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Publications Resulting from the Fundamental Research on Explosives Program

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PUBLICATIONS RESULTING FROM THE FUNDAMENTAL RESEARCH ON EXPLOSIVES PROGRAM

by

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ABSTRACT

The five-year Fundamental Research on Explosives Program at Los Alamos National Laboratory, begun in 1981, was the study of explosives behavior at a molecular level. The research team developed and tested a model of a simple explosive, liquid nitric oxide (NO), overcoming difficult problems to investigate its properties. Using recently developed high-speed technology, we conducted innovative experiments, such as those on high-density NO, on the molecular spectroscopy of shock-compressed materials, and on detonating liquid NO. We developed methods for calculating the thermodynamics of dense molecular systems and describing molecular-level chemistry. The team obtained theoretical and experimental equations of state for the products of detonating liquid NO and obtained the first coherent anti-Stokes Raman spectroscopy data in shock-compressed materials. The program created worldwide enthusiasm in detonation and shock wave physics and chemistry; the bibliography included in this report is the result of numerous requests for our results.

In October 1981, Los Alamos National Laboratory initiated a five-year program, known as the Fundamental Research on Explosives (FRE) Program, supported by the Laboratory's Institutional Scientific Research and Development funding. The program was a Laboratory-wide effort to apply state-of-the-art theory and experimentation to the behavior of explosives at a molecular scale. The primary goal of the program was to gain a fundamental understanding of the phenomenology of the explosive process. The plan was to investigate a simple explosive system in order to develop a model that contained most of the "real" chemistry and physics, with as much a priori input as possible, and to test this model against experiments. Heretofore, such a plan would have been virtually impossible because of inherent difficulties, such as the extremely short time scales involved in the process. The commonly observed time scales in order of magnitude are as follows: shock front, picoseconds; reaction zone, nanoseconds; and major heat release, nanoseconds.

The basic idea of the program was to investigate the properties of a prototypal explosive. This prototype had to be simple enough to limit the number of important chemical reactions, but it still had to be a condensed-phase explosive that would yield results applicable to practical explosives. Liquid nitric oxide (NO) was chosen as the explosive for investigation because of the homogeneity of the liquid phase. It offered the molecular simplicity of a diatomic molecule, and because earlier experiments[1] had shown the feasibility of conducting detonation experiments on this system. These experiments provided some useful information including the fact that liquid NO is a sensitive explosive with a detonation velocity of 5.6 mm/μs and an estimated detonation pressure of 100 kbar. The detonation products of liquid NO had been calculated to be the simple molecules, N_2 and O_2, for which there existed good theoretical data. In addition, liquid NO could be obtained in high purity and in a well-characterized form at Los Alamos.

The status of technology in theoretical molecular dynamics and computation capability and in modern spectroscopy indicated that perhaps the time for undertaking this kind of study had arrived. Certain high-speed instrumentation and techniques had recently been developed, and it was believed that these tools could be applied to studying the molecular-level chemistry of explosives. Examples of available instruments included the Cray computers and picosecond lasers. It was our task to adapt and modify these and many other instruments and techniques to help provide an insight into the role of molecular-level chemistry in explosives behavior.

Using this new technology, we sought to accomplish the following:

- Use theory and experiment together in a unified program to attain the confidence of accurately calculating the equations of state for both the explosives and their reaction products, as individual molecules and in mixtures of molecules.
- Test the basic assumptions of detonation theory using the real measured equation of state for the detonation products of a condensed-phase explosive.
- Test detonation theory as a description of real detonations (nonlaminar) to get a measure of the approximations of the laminar theory.
- Develop new techniques, especially new laser spectroscopic techniques, for the study of shock waves.
- Develop interest in detonation science among scientists who had not previously been involved in the field.

[1]J. B. Ramsay and W. C. Chiles, “Detonation Characteristics of Liquid Nitric Oxide,” in Proc., Sixth Symposium (International) on Detonation, 723 (1976).

- Produce a new sense of excitement and enthusiasm in the minds of the scientists who have been working for years in the field.

The FRE program produced a worldwide impact on the science of detonation and shock wave physics and chemistry. Much enthusiasm was exhibited by scientific investigators at Los Alamos, at sister Department of Energy and Department of Defense facilities, and from groups in Germany, France, and Canada. At Los Alamos, numerous scientists who previously had not held an interest in this field began their own investigations into explosives-related phenomena, which are continuing.

The FRE program was organized at Los Alamos as follows:

- Principal sponsoring directorate—Associate Directorate for Engineering Sciences (ADES)
- Program manager—L. A. Gritzo (M-Division Office)
- Project manager—T. Rivera (Group M-1)
- Technical advisory committee—D. Breshears (Group CHM-2), W. Fickett (Group M-3), B. L. Holian (Group T-4), and R. R. Ryan (Group INC-4)
- Participating divisions—Dynamic Testing (M), Design Engineering (WX), Isotope and Nuclear Chemistry (INC), Chemistry (CHM), Physics (P), and Theoretical (T)
- Participating groups—Explosives Technology (M-1), Detonation Physics (M-3), Shock Wave Physics (M-6), Fabrication and Assembly (WX-3), Isotope and Structural Chemistry (INC-4), Analytical Chemistry (CHM-1), Physical Chemistry (CHM-2), Photochemistry (CHM-4), Condensed Matter and Thermo Physics (P-10), Equation of State and Opacity (T-4), Theoretical Chemistry and Molecular Physics (T-12), and Detonation Theory and Application (T-14)

The researchers worked diligently to achieve their stated goals. Eventually, however, the program underwent a transition from a relatively diversified effort (Table I) to a focused set of teams (Table II). Some of the earlier gas-phase studies were found to be inadequate in describing the shocked (and detonating) condition of liquid NO. The highly excited gas phase and molecular beam cluster studies were discontinued in favor of condensed-phase techniques.

Table I. Early FRE Team Efforts

Theory

P. J. Hay (T-12)	Ab Initio Intermolecular Potentials
J. D. Johnson (T-4) and M. S. Shaw (T-14)	Thermodynamics of Dense Molecular Fluids
R. T. Pack (T-12)	Semi-Empirical Molecular Potentials
J. R. Stine (M-1)	Theoretical Chemical Dynamics

Hydrodynamics

W. C. Davis (M-3)	Detonation Physics
G. L. Schott (M-1)	Shocked-State Measurements
R. L. Mills (P10) and L. A. Schwalbe (WX-3)	Unreacted NO EOS
S. C. Schmidt (M-6)	Laser-Based Diagnostics of Shocked Material

Spectroscopy

S. F. Agnew (INC-4) and B. I. Swanson (INC-4)	Spectroscopy of Molecules At High Density
N. C. Blais (CHM-2)	Studies of Clusters Of Explosive Molecules
N. R. Greiner (CHM-1)	Detonation Products Chemistry
J. B. Cross(CHM-2)	Intermolecular Forces
D. S. Moore (CHM-4)	Laser-Based Diagnostics of Shocked Material
D. Schiferl (M-6)	Spectroscopy of Molecules at High Densities
J. J. Valentini (CHM-2) and N. S. Nogar (CHM-2)	Spectroscopy of Highly Excited Molecules

Table II. Later FRE Team Efforts

Theory

P. J. Hay (T-12) and R. R. Pack (T-12)	Theory of Reaction Mechanisms
J. D. Johnson (T-4) and M. S. Shaw (T-14)	Thermodynamics of Dense Molecular Fluids
J. R. Stine (M-1)	Theoretical Chemical Dynamics

Hydrodynamics

W. C. Davis (M-3) and G. L. Schott (M-1)	Detonation and Shocked-State Measurements

Continued on next page

Table II—*Continued*

Spectroscopy

S. C. Schmidt (M-6) and D. S. Moore (CHM-4)	Laser-Based Diagnostics of Shocked Material
S. F. Agnew (INC-4), B. I. Swanson (INC-4) and D. Schiferl (M-6)	Spectroscopy of Molecules at High Density
N. C. Blais (CHM-2) and N. R. Greiner (CHM-1)	Real-Time Detonation Studies

Thus, regarding the later FRE team efforts, the team of Blais and Greiner performed experiments on the real-time analysis of the reaction products of shocked, solid NO. The team of Agnew, Swanson, and Schiferl, using diamond anvil cells, conducted spectroscopic experiments on high-density NO. The team of Schmidt and Moore performed difficult but elegant experiments on the molecular spectroscopy of shock-compressed materials. The team of Davis and Schott performed the difficult hydrodynamic experiments on detonating liquid NO.

On the theoretical front were the teams of Shaw and Johnson, who developed theoretical molecular dynamics methods to calculate the thermodynamics of dense molecular systems, and Stine and D. W. Noid (not a FRE member), who developed semiclassical “chemical dynamics” methods to describe molecular-level chemistry. Hay and Pack employed ab initio and semi-empirical quantum mechanical methods to calculate chemical structures.

A major milestone was achieved when the team obtained both a theoretical equation of state (EOS) and an experimental EOS for the products of detonating liquid NO. Both methods, although completely independent of one another, yielded Hugoniot information that was in remarkably close agreement. The theoretical EOS work addressed deficiencies in the treatment of the anisotropy of molecules and in the mixing of fluids. A new, approximate variational method for sphericalization and mixing, and a new virial technique for mixing different species were developed.

The first coherent anti-Stokes Raman spectroscopy (CARS) data in shock-compressed materials were obtained. A two-stage light gas gun was used to accelerate a polycarbonate projectile to a desired velocity. The projectile struck a stainless-steel target plate producing a shock wave that ran forward into a 3-mm-thick liquid sample. CARS signals, produced in the shocked samples, were detected and recorded.

In the final analysis, the degree to which success is achieved for a program of fundamental research can be judged by the number and kind of resulting publications. After receiving requests from numerous scientists for the results of the FRE program, we composed the following bibliography from as many publications as we could find that were generated from the program. Even though years have passed since the conclusion of the program, much of the work and technical achievements reported are current, pertinent, and continuing.

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