NANO ENGINEERED ENERGETIC MATERIALS MURI

Summary

ARO Review of Nanoenergetic Materials Initiatives
MURI / DURINT Review
16-17 November 2005
Holiday Inn Aberdeen, Aberdeen, MD
Significant Accomplishments

- Real time shock compression of SAMs.
- Chemical reaction propagation in nanoenergetic materials with nanometer space and subnanosecond time resolution.
- Fast imaging and spectroscopy of energy release.
- Examination of Al cluster synthesis by reacting Al(I) halides with LiN(SiMe₃)₂.
- Synthesis of Al₁₂ icosahedral cluster capped by i-Bu groups.
- Studies investigating the synthesis of size selected Al clusters using metal hydride precursors as source agents- RAlH₂ has been targeted (R group – N(SiMe₃)₂ to produce a protective capping ligand.
- Studies have been initiated to examine the structure of clusters that are prepared directly in the analytical region of a UHV STEM instrument.
- Constructed custom uhv chambers with Al sources for building oxidizer-fuel (Al) interface model structures and analyzing reaction chemistry.
  - Infrared spectroscopy
  - X-ray photoelectron spectroscopy
  - Atomic force microscopy
- Did first studies to evaluate best nitroaromatic oxidizer self-assembled monolayer (SAM) structures to use.
- Did first analysis of Al reaction chemistry with room temperature oxidizer SAMs.
- In process of installing sample temperature control from cryo to elevated temperatures (~200 deg C).
• Development of a scalable parallel algorithm for ReaxFF MD simulations using spatial decomposition.
• Performed scalability test of the P-ReaxFF algorithm on an 800-processor Power4 system at DoD’s Artic Region Supercomputing Center - parallel efficiency and communication overhead with scaled workloads – 86,016 P atom RDX systems on P processors.
• To validate ReaxFF MD simulations of Al nanoparticles embedded in energetic crystal, MD simulation was performed of RDX molecule on Al (111) surface, in which interatomic forces were computed quantum mechanically (in framework of DFT).
• Flame propagation across thin films of nAl performed to understand role of Pe and Ra numbers on reaction front.
• Burning behavior of quasi-homogeneous mixtures of nAl – liquid water and nAl – liquid nitromethane analyzed.
• Fabrication and flame propagation of nano-energetic materials in microchannels underway.
• Developed and constructed high pressure RESS system for fabrication of nano RDX.
• Completion of 3-D flow modeling of RESS for fabrication of NEM.
• Multi-scale modeling of ignition and combustion of single aluminum particles.
Manuscripts submitted


“Nanotechnology energetic material dynamics studied with nanometer spatial resolution and picosecond temporal resolution”, Dana D. Dlott, Selezion A. Hambir, Hyunung Yu, Proceedings of 6ISICP conference (3/05).

“Thinking big (and small) about energetic materials”, Dana D. Dlott, Materials Science and Technology (submitted 5/5/05).

Papers published in peer-reviewed journals


Papers published in non-peer-reviewed journals or in conference proceedings


“Nanotechnology energetic material dynamics studied with nanometer spatial resolution and picosecond temporal resolution”, Dana D. Dlott, Selezion A. Hambir, Hyunung Yu, Proceedings of 6ISICP conference (3/05).


“Nanotechnology energetic material dynamics studied with nanometer spatial resolution and picosecond temporal resolution,” Dlott, D., (invited, keynote address), International Conference on Computational & Experimental Engineering and Sciences, Madeira, Portugal, (July ’04).


“Nanotechnology energetic material dynamics studied with nanometer spatial resolution and picosecond temporal resolution,” Dlott, D., (invited, plenary talk) Sixth International Symposium on Special Topics in Chemical Propulsion, Santiago, Chile (Mar. ’05).


Internal Collaborations/Interactions

- Dlott seminar at USC, April 2005
- Yetter seminar at USC, September 2005
- Vashishta seminar at UIUC, October 2005
- MURI Group meeting at USC, October 2005
- Nuzzo seminar at PSU, November 2005
- Nuzzo and Girolami interacting with Dlott on fabricating and analyzing SAMs on Al thin films and samples with monodisperse Al clusters in the size range of 10-70 atoms, 2005
- Vashishta, Rajiv, and Nakano interacting with Dlott on modeling of reactivity of SAMs on Al, 2005
- Yang, Yetter, and Son interacting on flame propagation of nAl mixtures, 2005
- Kuo and Yang interacting on supercritical fluid processing of nano energetic oxidizers, 2005
At Penn State, Dr. Steven F. Son has taken a year sabbatical from Los Alamos National Laboratory (LANL) to conduct collaborative research with Yetter, Kuo, Yang, and Allara on the MURI program. This collaboration will be continued through the duration of the program via graduate students spending summers at LANL.

Collaboration with Dr. Bryce Tappen and Dr. Blaine Asay of LANL on nanoenergetics established.

Kuo and Yetter have an existing program with Dr. Lee Harris at ARDEC on the development of advanced layered gun propellants. Nano energetic materials fabricated as part of this MURI will be used as ingredients in future formulations of these propellants.

Kuo and several members of his group as well as Yetter visited Picatinny Arsenal to confer with Mr. Victor Stepanov of New Jersey Institute of Technology (NJIT) and ARDEC about the RESS process. His advice and input was very helpful to the current work and collaborative interactions are planned for the future. During the 6th International Symposium on Special Topics in Chemical Propulsion, held in Santiago, Chile in March 2005, Kuo spoke with Professor Lev Krasnoperov of NJIT for the detailed operational process in the production of nano-crystalline RDX.

The Kuo group also consulted Dr. Jeff Morris of ARL this past year on solubility aspects for the RESS process. His familiarity with carbon dioxide and RDX reactions at elevated pressures were helpful in determining the pressure and temperature limits which were placed on the Penn State RESS system. While a visit was not made to his facility to see his Thar Technologies setup, photographs of his experimental facility were obtained and discussed. Dr. Morris also directed the team to past research on RESS systems and the most recent progress on the theoretical modeling of RDX solubility.

To increase communication and collaboration between the CACS group at USC and the theoretical chemistry group at ARL, Dr. Brad Forch and Dr. Kevin McNesby visited the CACS facilities, including a tour of the Data Visualization Center and the parallel computing labs. Dr. McNesby also gave a seminar on his research during the visit.

The CACS graduate student, Richard Clark, visited ARL in Maryland during August 2005. During his weeklong visit, he gave a presentation to the theoretical chemistry group and met with most of the group’s researchers individually. Richard Clark enjoyed the opportunity to discuss areas of future research collaborations with Dr. Brad Forch, Dr. Maggie Hurley, and Dr. Betsy Rice. The relationships developed during the visit will increase regular communications between CACS and ARL and will enhance opportunities for future collaborations. Another graduate student, Richard Seymour, will spend the 2006 summer at ARL as part of the continuing collaborations. CACS researchers and graduate students are using DoD supercomputing facilities including the supercomputer at ARL for large-scale simulations for NEEM research. The USC group has also been collaborating with the Goddard group at Caltech on modeling of energetic materials.

At UIUC, Diott has discussed his research extensively with collaborators at the DOE labs LANL and Argonne.
• Annual Review Meeting
• Participation in Relevant Scientific Meetings
• Distribution of Annual Report, Publications and Presentations of Team Members on CD to Review Panel Members
• Webpage established: www.NEEM.psu.edu
  – Program description
  – Links to team member websites
  – Downloadable material for distribution including annual reports and technical publications
Continued Commitment to Education

- Participation at technical meetings – PSU, UIUC, and USC students presenting papers at technical meetings.
- Summer interns at DoD and DoE laboratories – PSU graduate student to conduct research at LANL during summer 2006 – USC students visit ARL during summers of 2005 and 2006.
- Graduate Course “Combustion of Energetic Materials” taught by Dr. Steve Son at PSU during the Fall 05
- Graduate student and post-doc exchange between PSU, UIUC, and USC planned for a week duration during the summer of 2006 in PSU laboratories to further develop fundamental research and training in multidisciplinary fields of study including energetic materials, nanotechnology, spectroscopy, theoretical chemistry, combustion.
- Graduate student and post-doc conference around DoD laboratory to enhance student participation and understanding of important DoD relevant research under proposal consideration.