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OFFICE OF NAVAL RESEARCH
END-OF-YEAR REPORT*

for

01 December 1988 through 30 September 1989

Contract # N00014-89-WX-24146

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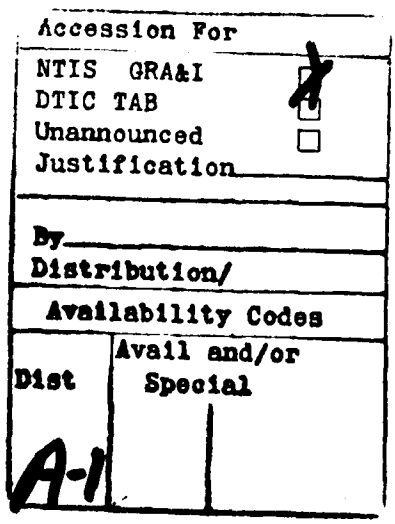
TECHNICAL REPORT # 6

SIMULATIONS OF REACTIVE COLLISIONS IN DETONATING SOLIDS

Carter T. White and Donald W. Brenner

Code 6119, Chemistry Division
Naval Research Laboratory
Washington DC 20375-5000

30 September 1989



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Washington DC 20375-5000

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END-OF-YEAR REPORT (Part I)
Contract # N00014-89-WX-24146

PART I

a. Papers Submitted to Refereed Journals (not yet published):

1. D.W. Brenner, C.T. White, M.L. Elert, and F. E. Walker
"Chemical Model for Intrinsic Detonation Velocities",
Int. J. Quantum Chem. (in press).

b. Papers Published in Refereed Journals:

1. M.L. Elert, D.M. Deaven, D.W. Brenner, and C.T. White,
"One-Dimensional Molecular-Dynamics Simulation of the Detonation of Nitric Oxide", *Phys. Rev. B (Rapid Comm.)* **39**, 1453 (1989).

2. J.W. Mintmire, B.I. Dunlap, D.W. Brenner, R.C. Mowrey, H.D. Ladouceur, P.P. Schmidt, C.T. White, and W.E. O'Grady,
"Chemical Forces Associated with Deuterium Confinement in Palladium",
Phys. Lett. A **138**, 51 (1989).

c. Books (and sections thereof) Submitted for Publication:

1. M.L. Elert, D.W. Brenner, and C.T. White,
"Some One-Dimensional Molecular Dynamics Simulations of Detonation",
1989 APS Topical Conference on Shock Compression of Condensed Matter, (in press).

2. D.W. Brenner, M.L. Elert, and C.T. White,
"Incorporation of Reactive Dynamics in Simulations of Chemically Sustained Shock Waves", *1989 APS Topical Conference on Shock Compression of Condensed Matter*, (in press).

d. Books (and sections thereof) Published: None

e. Technical Reports Published and Papers Published in Non-Refereed Journals:

1. C.T. White, M.L. Elert, and D.W. Brenner
"Simulations of Detonating Chains",
Proceedings of the ONR-Sandia Workshop on Energetic Materials Initiation Fundamentals, Published by the Chemical Propulsion Information Agency.

2. D.W. Brenner, C.T. White, and M.L. Elert
"Simulations of Reactive Collisions in Condensed Phases: Application to Detonating Solids", Proceedings of the ONR-Sandia Workshop on Energetic Materials Initiation Fundamentals, Published by the Chemical Propulsion Information Agency.

f. Patents Filed: None

g. Patents Granted: None

h. Invited Presentations:

1. C.T. White, M.L. Elert, and D. W. Brenner,
"Simulations of Detonating Chains",
ONR-Sandia Workshop on Energetic Material Initiation Fundamentals,
Livermore CA, December 1989.

2. D.W. Brenner, M.L. Elert, and C.T. White,
"Simulations of Reactive Collisions in Condensed Phases: Application to Detonating Solids", ONR-Sandia Workshop on Energetic Material Initiation Fundamentals,
Livermore CA, December 1989.

3. C.T. White, "Simulations of Chemically Sustained Shock Waves in Molecular Solids", Dept. Colloquium, University of NM, Albuquerque NM, March 1989.

4. C.T. White, D.W. Brenner, and M.L. Elert,
"Modeling Reactive Collisions in Molecular Solids",
ONR Workshop on Theoretical Chemistry,
George Washington University, Washington DC, April 1989.

5. D.W. Brenner, "Molecular-Dynamics Simulations of Chemically-Sustained Shock Waves in Solids", Xerox Webster Research Center, Webster NY, June 1989.

i. Contributed Presentations:

1. D.W. Brenner, C.T. White, and M.L. Elert,
"Simulations of Reactive Collisions in a Molecular Solid",
March Meeting of the APS, St. Louis MO, March 1989,
[*Bull. Am. Phys. Soc.* **34**, 608 (1989)].

2. C.T. White, D.W. Brenner, M.L. Elert, and F.E. Walker,
"Molecular Dynamics Simulations of Shock Waves in Model Energetic Materials",
1989 Sanibel Symposia, St. Augustine FL, April 1989.

3. D. W. Brenner, C.T. White, and M.L. Elert,
"Simulation of a Chemically-Sustained Shock Wave in a Molecular Solid",
Conference of the Dynamics of Molecular Collisions, Asilomar CA, July 1989.

4. D.W. Brenner, C.T. White, and M.L. Elert
"Reaction Dynamics of a Chemically-Sustained Shock Wave",
1989 APS Topical Conference on Shock Compression of Condensed Matter,
Albuquerque NM, August 1989 [*Bull. Am. Phys. Soc.* 34, 1722 (1989)].

5. M.L. Elert, D.W. Brenner, and C.T. White
"Some One-Dimensional Molecular Dynamics Simulations of Detonations",
1989 APS Topical Conference on Shock Compression of Condensed Matter,
Albuquerque NM, August 1989 [*Bull. Am. Phys. Soc.* 34, 1722 (1989)].

j. Honors/Awards/Prizes: None

k. Number of Graduate Students Receiving Full or Partial Support on Contract: None

l. Number of Postdoctoral Fellows Receiving Support on ONR Contract: One

END-OF-YEAR REPORT (Part II)
Contract # N00014-89-WX-24146

PART II

a. Principal Investigator:

Dr. Carter T. White
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Washington DC, 20375-5000

b. Cognizant ONR Scientific Officer:

Dr. Donald H. Liebenberg
Code 1112AI
Office of Naval Research
Arlington VA, 22217-5000

c. Current Telephone Number: (202)-767-3270

d. Brief Description of Project:

This project uses molecular dynamics simulations to study the short-time chemistry and physics of detonating solids. A variety of condensed phase systems are studied ranging from one-dimensional chains to complex molecular solids. This research first requires the development of potentials capable of realistically modeling shock-induced chemical reactions in energetic molecular solids. Molecular dynamics simulations using these potentials are then carried out to study the role of molecular-scale chemistry in the initiation and propagation of solid-state detonations. This research addresses a number of fundamental issues including: (i) whether concerted chemical reactions at or near the shock front sustain a detonation; (ii) whether parallels can be drawn between gas-phase reactions and detonations; and, (iii) whether molecular scale dynamics can provide insight into making safer explosives.

e. Significant Results During FY 89:

Many-body 'chemical' forces were incorporated into a molecular dynamics simulation of a detonating one-dimensional chain using the LEPS formalism.[h1] Parameters of the forces were chosen appropriate for modeling the condensed-phase detonation of nitric oxide according to the reaction, $2NO \rightarrow N_2 + O_2$. The simulations displayed a self-propagating shock front with a stable velocity which was an intrinsic property of the system. For initially overdriven detonations the detonation velocity converged to this stable intrinsic velocity over a period of several picoseconds. During this time the reaction efficiency of nitric oxide behind the front was noticeably decreased, indicating a relationship between reaction kinetics and the steady-state detonation velocity. This study was the first molecular dynamics simulation of a detonating system that used realistic endothermic bond-breaking and exothermic bond-forming chemical reactions.

The concept of incorporating realistic chemical reactivity into simulations of detonations was successfully extended to higher dimensions using the Tersoff many-body bonding formalism.[h2,h5] Tersoff potentials were also used to further study one dimensional chains.[h4] The Tersoff formalism had only previously been applied to group IV solids, and so our efforts were the first to extend it to reacting molecular solids. Using

a two-dimensional crystal composed of diatomic molecules as a model energetic material, the simulations displayed properties of real detonating systems such as initiation behind a leading shock wave, an intrinsic detonation velocity that was in agreement with typical experimental velocities, and a following flow.[h5] Comparison of few-body reaction dynamics in the gas phase with atomic velocities near the shock front suggested that the intrinsic detonation velocity is influenced by endothermic bond breaking reactions.[h2] Further support for this hypotheses came from simulations of a molecular solid which used a potential energy function that was identical to the energetic solid except that net exothermic bond formation was not included. The picture that is emerging from these initial studies is that the detonation velocity is limited to just above the threshold required for endothermic molecular dissociation at the shock front.

f. Summary of Plans for FY 90:

The results obtained in the first nine months of this contract have demonstrated that our molecular based simulations provide a good starting point for describing many of the properties of detonating solids. In the coming year we plan to extend our current simulation techniques to larger and more diverse systems. This phase of the project will require the development of potential energy functions that can begin to model more complicated molecular solids (e.g. those containing conjugated rings and strained cage structures). Next year we also plan longer computer runs to further link the atomic-scale behavior observed in our simulations to well-established 'macroscopic' models of detonation. Finally, we expect to begin studies of defects which are thought to play an important role in the initiation of detonations. With our techniques we can include defects in the simulation both in the form of structural imperfection (e.g. vacancies and grain boundaries) and chemical impurities (e.g. reactive radicals and high mass atoms).

g. Current Graduate Students and Postdoctorals Working on this Project:

Dr. Phuoc X. Tran (full-time ONT post-doc)

h. Technical Reports Submitted to ONR During the Past Year:

1. M.L. Elert, D.M. Deaven, D.W. Brenner, and C.T. White, "One-Dimensional Molecular-Dynamics Simulation of the Detonation of Nitric Oxide", *Phys. Rev. B (Rapid Comm.)* **39**, 1453 (1989).

2. D.W. Brenner, C.T. White, M.L. Elert, and F. E. Walker "Chemical Model for Intrinsic Detonation Velocities", *Int. J. Quantum Chem.* (in press).

3. J.W. Mintmire, B.I. Dunlap, D.W. Brenner, R.C. Mowrey, H.D. Ladouceur, P.P. Schmidt, C.T. White, and W.E. O'Grady, "Chemical Forces Associated with Deuterium Confinement in Palladium", *Phys. Lett. A* **138**, 51 (1989).

4. M.L. Elert, D.W. Brenner, and C.T. White, "Some One-Dimensional Molecular Dynamics Simulations of Detonation", *1989 APS Topical Conference on Shock Compression of Condensed Matter*, (in press).

5. D.W. Brenner, M.L. Elert, and C.T. White, "Incorporation of Reactive Dynamics in Simulations of Chemically Sustained Shock Waves", *1989 APS Topical Conference on Shock Compression of Condensed Matter*, (in press).

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