamics observed 60 picoseconds behind a solid-state shock front

Authors: I-Yin Sandy Lee, Jeffrey R. Hill, Honoh Suzuki, Bruce J. Baer and Eric L. Chronister, and Dana D. Dlott

Volume 103 Pages 8313-821 Month Published: Nov Year: 1995

8. Name of Journal: Chemical Physics Letters

Title of Article: A new method for studying picosecond dynamics of shocked solids: application to crystalline energetic materials

Authors: David E. Hare, Jens Franken and Dana D. Dlott

Volume 244 Pages 224-230 Month Published: Oct Year: 1995

9. Name of Journal: Time-resolved Vibrational Spectroscopy VII (book of conference abstracts).

Title of Article: Time-resolved Two-dimensional Vibrational Spectroscopy and its Application to High Explosives

Authors: Xiaoyu Hong and Dana D. Dlott

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10. Name of Journal: Time-resolved Vibrational Spectroscopy VII (book of conference abstracts).

Title: Picosecond time-resolved coherent Raman temperature-pressure jump spectroscopy

Authors: David E. Hare, Jens Franken and Dana D. Dlott

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11. Name of Journal: Shock Compression of Condensed Matter--1995 (book of conference abstracts).

Title of Article: Ultrafast spectroscopy of the first nanosecond

Authors: I-Yin Sandy Lee, David E. Hare, Jeffrey R. Hill, Jens Franken, Honoh Suzuki, Dana D. Dlott, Bruce J. Baer and Eric L. Chronister

Volume 370 Pages 905-908 Month Published: Year: 1995

12. Name of Journal: Decomposition, Combustion and Detonation Chemistry of Energetic Materials, Mat. Res. Soc. Symp. Proc.

Title of Article: Ultrafast dynamics of shock waves and shocked energetic materials

Authors: David E. Hare, I-Yin Sandy Lee, Jeffrey R. Hill, Jens Franken, Honoh Suzuki, Bruce J. Baer, Eric L. Chronister and Dana D. Dlott

Volume 418 Pages 337-348 Month Published: Year: 1996

13. Name of Journal: Decomposition, Combustion and Detonation Chemistry of Energetic Materials, Mat. Res. Soc. Symp. Proc.

Title of Article: Vibrational energy transfer in high explosives: nitromethane

Authors: Xiaoyu Hong, Jeffrey R. Hill and Dana D. Dlott

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14. Name of Journal: Journal of Applied Physics

Title of Article: Ultrahigh time resolution vibrational spectroscopy of shocked molecular solids

Authors: Selezion A. Hambir, Jens Franken, David E. Hare, Eric L. Chronister, Bruce J. Baer and Dana D. Dlott

Volume 81 Pages 2157-2166 Year: 1997.

15. Name of Journal: Shock Waves

Title of Article: Shock waves in molecular solids: ultrafast vibrational spectroscopy of the first nanosecond

Authors: Jens Franken, Selezion Hambir, David E. Hare and Dana D. Dlott

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Name of Journal: Physical Review Letters

Title of Article: Ultrafast Raman spectroscopy of shock fronts in molecular solids

Authors: Guray Tas, Jens Franken, Selezion A. Hambir and Dana D. Dlott

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Name of Journal: Journal of Applied Physics

Title of Article: Coherent Raman spectroscopy of nanoshocks

Authors: Guray Tas, Selezion A. Hambir, Jens Franken, David E. Hare and Dana D. Dlott

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Technical summary

The project focuses on understanding the initial steps of energetic material ignition at the molecular level, with the long-range goal of understanding the fundamental mechanisms of the sensitivity of energetic materials. Our efforts involve three distinct, but ultimately related projects: (1) understanding the detailed behavior of solid-state molecules immediately behind a shock front; (2) developing new diagnostic techniques and using them to investigate the picosecond time scale behavior of insensitive energetic materials under shock loading conditions; and (3) studying molecular mechanical energy transfer in condensed energetic materials.

In what follows, reference numbers (x) refer to the above publication list.

In order to learn about the first two issues listed above, we need to shock energetic solids and monitor their physical and chemical response with very high time, space, and frequency resolution. The idea is to better understand the elementary events in shock initiation of energetic materials. At the beginning of the project we used a very primitive method of generating and detecting shock waves (1). The generation method used metal foils, following earlier research, and the detector was just a camera which took photomicrographs of the shock in a polymer film. We had risetimes of a few hundred ps. We then developed spectroscopic probe methods. Spectroscopy is preferred because it provides molecular-level information. We tried a coherent Raman method (CARS) (2) which had a great deal of promise because it had the potential of telling us the shocked material's temperature, pressure and composition. However the CARS apparatus did not make a good shock wave, and the experiment was limited to polymer films. The metal foil apparatus, which made a pretty good shock wave, was coupled with spectrographs, and a study was made of strongly absorbing dye molecules in a polymer film (7). This study was the first ever observation of molecular dynamics right behind a shock front. However this method was limited by the balkiness of the laser, and the fact that absorption spectroscopy is not very good for the desired energetic materials. Next we figured out how to extend the CARS experiments so energetic materials could be studied (8). That involved using very fine particles of energetic material doped in a polymer layer. The technique, with subsequent modifications, proved quite versatile, and it became possible to see shock effects in virtually any energetic material, including insensitive explosives NTO and TATB. Still we were limited by the problem that the CARS laser didn't make a very good shock wave. Eventually we figured out how to make a really great shock wave using the CARS apparatus. That involved inventing a new type of polymer shock generation layer assembly (14), and a new detection scheme using a polycrystalline layer of anthracene. Then the shock we were making was so great, in the sense that it had such a fast risetime, that we couldn't even measure how fast it was. We developed an improved sample system and a new method of spectral analysis, and we were finally able to see the risetime of the shock front was <25 ps. Now I am very happy because we seemingly have it all together. We can produce very nice and reproducible shocks and we can use and probe energetic materials. There is still a lot of room for future development, however. First the shock pressure needs to be increased a bit from the present maximum of ~45 kilobars, in order to cause chemical reactions in insensitive energetic materials. Second we need to develop femtosecond detection schemes to be able to really get at the shock front. Whatever happens in the future, we have made great strides in shock generation and detection, and our group is arguably the world leader in this area now.

In order to learn about the third issue of molecular energy transfer, we need to develop new kinds of time-resolved vibrational spectroscopy to monitor the flow of mechanical energy in energetic materials. We have developed a "two-dimensional vibrational spectroscopy", which is a combination of infrared (IR) and anti-Stokes Raman spectroscopy. In this technique, an intense infrared pulse is tuned to excite a specific, selected vibrational state of an energetic material, and a subsequent visible probe pulse elicits the anti-Stokes Raman spectrum. In anti-Stokes Raman, the instantaneous intensity of a particular transition is proportional to the occupation number of the mode responsible for that transition, so this probing technique gives an instantaneous snapshot of how much energy is where in the molecule. Using a ps YLF laser, we obtained some very interesting results on a model system for condensed phase explosives, liquid nitromethane (NM). We were able to monitor energy flow through the NM molecules on the ~50 ps time scale (3). In addition, we were able to monitor the transfer of energy from other molecules to NM. The most interesting finding was that mechanical energy could be trapped for what seems to be a long time, ~25 ps, in symmetric stretching modes of the nitro group. Furthermore, in mixtures of NM and other molecules, specifically alcohols, exciting the alcohol molecule also resulted in energy trapping in the nitro group. This channeling and trapping into the nitro group was totally unexpected, and might provide insights into why nitro groups are found in almost all technologically important energetic materials. There were several difficulties in using our YLF laser, primarily the very long pulse duration of ~80 ps. We put much time and effort into improving it, but ultimately turned to a new type of laser, Ti:sapphire. We have now finished a Ti:sapphire laser which is the envy of other vibrational spectroscopists, which has time resolution of ~0.5 ps. We have remeasured NM with much better time resolution and have some preliminary data which is very interesting. We will now extend this instrument to other energetic material systems.