SYMPOSIUM H

Multifunctional Energetic Materials

November 28 - 30, 2005

Chairs

Alexander Gash	Lawrence Livermore National Laboratory
Naresh Thadhani	Georgia Institute of Technology
William Wilson	Defense Threat Reduction Agency
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This volume may be published in print format after the meeting.

* Invited paper

SESSION H1: Synthesis and Processing I
Chair: Adam Cumming
Monday Morning, November 28, 2005
Room 301 (Hynes)

8:30 AM *H1.1
Reactive Nanocomposite Powders: Synthesis by Arrested Reactive Milling and Characterization. Edward L. Dreizin, Mirko Schoenitz, Mikhaylo Trunov, Swati Umbrajkar, Xiaoying Zhu, Salil Mohan and Vern Hoffmann; Mechanical Engineering, NJ Institute of Technology, Newark, New Jersey.

9:00 AM H1.2
Synthesis and Characterization of Dual Functional Energetic Structural Materials Roussislava Zaharieva and Sathyanaraya Hanagud; Aerospace Engineering, Georgia Institute of Technology, Atlanta, Georgia.

9:15 AM H1.3
Novel Energetic Composite Materials. Jun Nable and Andrew Sherman; Powdermet Inc., Euclid, Ohio.

9:30 AM *H1.4
Reactive Multilayer Foils for Structural Energetic Applications. Timothy Weihs, [1]Department of Materials Science and Engineering, Johns Hopkins University, Baltimore, Maryland; [2]Reactive NanoTechnologies, Hunt Valley, Maryland.

10:00 AM BREAK

10:30 AM H1.5
Self-assembled Ordered Energetic Composites of CuO Nanorods and Nanowells and Al Nanoparticles with High Burn Rates. Rajesh V. Shende[1], Senthil Subramaniam[1], Steve Apperson[1], Shameem Hasan[1], Shantanu Bhattacharya[1], Yuanfang Gao[1], Maruf Hossain[1], Shubhra Gangopadhyay[1], Paul Redner[2], Deepak Kapoor[2] and Steven Nicolich[2]; [1]Electrical and Computer Engineering, University of Missouri, Columbia, Missouri, Missouri; [2]U.S. Army, ARDEC, Picatinny, New Jersey.

10:45 AM *H1.6
Low Density Metals Through Combustion Synthesis. Bryce Tappan, Los Alamos National Lab, Los Alamos, California.

11:15 AM *H1.7
The Application of Energetic SHS Reactions in the Synthesis of Multi-functional Bone Tissue Engineering and Drug Delivery Systems. John Jeremy Moore[1], Doug Burkes[1], Reed Ayers[1], Guglielmo Gottoli[1], Hu Chun Yi[2] and Jacques Guigne[2]; [1]Metallurgical and Materials Engineering, Colorado School of Mines, Golden, Colorado; [2]Guigne Space Systems Inc (GSSI), Golden, Colorado.

11:45 AM H1.8
Reactive Binary Al-Li Powders Prepared by Mechanical Alloying. Xiaoying Zhu, Mirko Schoenitz and Edward L. Dreizin; New Jersey Institute of Technology, Newark, New Jersey.

SESSION H2: Synthesis and Processing II
Chair: Reed Ayers
Monday Afternoon, November 28, 2005
Room 301 (Hynes)

1:30 PM *H2.1
Linear Cellular Alloys in Lightweight Steels and Composites: Fabrication, Quasi-static and Dynamic Properties Joe Cochran[1], Justin Clark[1], David McDowell[2,1], Thomas Sanders[1] and Naresh Thadhani[1]; [1]Materials Science and Technology, Georgia Institute of Technology, Atlanta, Georgia; [2]Mechanical Engineering, Georgia Institute of Technology, Atlanta, Georgia.

2:00 PM *H2.2
Polymer-Coated Ultra-Fine Particles. Patrick Brousseau[1] and Charles Dubois[2]; [1]Energetic Materials, DRDC Valcartier, Val-Belair, Quebec, Canada; [2]Department of Chemical Engineering, Ecole Polytechnique de Montreal, Montreal, Quebec, Canada.

2:30 PM BREAK

3:30 PM *H2.3
Product design of particulate energetic materials Ulrich Teipel[1], Ulrich Foerter-Barth[2] and Michael Herrmann[2]; [1]Particle Technology, University of Nuremberg, Nuremberg, Germany; [2]Energetic Materials, Fraunhofer Institute for Chemical Technology, Pfinztal, Germany.

4:00 PM H2.4
Control of the Structural Refinement in Al-MoO_3 Nanocomposites Prepared by Arrested Reactive Milling. Swati M. Umbrajkar, Mirko Schoenitz and Edward L. Dreizin; Mechanical Engineering, New Jersey Institute Of Technology, Newark, New Jersey.

4:15 PM H2.5
Synthesis of Branched Phosphazene Based Energetic Materials Barny William Greenland[1], Joachim Steinke[1], David Widdowson[1], Peter Golding[2] and Steve Trussell[2]; [1]Chemistry Department, Imperial College, London, United Kingdom; [2]AWE, Aldermaston, United Kingdom.

4:30 PM *H2.6
Mechanically Alloyed Al-based Materials. Huey Hoon Hng, School of MS&E, Nanyang Technological University, Singaproe, Singapore.

SESSION H3: Characterization
Chair: Patrick Brousseau
Tuesday Morning, November 29, 2005
Room 301 (Hynes)

8:15 AM *H3.1
Ultrafast Dynamics of Nanotechnology Energetic Materials. Hyunung Yu, Selezion A. Hambir and Dana D. Dlott; School of Chemical Sciences, University of Illinois, Urbana, Illinois.

8:45 AM H3.2
On-Chip Initiation and Burn Rate Measurements of Thermite Energetic Reactions. Steven Apperson[1], Shantanu Bhattacharya[1], Yuanfang Gao[1], Senthil Subramanian[1], Shameem Hasan[1], Maruf Hossain[1], Rajesh V. Shende[1], Shubhra Gangopadhyay[1], Paul Redner[1], Deepak Kapoor[2] and Steven Nicolich[2]; [1]Electrical and Computer Engineering, University of Missouri, Columbia, Missouri, Missouri; [2]U.S. Army, ARDEC, Picatinny Arsenal, Picatinny, New Jersey.

9:00 AM *H3.3
Overview of Nanoscale Energetic Materials Research at Los Alamos. Steven F. Son, Lawrence Livermore National Laboratory,

Livermore, California.

9:30 AM H3.4
Protocols for in vitro toxicity screening of aluminum nanoparticles. Maria Palazuelos[1,4], David Moraga[2], Brij Moudgil[1,3], Mick Popp[2] and Kevin William Powers[1]; [1]Particle Engineering Research Center, University of Florida, Gainesville, Florida; [2]Interdisciplinary Center for Biotechnology Research, University of Florida, Gainesville, Colorado; [3]Materials Science and Engineering, University of Florida, Gainesville, Colorado; [4]Department of Chemical Engineering, University of Florida, Gainesville, Florida.

9:45 AM BREAK

10:15 AM *H3.5
Understanding and Tuning the Reactivity of NanoEnergetic Materials. A. Prakash, A. Rai, A. McCormick and Michael R. Zachariah; University of Maryland and NIST, College Pak, Maryland.

10:45 AM H3.6
Substrate Effects in Electrical Initiation of Nanolaminate Thin Films Joseph W. Tringe, Alexander E. Gash and Troy W. Barbee; Chemistry & Materials Science Directorate, Lawrence Livermore National Laboratory, Livermore, California.

11:00 AM *H3.7
Inorganic Nanoparticles for Gun Propellants. Barbara Baschung, ISL, Saint-Louis, France.

11:30 AM *H3.8
Energy Release Characteristics of Impact-Initiated Energetic Materials Richard G. Ames, Naval Surface Warfare Center, Dahlgren Division, Dahlgren, Virginia.

SESSION H4: Mechanisms I
Chair: Randall Simpson
Tuesday Afternoon, November 29, 2005
Room 301 (Hynes)

1:30 PM *H4.1
The Effect of Nanopowder Attributes on Reaction Mechanism and Ignition Sensitivity of Nanothermites. Jan A. Puszynski, Christopher Bulian and Jacek J. Swiatkiewicz; SD School of Mines and Technology, Rapid City, South Dakota.

2:00 PM H4.2
Aluminum Activation Mechanisms Curtis E. Johnson, Timothy J. Foley and Kelvin T. Higa; Research Department, NAVAIR, China Lake, California.

2:15 PM H4.3
Ignition of Aerosolized Reactive Particles at High Heating Rates. Salil Mohan, Yuriy L. Shoshin and Edward L. Dreizin; Mechanical Engineering, New Jersey Institute of Technology, Newark, New Jersey.

2:30 PM BREAK

3:30 PM *H4.4
The effect of slow heating rates on the reaction mechanisms of nano and micron composite thermite reactions Michelle L. Pantoya and John J. Granier; Mechanical Engineering Dept, Texas Tech University, Lubbock, Texas.

4:00 PM *H4.5
Evolution and Revolution - Changing Energetics Technology. Adam S. Cumming, Energetics Technology, DSTL Fort Halstead, Kent, United Kingdom.

4:30 PM H4.6
Study of Melting and Oxidation of Nanometer Size Aluminum Powders. Swati M. Umbrajkar, Mikhaylo Trunov, Mirko Schoenitz and Edward L. Dreizin; Mechanical Engineering, New Jersey Institute Of Technology, Newark, New Jersey.

4:45 PM H4.7
Combustion Mechanisms of Nanocomposite Al/PTFE. Dustin T. Osborne and Michelle L. Pantoya; Mechanical Engineering Dept, Texas Tech University, Lubbock, Texas.

SESSION H5: Poster Session
Tuesday Evening, November 29, 2005
8:00 PM
Exhibition Hall D (Hynes)

H5.1
Density of RDX Crystals Grown During High Acceleration in an Ultracentrifuge. Mary Y. D. Lanzerotti[1], Richard Z. Squillace[1], Alex Gandzelko[1] and Jagadish Sharma[2]; [1]U. S. Army ARDEC, Picatinny Arsenal, New Jersey; [2]Carderock Division, Naval Surface Warfare Center, West Bethesda, Maryland.

H5.2
Theoretical and Experimental Study of the Vibrational Spectroscopy of 2,4-Dinitroimidazole. Jennifer A. Ciezak and Samuel F. Trevino; ARL/NIST, Gaithersburg, Maryland.

H5.3
Assessment of Deposition and Clearance Fractions using the Icrp 66 Lung Model for Airborne Nanomaterials. Charles Jenkins[1], Jorge Hurtado[2], Wesley E. Bolch[2] and Chang-Yu Wu[1]; [1]Dept. of Environmental Engineering Sciences, University of Florida, Gainesville, Florida; [2]Dept. of Nuclear and Radiological Engineering, University of Florida, Gainesville, Florida.

H5.4
Atomistic Simulations of PETN Molecular Nanocrystalline Particles Theodore Golfinopoulos[1], Longguang Zhou[1], Hanchen Huang[1] and Richard H. Gee[2]; [1]Mechanical, Aerospace, and Nuclear Engineering, Rensselaer Polytechnic Institute, Troy, New York; [2]Chemistry and Chemical Engineering Division, Lawrence Livermore National Laboratory, Livermore, California.

H5.5
New Approach for Large-Scale Production of Carbon Single-Walled Nanotubes: Synthesis of Small Diameter Nanotubes. E. Mora[1], T. Tokune[2] and A. R. Harutyunyan[2]; [1]Physics Department, The Ohio State University, Columbus, Ohio; [2]Honda Research Institute, Columbus, Ohio.

H5.6
Patterning PETN and HMX using Dip Pen Nanolithography. Omkar A. Nafday[1,2], Brandon L. Weeks[1], Jason Haaheim[2] and Ray Eby[2]; [1]Chemical Engineering, Texas Tech University, Lubbock, Texas; [2]Sales and Applications, NanoInk Inc., Chicago, Illinois.

SESSION H6: Mechanisms II
Chair: Jan Puszynski
Wednesday Morning, November 30, 2005
Room 301 (Hynes)

8:15 AM *H6.1
Shear Localization and Initiation of Chemical Reactions in Energetic Materials Under Dynamic Loading. Vitali F. Nesterenko[1,2] and Jing Cai[1]; [1]Materials Science and Engineering Program, University of California at San Diego, La Jolla, California; [2]Department of Mechanical and Aerospace Engineering, University of California at San Diego, La Jolla, California.

8:45 AM H6.2
Shock-Induced Chemical Reactions in Organic Liquids. Dana M. Dattelbaum, Stephen A. Sheffield, David L. Robbins, Richard L. Gustavsen, Robert R. Alcon, Joseph M. Lloyd and Pete Chavez; Los Alamos National Lab, Los Alamos, New Mexico.

9:00 AM *H6.3
Hot Spots in Energetic Crystals from Dislocation Pile-up Avalanches. William R. Grise, Department of Industrial and Engineering Technology, Morehead State University, Morehead, Kentucky.

9:30 AM H6.4
Role of Constituent Configuration on Shock-Induced Reactions in a Ni+Al Powder Mixture. Daniel Eakins and Naresh Thadhani; Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia.

9:45 AM H6.5
Dynamic Impact Characterization of Epoxy-Cast Al+Fe2O3 Mixtures Louis Ferranti and Naresh N. Thadhani; Materials Science & Engineering, Georgia Institute of Technology, Atlanta, Georgia.

10:00 AM BREAK

10:30 AM H6.6
Shear Initiated Reactions in Energetic and Reactive Materials. Denise Meuken[1], M. Martinez Pacheco[2], H. J. Verbeek[1], R. H. B. Bouma[1] and L. Katgerman[2,3]; [1]Energetic Materials, TNO Defense Security and Safety, Rijswijk, Netherlands; [2]Netherlands Institute for Metals Research, Delft, Netherlands; [3]Delft University of Technology, Delft, Netherlands.

10:45 AM *H6.7
Lattice Deformation and Shear Bands Formed in Crystalline Solids by Shock or Impact. C. S. Coffey and J. Sharma; Research and Technology, Indian Head Div, NSWC, Indian Head, MD., Maryland.

SESSION H7: Theory and Modeling
Chair: Jan Puszynski
Wednesday Morning, November 30, 2005
Room 301 (Hynes)

11:15 AM *H7.1
Theoretical Chemical Characterization of Energetic Materials. Betsy M. Rice, Ballistics and Weapons Concepts Divison, U. S. Army Research Laboratory, Aberdeen Proving Ground, Maryland.

11:45 AM H7.2
Atomistic and mesoscale modeling of mechanical and chemical processes in energetic materials. Alejandro Strachan[1], Adri van Duin[2], William Goddard[2] and Brad Holian[3]; [1]Materials Engineering, Purdue University, West Lafayette, Indiana; [2]Caltech, Pasadena, California; [3]Los Alamos National Laboratory, Los Alamos, New Mexico.

SESSION H8: Theory II
Chair: Michael Zachariah
Wednesday Afternoon, November 30, 2005
Room 301 (Hynes)

1:30 PM *H8.1
Atomistic Studies of Fundamental Properties and Processes in Energetic Materials: Relevance to Mesoscale Initiation Phenomena. Thomas (Tommy) D. Sewell, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico.

2:00 PM *H8.2
Characterising and Modelling the Response of Polymer-Bonded Explosives (PBXs) to High-Rate Loading. William G. Proud[1], M. W. Greenaway[1], C. R. Siviour[1], J. E. Field[1], D. Porter[2], P. Gould[2], P. D. Church[3] and I. G. Cullis[3]; [1]Physics and Chemistry of Solids Group, Cavendish Laboratory, Cambridge, United Kingdom; [2]QinetiQ, Farnborough, Farnborough, United Kingdom; [3]QinetiQ, Fort Halstead, Kent, United Kingdom.

2:30 PM BREAK

3:30 PM H8.3
Shock-Wave Propagation Study in Single Crystalline fcc-Al and ?-Fe2O3 and Their Interface Using Classical Molecular Dynamics Simulations. Vikas Tomar and Min Zhou; Mechanical Engineering, Georgia Institute of Technology, Atlanta, Georgia.

3:45 PM H8.4
Plastic deformation of semiconducting nanoparticles during a shock wave from first-principles molecular dynamics. Matteo Cococcioni[1,2], Gerbrand Ceder[1,2] and Nicola Marzari[1,2]; [1]Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; [2]Institute for Soldier Nanotechnology, Massachusetts Institute of Technology, Cambridge, Massachusetts.

4:00 PM H8.5
Molecular dynamics simulation of shock-induced chemical, mechanical and thermal processes in nanostructured metastable composites. Shijin Zhao[1], Timothy Germann[1] and Alejandro Strachan[2]; [1]Los Alamos National Lab, Los Alamos, New Mexico; [2]Materials Engineering, Purdue University, West Lafayette, Indiana.