**Title:** Simulations of Reactive Collisions in Detonating Solids (End-Of-Year Report)

**Authors:** Carter T. White and D. W. Brenner

**Report Date:** End-Of-Year Report, 8/12/89 to 8/9/90

**Abstract:**

(U) End-Of-Year Report for ONR project entitled "Simulations of Reactive Collisions in Detonating Solids"
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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SIMULATIONS OF REACTIVE COLLISIONS IN DETONATING SOLIDS

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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:

   "One-Dimensional Molecular-Dynamics Simulation of the Detonation of Nitric

   Schmidt, C.T. White, and W.E. O'Grady,
   "Chemical Forces Associated with Deuterium Confinement in Palladium",

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",

2. D.W. Brenner, M.L. Elert, and C.T. White,
   "Incorporation of Reactive Dynamics in Simulations of Chemically Sustained Shock

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.

   "Simulations of Reactive Collisions in Condensed Phases: Application to Detonating
   Initiation Fundamentals, Published by the Chemical Propulsion Information
   Agency.

f. Patents Filed: None

g. Patents Granted: None
h. Invited Presentations:


i. Contributed Presentations:


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
PART II

a. Principal Investigator:

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Dr. Donald H. Liebenberg
Code 1112AI
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Arlington VA, 22217-5000

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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.\(^{1}\) Parameters of the forces were chosen appropriate for modeling the condensed-phase detonation of nitric oxide according to the reaction,

\[ 2\text{NO} \rightarrow \text{N}_2 + \text{O}_2. \]

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.\(^{2,3}\) Tersoff potentials were also used to further study one dimensional chains.\(^{4}\) 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. 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:


Carter T. White  
Theoretical Chemistry Section  
Chemical Dynamics and Diagnostics Branch  
Chemistry Division, Code 6119

Donald W. Brenner  
Theoretical Chemistry Section  
Chemical Dynamics and Diagnostics Branch  
Chemistry Division, Code 6119
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