Chemistry and Materials Science
Directorate News

Providing scientific excellence and leadership that meets and anticipates the needs of the Laboratory's programs

July 2003
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Inside This Issue

Message from the Associate Director

In the Chemistry and Materials Science (CMS) Directorate, we pride ourselves on our long-standing history of scientific and technical excellence, as well as our sound operational and business practices. Nevertheless, we have our share of vulnerabilities, particularly in the areas of safety and security, as we manage many chemical laboratories and sensitive nuclear materials.

I would like to take this opportunity to reiterate my personal commitment and that of my staff: We will take prompt and effective action to aggressively resolve any issues of safety and security that may surface in the course of our operations. Furthermore, we will ensure that we will protect, not punish, those who bring up these issues as they occur.

A series of events at Los Alamos and now at our Laboratory has—in the

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A Corner on Science
Plutonium Research Made Smaller but Better

CMS researchers in the Materials Science and Technology Division (MSTD) recently overcame a major impediment in plutonium research by demonstrating how a transmission electron microscope (TEM) can be used to solve a 50-year-old problem caused by the absence of large single crystals of Pu.

Pu exists in several forms, including the monoclinic α phase and the face-centered cubic δ phase. Despite efforts to refine sample-preparation techniques, Pu experimenters are almost always reduced to using single-phase, polycrystalline samples. Such samples significantly limit the effectiveness of most surface-sensitive electron spectroscopies, including synchrotron-radiation-based measurements such as x-ray absorption spectroscopy (XAS) and photoelectron spectroscopy.

With these techniques, the best measurements are made on single-crystalline surfaces and are invariably linked to the direct confirmation of surface ordering via diffraction techniques such as low-energy electron diffraction. But because Pu samples are usually

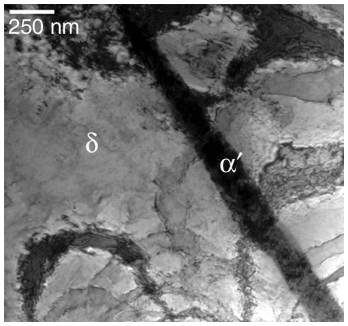

Fig. 1. A bright-field transmission electron microscopy image of the partially transformed, two-phase α′- and δ-Pu structure used in the experiment by **Kevin Moore** and his MSTD colleagues.

polycrystalline, uncertainties concerning the samples' geometric structures persist. These uncertainties compromise the utility of such measurements, limiting our understanding of the Pu electronic structure.

CMS scientist **Kevin Moore** and his MSTD colleagues have solved this phase-identification problem by using a TEM in two very different ways to determine the electronic structure of a partially transformed, two-phase α′- and δ-Pu structure (Fig. 1).

First, with the help of the MSTD TEM, which provides exceptional spatial resolution, the researchers determined the crystallinity of various microscopic sections of a polycrystalline foil. They then used the microscopic focusing

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In Memoriam
Maria Bartelt

by Jim De Yoreo and Chris Krenn

Maria Bartelt, dressed in the light-blue hat and uniform worn by science students at the Universidade de Aveiro in Portugal, at her graduation parade in 1984.

Maria Bartelt, physicist and scientific capability leader for Computational Materials Science in CMS, passed away at the age of 41 on June 23, due to complications from an opportunistic infection. Maria had been battling non-Hodgkins lymphoma for more than a year. She is survived by her husband, **Tim**; her twin sister, **Maria de Fátima Taveira Pires de Carvalho**; an older sister, **Dalila Carvalho**; her mother, **Arcilia Gomes Taveira**; and her beloved parrot, Spike. A service in Maria's honor was held on Saturday, June 28, at the East Gate Auditorium.

Maria started her career as a research assistant at the Universidade de Aveiro in Portugal, where she received her diploma in theoretical, solid-state physics in 1984 for her work on amorphous systems. She received her master's degree in physics in 1989 and her Ph.D. in physics in 1991 from Clarkson University under **Vladimir Privman**. Maria was awarded the Graduate Student Distinction Prize and membership in the ΦΚΦ Honor Society for her work on surface and size effects in statistical mechanics, particularly irreversible adsorption, polymers, and interfaces.

After receiving her Ph.D., Maria became a postdoctoral research associate at Iowa State University in Ames, Iowa, where she began a long and fruitful collaboration with **James Evans** in the field of thin-film epitaxy. Maria remained at Iowa State until 1996, publishing an impressive series of highly cited papers on a number of topics, including the following: submonolayer nucleation and growth

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chemistry & materials science CMS

Chemistry and Materials Science Directorate

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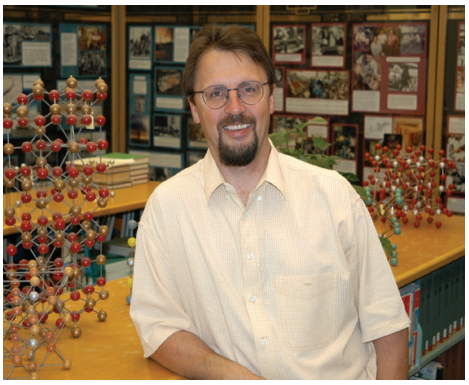
National Nuclear Security Administration

Interview With...
Vasily Bulatov



Before coming to work at the Laboratory in 1999, CMS materials physicist **Vasily Bulatov** had spent several years collaborating with scientists in the Physics and Advanced Technologies (PAT) Directorate on projects investigating the dynamics of materials. Although Vasily's areas of interest and expertise matched closely with the needs of the Laboratory's program in material dynamics, he did not seriously consider employment at Livermore because, as a non–U.S. citizen, he could not be offered a career position. Or so Vasily thought until he began working with **Tomás Díaz de la Rubia**, our current associate director.

At the time, Vasily, a native of Moscow, was a research scientist at the Massachusetts Institute of Technology (MIT). Tomás invited Vasily to reconsider joining the Laboratory. When Vasily explained his hesitation, Tomás investigated and discovered that foreign nationals could indeed hold career positions. Vasily then interviewed for and eventually accepted a career position in CMS.

Vasily is now a co–principal investigator of the Dynamics of Metals Program and has served as the Computational Materials Science Group leader. He is also writing a book, tentatively titled *Computer Modeling of Dislocations*, to be published by Oxford University Press. Vasily credits Tomás with not only bringing him to the Laboratory but also for being his mentor, advocate, and friend. Vasily believes that Tomás's guidance and support were crucial in helping him transition from academia to the Laboratory.

Joining a national laboratory and becoming a U.S. citizen were not part of Vasily's original plans when he came to the United States in 1990 to work with

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In Memoriam

Continued from page 1

of islands, multilayer kinetic roughening, and spatial organization during nonequilibrium random sequential adsorption.

In 1996, Maria left Iowa State to become a physicist in the Computational Materials Science Department at Sandia National Laboratory in Livermore, where she continued her work on thin-film growth and expanded her research to include electromigration and stress voiding in interconnects, the creation of dislocation boundaries during metal deformation, and dislocation networks in the complex plastic zones formed during indentation and fracture.

Maria joined Lawrence Livermore in 2000. She continued her work on dislocation dynamics and became increasingly involved in simulating the growth of molecular crystals under near-equilibrium conditions from solutions. Most recently, she was working on a kinetic Monte Carlo approach to predict the templated nucleation and growth of macromolecular structures formed at nanoscale chemical patterns on surfaces. Until her death, Maria remained an associate scientist for the Institute for Physical Research and Technology at Iowa State.

Over the course of her remarkably productive career, Maria published more than 70 journal articles, book chapters, and proceedings; delivered many invited talks at national and international conferences; and organized numerous symposia. She was a recognized leader in her field.

But for those of us who had the great fortune to work with Maria, the statistics on her accomplishments tell little about what she meant to us. Maria was a person of deep principles, profound determination, and unquenchable optimism; she never uttered a negative word. She cared genuinely about the welfare of her friends, colleagues, and group members, and her door was always open to offer a sympathetic ear or useful advice. Maria always had a smile to show the world, and by her positive example, she made those around her smile as well. She was a good person. We are better for having known Maria, and we will miss her. ■

CMS Notable Publications

by Michael Fluss

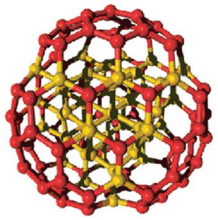
Bucky Diamonds Are a Scientist's Best Friend

No, it's not the *Seven Year Itch*! Livermore scientists from CMS and PAT collaborated in a combined experimental and theoretical effort to study the structure and properties of curious nanodiamond materials found in detonations and meteorites.

This work was highlighted in articles published in *Materials Update* and *Physical Review Focus*. The *Materials Update* article emphasized that "nanoscale particles of diamond produced in detonations and seen in meteorites might have fullerene-like coats," while the *Physical Review Focus* article noted, "...[T]his new family of carbon clusters may provide new insights for the development of optoelectronics—futuristic devices that process both light and electrical signals."

The noteworthy paper is "Quantum confinement and fullerenelike surface reconstructions in nanodiamonds" by **Jean-Yves Raty**, **Giulia Galli**, **Christoph Bostedt**, **Tony van Buuren**, and **Lou Terminello** (*Phys. Rev. Lett.* 90, 037401, [2003]). The authors reported x-ray absorption and emission experimental results and ab initio calculations, showing that the diameter of carbon diamond must be reduced to 2 nm before there is an observable optical-gap increase. Such results differed from observations of Si and Ge, in which quantum-confinement effects persisted at sizes up to 6–7 nm.

The authors' calculations also showed that the surface of nanodiamond particles larger than 1 nm reconstructed in a fullerene-like manner, giving rise to a new family of carbon clusters: bucky diamonds. The signatures of these surface reconstructions were compatible with the pre-edge features observed in measured absorption spectra.



Ball-and-stick representation of a bucky diamond cluster with a diamond core (yellow) and a fullerene-like reconstructed surface (red). Unlike Si and Ge, this nanodiamond exhibits very weak quantum-confinement effects.

Publication URL
http://link.aps.org/abstract/PRL/v90/e037401

New Si–C Linking Method for Rounding Up Biomolecules

Instead of herding cattle, Livermore scientists are learning how to round up biomolecules, the stars of multidisciplinary chemistry, materials, and bioscience research.

Bradley Hart, **Sonia Létant**, **Staci Kane**, **Masood Hadi** (Sandia), **Sharon Shields**, and **John Reynolds** attached biomolecules to porous Si by using a novel linking method that forms a direct Si–C bond on the surface and that retains the photoluminescence of porous Si.

This approach, which is described in "New method for attachment of biomolecules to porous silicon" (*Chem. Comm.* 3, 322 [2003]), involves covalently modifying the hydride-terminated surface of porous Si with an organic linker. The linker is then used to covalently attach various molecules to the surface, including small molecules such as fluorescent probes and large biomolecules such as proteins and enzymes.

The new linking system, which is less synthetically laborious and less deleterious to the photoluminescence of porous Si than other methods, capitalizes on an attachment method that forms a direct Si–C bond through Lewis acid-catalyzed hydrosilylation. Traditional protein crosslinking chemistry is then used to form covalently bound systems available for binding a variety of molecules.

Publication URL
http://pubs.rsc.org/ej/CC/2003/b209453c.pdf?&Yr=2003&VOLNO=%20&Fp=322&Ep=323&JournalCode=CC&Iss=3

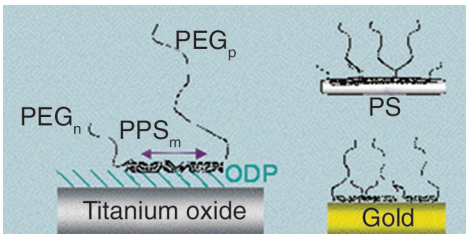
Stable Antifouling Surfaces to Keep Your Biosensors Clean

Good housekeeping is important—even at the molecular level! The performance of devices used in biological assays, DNA screening, proteomic arrays, and cell organization is subject to fouling and degradation, which means that advances in biotechnology are impeded by the limitations of antifouling surface materials.

However, significant advances in biomaterials surface chemistry have led to the development of an assembly-based, surface-modification process that yields stable, biofouling-resistant surfaces. CMS scientist **Jean Bearinger** is the lead author of "Chemisorbed poly(propylene sulphide)-based copolymers resist biomolecular interactions," (*Nat. Mater.* 2, 259 [2003]), which describes research that she accomplished while working in **J. Hubbell's** group in Zurich, Switzerland.

In a companion guest article, "Stable antifouling surfaces," **Ralph Nuzzo** of the University of Illinois describes interfaces as central to the structures and processes that support life. Ralph remarks that molecular assembly provides new capabilities for controlling biomolecular interactions at materials surfaces.

Ralph notes that Jean and her colleagues "report a significant advance in biomaterials surface chemistry—the development of an assembly-based process for surface modification that yields strongly biofouling-resistant surfaces of exceptional stability." He also states, "The lessons learned in this work suggest important new directions for research into surface-mediated assembly—ones that embrace molecular designs based on polymeric amphiphiles—and offer the hope that practical systems can be developed for diagnostic and microfluidic applications."



Block copolymers consisting of the poly(ethylene glycol) (PEG) and poly(propylene sulphide) (PPS) sulfamers passivate hydrophobic and gold surfaces. Surface examples include self-assembled monolayers of octadecyl phosphate (ODP) on TiO_2 and polystyrene (PS).

Publication URL
http://www.nature.com/cgi-taf/DynaPage.taf?file=/nmat/journal/v2/n4/full/nmat851.html&filetype=pdf ■

Building 155 Is Open and Ready for Science

A ribbon cutting ceremony was held on April 16 to officially open Building 155, providing 65 additional offices for workers in the adjacent Isotope Sciences Facility (Building 151) and a new home for the Chemical Biology and Nuclear Science Division office. The design of the 22,000-square-feet, two-story building began in May 2000, and construction started in September 2001. The facility was finished in February 2003, and the Department of Energy approved its use on April 17.

CMS administrators **Bonnie McGurn** (left) and **Brynn Bollinger** (right) examine the new adjustable document reader/projector in the Building 155 auditorium.

Al Ramponi (left), division leader of the Chemical Biology and Nuclear Science Division, which is now housed in Building 155, and **Al Moser** (right), CMS operations manager, speak at the April 16 ribbon cutting ceremony.

CMS Associate Director **Tomás Díaz de la Rubia** cuts the ribbon to officially open Building 155.

Office moves into the new building began on April 18 and are almost complete. The second floor is now a limited area, requiring a Q clearance for entry, while office space for CMS staff with P clearances is on the first floor. The first floor also features a state-of-the-art, 150-seat auditorium with outstanding acoustics and video projection features, electronic controls, an adjustable podium, and an adjustable document reader/projector.

CMS would like to thank **Barbara Pulliam**, the CMS project manager, and **Michael Atkinson**, the Plant Engineering project manager, for all their work in making sure that Building 155 was completed on time and within the $8.4 million budget. ■

Division Name Change—ANCD Is Now CBND

The Analytical and Nuclear Chemistry Division has been renamed the Chemical Biology and Nuclear Science Division (CBND) in light of a recent realignment in the division's strategic mission.

The new name reflects the division's emphasis on characterizing, detecting, and modeling biochemical systems, which builds on the division's core competencies in nuclear chemistry, radiation detection and measurement, and isotope geochemistry. The name also shows the division's commitment to positioning itself at the intersection of Laboratory programs in nuclear science, chemical sciences, and bioanalytical chemistry.

CBND staff began moving into Building 155 on April 18. The division office is now in the Room 1143 suite located on the south side of the first floor. ■

Building 151 Seismic Update

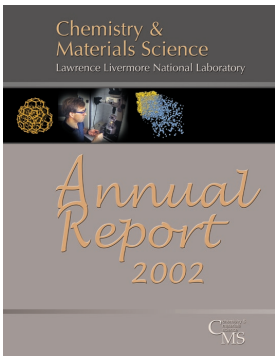
Exterior drilling on Building 151 is complete! Thanks to all residents for their patience and understanding during the 30-day window we dedicated for this phase of the project.

Work on the seismic upgrade of Building 151 is progressing well.

The building's exterior rebars and forming are progressing well. During the weekend of June 13–15, we x-rayed the construction areas inside Building 151 to obtain a more accurate picture of hidden structures within the building's walls and floors. The construction crews are now using these x-ray radiograms as a map to help guide them through existing electrical conduits, pipes, plumbing, and rebars when drilling into the building's walls, floors, and roof.

We anticipate completing the seismic upgrade of Building 151 in September. Please contact **Barbara Pulliam** (ext. 3-4680), the CMS project manager, or **Bryan Bandong** (ext. 3-0855), the programmatic point of contact, if you have any questions about the seismic upgrade or its impact on your programmatic work. ■

Hot Off the Press: The 2002 Annual Report



Thanks to the contributions of many CMS employees, we are proud to announce the publication of our *2002 Annual Report*! Preliminary copies were given to the May Director's Review Committee (DRC). Laboratory Director **Michael Anastasio** also received a copy as part of our directorate's Appendix F submittal.

The Annual Report describes groundbreaking research conducted in 2002 within the four CMS research theme areas, as well as accomplishment highlights of each division, institute, and center in CMS. We thank everyone who contributed to the Annual Report and hope that you enjoy the resulting showcase of your work. Thanks also to all who provided administrative support and to the many authorized derivative classifiers who reviewed the articles.

We'd like to acknowledge our Information Application Services Team, who worked hard under the direction of **Theresa Healy** to pull together the Annual Report in time for the May DRC, and **Michael Fluss**, the scientific editor for the Annual Report. The team also received strong art support from **Alexandria Ballard** and **Galen Hazelhofer** in Innovative Business and Information Services.

The Annual Report will be distributed to all CMS employees in July, and a PDF version is available at http://www-cms.llnl.gov/news/ann_rpt.html. Contact Theresa Healy (ext. 4-4221) if you have any suggestions for next year's Annual Report. ■

It's Our Turn to Sponsor the 2003 Run for HOME!

CMS is sponsoring this year's Run for HOME, the kick-off event for the Laboratory's annual Helping Others More Effectively (HOME) campaign. To encourage the participation of all Laboratory employees by accommodating alternate work schedules, the 2003 run will be held on Thursday, October 30, instead of on Halloween as in previous years.

The theme for the 2003 Run for HOME is Team America—Three Cheers for the Red, White, and Blue. CMS has also chosen a special costume category: American Heroes and Patriotic Icons.

The red, white, and blue colors and the flag motif in the 2003 HOME logo symbolize the strong patriotism and national pride of Laboratory employees. The logo also conveys the main message of the HOME campaign: to extend help to others in our community who are in need.

To be successful, the run will need many volunteers from CMS, so keep an eye out for future announcements on ways you can help. For more information about the run, contact **Al Moser** (ext. 3-0326), chair of the Run for HOME committee, or **Jana Marden** (ext. 2-6091), principal assistant to the chair. ■

Meet the New Information Application Services Team

In April, CMS bid a fond farewell to technical writer/editor **Dabbie Bowron** (formerly Schleich), who has left CMS after seven years of faithful service to work with **Denise Robinson**, the Laboratory's institutional facility manager.

Stephanie Shang was selected in May as Dabbie's replacement. Stephanie is a senior technical writer/editor with more than ten years of experience at the Laboratory. Her primary duty is to support the publication and communication needs of the CMS associate director (AD) and his staff. Stephanie is a familiar face in CMS, especially among staff embedded in the Weapons Program. Prior to joining CMS, she supported three ADs in the Defense and Nuclear Technologies Directorate: **George Miller**, **Michael Anastasio**, and most recently, **Bruce Goodwin**.

Technical writer/editor **Emmeline Chen** joined CMS in February and worked with Dabbie to colead the *2002 Annual Report*. Emmeline is available to help CMS scientists and staff with their journal articles, presentations, posters, or other writing/editing needs. Emmeline grew up in Livermore and interned in CMS and BBRP during high school and college. She has a Ph.D. in social psychology from New York University. She also holds an M.A. in psychology and a B.A. in English from Stanford University.

The newest addition to the team is **Missy Davidson**. Missy, who has a B.A. in communication design from California State University, Chico, laid out the *2002 Annual Report* and *Facts & Figures 2003*. Missy and technical illustration specialist **Scott Dougherty** can provide art support, design, and layout for figures, publications, posters, and presentations.

The Information Application Services Team (from left to right: **Stephanie Shang**, **Theresa Healy**, **Karen Rath**, **Emmeline Chen**, **Missy Davidson**, and **Marleen Emig**; not pictured: **Scott Dougherty**).

Rounding out the team are Web editor **Karen Rath** and Webmaster **Marleen Emig**, who are working to design and update the CMS internal and external Web sites.

Please contact **Theresa Healy** (ext. 4-4221), the manager of the Information Application Services Team, if you have any questions about how the team members can support you. ■

Nuclear Science Internship Program

NSIP recruitment poster.

This year's Nuclear Science Internship Program (NSIP), which is cosponsored by the Glenn T. Seaborg Institute and the U.S. Department of Energy, began on June 16 and continues until August 8. Twenty-two students are affiliated with NSIP this summer. These students will be mentored by nuclear scientists at the Laboratory, including those in our Chemical Biology and Nuclear Science Division.

The goal of NSIP is to provide graduate and undergraduate students with a structured research program in radiation detection, biomedical applications, computational biochemistry, isotope geochemistry, or radiochemistry. NSIP also features seminars with leading nuclear scientists, tours of Laboratory facilities, and introductions to the major programs at Livermore. This year's NSIP is being coordinated by **Christine Hartmann Siantar**, **David Smith**, and **Douglas Phinney** from the Glenn T. Seaborg Institute. ■

Kudos to CMS Staff and Students

CMS proudly recognizes the following accomplishments:

- A paper coauthored by **Olgica Bakajin**, a Lawrence fellow working within CMS, was recently accepted for publication in *Science*. The article, "Microfabricated mixer for time-resolved single molecule protein folding" by **E. Lipman**, **B. Schuler**, **O. Bakajin**, and **W. Eaton**, discusses protein folding work that Olgica conducted in collaboration with scientists at the National Institutes of Health. This research marks the first time protein folding has been monitored on the single-molecule level.

- **Raymond Friddle**, a graduate student working in the BioSecurity and Nanosciences Laboratory, won the best scientific poster prize at the 2003 Nanoscience and Bionanoscience Research Meeting. Raymond's poster, "DNA compaction by yeast mitochondrial packing protein ABF2p," was coauthored by **R. Baskin** and **A. Noy**. The meeting was held on June 11 at Lawrence Berkeley National Laboratory and gathered leading researchers for an exchange of recent advances in nanoscience.

- **Sarah Nelson**, a graduate student participating in this year's Nuclear Science Internship Program, is the recipient of the 2003 American Institute of Chemists Award. This award is given each year to the most outstanding graduating senior in chemistry, biochemistry, and chemical engineering at UC Santa Barbara (UCSB). Sarah was nominated for this award by the Dean of the UCSB College of Letters and Science. ■

CMS-Organized Symposia at the 2003 Materials Research Society Fall Meeting

CMS materials scientist **Jim Tobin** is organizing a four-day symposium, "Actinides: Basic Science, Applications, and Technology," for the Fall 2003 meeting of the Materials Research Society (MRS), to be held from December 1 to 5 in Boston. The symposium will focus on fundamental actinide science and its role in resolving the technical challenges posed by the complex electronic structure of actinide materials. Both basic and applied experimental approaches to actinide science, as well as theoretical modeling and computational simulations, will be discussed in the symposium.

Another symposium at the 2003 MRS Fall Meeting, "Synthesis, Characterization, and Properties of Energetic/Reactive Nanomaterials," is being co-organized by **Randy Simpson**, the division leader of the Chemistry and Chemical Engineering Division. This symposium will examine the new dimension in applications of energetic and reactive materials that has been introduced by the advent of nanomaterials. The symposium will also bring together fundamental studies on the synthesis, characterization of structure, and evaluation of properties of energetic/reactive nanomaterials for applications relevant to pyrotechnics, propellants, and explosives.

The call for symposium papers was issued in March, and submissions were due in June. Additional information about the 2003 MRS Fall Meeting is available online at http://www.mrs.org/meetings/fall2003. ■

CMS New Hires—Welcome Aboard!

CBND	Christopher Bailey	Ph.D.	1997	Chemistry	Yale University
CBND	W. Henry Benner	Ph.D.	1977	Environmental science and engineering	University of Florida
CBND	Peter Weber	Ph.D.	2002	Geography	University of California, Berkeley
CChED	Jennifer Blank	Ph.D.	1993	Geochemistry	California Institute of Technology
CMS infrastructure	Timothy Roberts	M.S.	1983	Industrial health and safety	University of Washington
CMS infrastructure	Julie Sedillo				
MSTD	Zurong Dai	Ph.D.	1996	Materials science	University of Science and Technology, China
MSTD	Robert Klatt				
MSTD	Scott McCall	Ph.D.	2000	Physics	Florida State University

Congratulations to the CMS Directorate Award Recipients from May 2003!

Hal Graboske Award of Excellence

William Wilson
Excellence for outstanding vision and tireless commitment displayed in defining and establishing the BioSecurity and Nanosciences Laboratory.

Exceptional Service Awards

Krishnan Balasubramanian
Recipient of the distinguished 2003 Robert S. Mulliken Award

Jennifer Szutu
Exceptional service to CMS in the area of labor law

CMS award recipients (clockwise from top left: **Cherie Napier**, **Mark Stoyer, Jim Tobin**, and **Krishnan Balasubramanian**) with CMS Associate Director **Tomás Díaz de la Rubia.**

Yolanda Villa
Outstanding contributions and perseverance in the CMS 2003 property audit

Distinctive Service Awards

Everett Guthrie
Sustained excellence in environmental radiochemistry

Mark Stoyer and Cherie Napier
Outstanding achievement in restarting the InterLaboratory Working Group conference series

Jim Tobin
Outstanding achievement in organizing the 2nd International Workshop on Spin Orbital Magnetism in Actinides in October 2002

Excellence in Publication Awards

John Elmer and Peter Terrill
Recipient of the distinguished 2003 Warren F. Savage Award for "Joining depleted uranium to high-strength aluminum using an explosively clad niobium interlayer"

Giulia Galli Gygi, Lou Terminello, Tony van Buuren, Christoph Bostedt, and Jean-Yves Raty
"Quantum confinement and fullerenelike surface reconstructions in nanodiamonds"

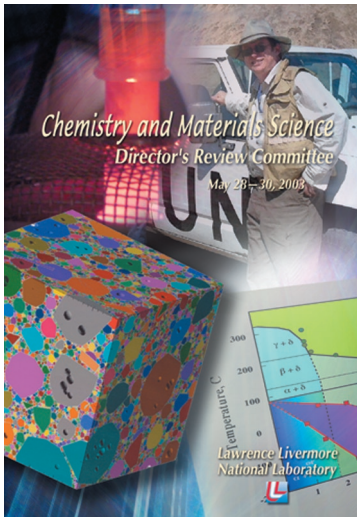
Ian Hutcheon
"Lead isotopic ages of chondrules and calcium–aluminum-rich inclusions"

M. Riad Manaa
"Discovery of the stable structure of buckyball $C_{48}N_{12}$"

Summer Is Here, and So Are the Summer Students...

Please extend a warm welcome to all new and returning CMS summer students, who are listed below:

Coby Adamczyk
Firas Akasheh
Zaheer Ali
Christopher Anderson
Vered Anzenberg
Michal Bajdich
Shannon Bays
Bryan Bednarz
Nadav Ben-Barak
Candyce Boyd
Audrey Britten
Juan Brown
Tim Cao
Aaron Cavosie
Giancarlo Cicero
Christopher Cummings
Lilian Davila
Kevin Demarco
Neil Drummond
Vernessa Edwards
Tyesha Farmer
William Farmer
Raymond Friddle
Lisa Friedman
Franco Gagliardi
Janine Garnham
Gabrielle Gaustad
Joseph Gezo
Allan Gu
Gabrielle Gustad
Benjamin Hackel
Leonard Harris
Bryna Hazelton
David Heringer
Jeremy Hicks
Yunfeng Hu
Melissa Huang
Brett Isselhardt
Dimitri Ivanov
Carl Jannetti
Katharine Jensen
Junhwan Jeon
Erin Jordan
Justin Kao
Brent Kraczek
Miki Kurimoto
John Kurylo
Elizabeth Lara
Elodie Leveugle
Steven Lieberman
Rong (Ron) Liu
Leonard Lucas
Laura Ludvigson
Justin Mach
Manu Manu
Lane Martin
John McDonald
Douglas McGregor
Abigail Miller
Michael Miller
Nathan Miller
Keara Moore
Daniel Murphy
Sarah Nelson
Jenet Peng
Erik Peterson
Kristina Pohaku
Shauntel Poulson
Navdeep Sekhon
Peter Situ
David Sprehn
Carlos Valdez
Aaron Weston
Christopher Young



May Director's Review Committee Gives CMS High Marks

by Jeff Kass

CMS again received high praise from the Director's Review Committee (DRC) after a meeting held from May 28 to 30. This second and final DRC meeting for FY03 focused on CMS stockpile stewardship work, operations, and workforce. The meeting also featured CMS research in two major areas: plutonium science and energetic materials and technology.

The committee of 15 distinguished scientists was led by **Thomas Tombrello**, the chair of the Physics, Mathematics, and Astronomy Division at the California Institute of Technology. The committee listened to presentations by CMS staff, viewed posters about our research, and met with small groups of scientists. The members then recorded their findings and provided useful assessments and comments on our work.


T. Díaz de la Rubia


L. Terminello


J. Wong


P. Allen


B. Wolfer


A. Schwartz


A. Hamza


B. Sadigh


A. Kubota


K. Moore


J. Tobin


K. Blobaum


C. Krenn


M. Suhr

Introductory Session

After welcoming the committee, **Tomás Díaz de la Rubia**, the CMS associate director, described the status of CMS efforts in support of the Laboratory's national-security mission and provided insight into our directorate's strategy. Tomás reaffirmed that maintaining the nation's nuclear stockpile remains the primary mission of CMS. He then discussed the great opportunities for scientific research and programmatic benefits that will be provided by the National Ignition Facility (NIF). Tomás also explained that the emerging homeland security mission will challenge CMS and the Laboratory to detect, interdict, and respond to chemical, biological, and nuclear weapons of mass destruction. These challenges provide CMS with the opportunity to define the long-range science of counterterrorism. Last, Tomás described the science and technology plans being developed by the Laboratory and the leading role that CMS is playing in many of these elements.

Ed Moses summarized the status of NIF, which is being activated and operated concurrently as an experimental facility. This approach is generating a high level of excitement among the experimentalists who are now deeply involved in planning experiments. As senior CMS management personnel have noted, "NIF will define science at LLNL for the next 25 years." This timely realization assures a valuable focus for CMS on equation-of-state studies, target fabrication (nanoscience), and other issues. The degree to which CMS and other Laboratory organizations will engage the challenges and opportunities presented by NIF will, in large part, determine Livermore's future success.

Stockpile Stewardship Session

Charlie Verdon, the A Program leader, presented an excellent overview of the Stockpile Stewardship Program and the role of CMS in helping the Laboratory maintain this important program. The talk began with a history of the program and a description of the four weapon types in the stockpile for which Livermore is responsible. Key Laboratory contributions to the overall program include plutonium capabilities, NIF, JASPER and hydrotest facilities, and the Advanced Simulation and Computing (ASCI) Program. CMS plays a critical role in many of these with our strong plutonium science research, NIF target fabrication efforts, and energetic-materials work, among others. The talk also described the various stockpile life extension plans that are underway or planned and the revitalization of the production complex.

Charlie McMillan, the B Program leader, highlighted the role of CMS in his program. B Program relies on CMS for basic materials science, materials modeling codes such as CHEETAH, and basic input to design and safety-analysis codes. CMS staff operate as an integral part of B Program and are viewed as such. Charlie stressed that no "we–they" mentality exists between CMS staff and other B Program staff.

Plutonium Session

Lou Terminello gave an excellent overview of CMS activities in support of weapons stockpile and performance. He provided the committee with a framework for understanding the program elements that would be described in the talks and posters on Pu science. Lou also explained how the different CMS research groups interact.

Presentations

Joe Wong presented results from a recent study that led to the first measurements of complete phonon-dispersion curves for any Pu-bearing material. The keys to the experiment's success were the fabrication of very large-grained samples through a novel approach and the use of an extremely fine-focused beam. Joe's results provide important insight into the basic nature of Pu and its alloys.

Pat Allen described efforts to predict the phase diagram of Pu–Ga–Fe, experiments to verify these predictions, and extended x-ray absorption fine-structure studies of Ga in α' martensite. Results provided the first calculation of this important ternary system and the discovery of new structure–property relationships.

Bill Wolfer provided an elegant discussion of how Ga stabilizes the δ phase in Pu alloys, changes the densities, creates different α' structures, and affects the martensite transformation. The large and opposite misfit of Ga in the α and δ phases is now explained for the first time. The now validated first-principles theory is being used to obtain fundamental parameters for radiation-damage-induced defects.

Adam Schwartz reported the mechanisms of radiation damage in Pu. Alpha particle decay results in the

Continues ➤

injection of energetic He (5 MeV) with the concomitant recoil of U (86 keV). The agglomeration of He with vacancies forms bubbles that may eventually result in swelling. The recoiling U produces dense, cascade damage and transient shock waves. The damage formation, mainly bubble formation, was studied by positron, optical, and transmission electron microscopy. The effects of aging on bubble density and size distribution were modeled and matched to experimental observations. Understanding this behavior is critically important to assess stockpile aging.

Posters

Alex Hamza described the design of a special-purpose apparatus for angle-resolved photoelectron spectroscopy. To prepare suitable actinide samples for these measurements, a laser evaporation and transfer system that has been tested with U was devised and is in the process of being approved for use with Pu.

Babak Sadigh presented the results of density-functional-theory calculations on δ-Pu and α-Pu using the software package VASP with spin polarization and generalized gradient approximation. Spin-polarized density functional theory can reproduce the cohesive energy and equivalent volume of the δ phase. Calculations involving the geometry of the α phase were in good agreement with experimental results, and important effects of Ga on the stability of the δ phase were identified.

Alison Kubota displayed molecular dynamics simulations, principally of collision-cascade-mediated phenomena in metals. Lattices of several millions of atoms were modeled using the embedded-atom method for Cu or Ni. To simulate the 1.3-nm He bubbles present in Pu, 1.0-nm He bubbles were embedded in Cu lattices and were subjected to cascade interactions. For the first time, the ejection of He atoms from the bubbles was observed, suggesting that the bubbles are dynamically stable. This work is very important for understanding the long-term aging mechanism for Pu.

The complexity of allotropic states in metallic Pu has led to continued uncertainty about its 5f electronic structure. The inability to grow large crystals, in addition to the radioactive perturbations of the crystalline systems, prevents the use of normal spectroscopic methods to study the electronic structure of Pu in sufficient detail. **Kevin Moore** described how a combination of high energy-electron energy loss spectroscopy (HE-EELS), transmission electron microscopy, and synchrotron X-ray absorption spectroscopy (XAS) are being used to address this problem. The HE-EELS and XAS data from both types of spectroscopy showed a large continuum with no prepeak structure, which was interpreted as direct evidence for the filling of the 5f 7/2 level. This indicates spin-orbit splitting of the 5f states of Pu. Such spin-orbit splitting must involve j-j coupling and not Russell–Saunders (i.e., LS) coupling, thus resolving a long-standing and important scientific issue.

Jim Tobin presented details about a work-in-progress that proposes to use spin-resolved photoelectron spectroscopy to probe spin sensitivity in nonmagnetic samples, such as Pu. Jim showed that both spin polarization and orbital polarization must be included in the models, a critical point for success.

Kerri Blobaum and **Chris Krenn** described the martensite and austenite start temperatures in Pu–Ga alloys. They also presented a model to understand the double-C time–temperature–transformation curve. Results suggest that the accepted crystallography is incomplete, and transmission electron microscopy is underway to examine the crystallography more completely.

Adam Schwartz summarized the major issues involved with the aging of Pu–Ga alloys. These issues include void swelling, density changes, dynamic properties, equation of state, and vulnerability. The poster provided a clear and effective summary of the extensive effort investigating these issues.

Bill Wolfer and **Mike Suhr** presented a poster on the theory of accelerated aging in Pu. Their research used temperature and ^{238}Pu as aging accelerants. The modeling they conducted provides crucial understanding for the accelerated-aging effort.

Karen Dodson and **Bart Ebbinghaus** described the recent successful fabrication of Pu accelerated-aging alloys and the characterization of these alloys in their unaged condition. Very good progress has been made on this difficult task.

Bill McLean and **Long Dinh** presented a well-developed model describing Pu corrosion. The model established a link between coupon tests and full-scale behavior.

Energetic-Materials Session

Randy Simpson provided an overview of the links between basic research and production for energetic materials. Precision storage and manipulation of chemical energy are required in nuclear weapons. Major issues include understanding and controlling high-energy materials so that they can be safely stored and exploded in a predictable and precise manner. To this end, the program has dedicated a large effort to developing computational and modeling tools that can use information from molecular-scale processes to simulate the behavior of systems. This vibrant and innovative energetic-materials effort integrates basic research with programmatic deliverables.

Presentations

Riad Manaa described a study using density-functional-theory techniques to predict the structure of azafullerenes with a molecular composition of $C_{48}N_{12}$. The structural, electronic, and conductive properties of these fullerenes were fine-tuned. The ground-state structure and IR signature of the fullerene-like $C_{48}N_{12}$ were also determined. The presentation was a summary of Riad's recent, award-winning paper.

Al Nichols reported on the use of thermal explosion modeling as a tool to predict the response of weapons to thermal insults. The only fully coupled thermal–chemical–hydrodynamic capability has been developed and is being

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K. Dodson


B. Ebbinghaus


B. McLean


L. Dinh


R. Simpson


R. Manaa


A. Nichols


L. Fried


J. Crowhurst


A. Goncharov


G. Overturf


R. Gee


A. Gash


J. Maienschein


C. Tarver


J. Molitoris


R. Schmidt

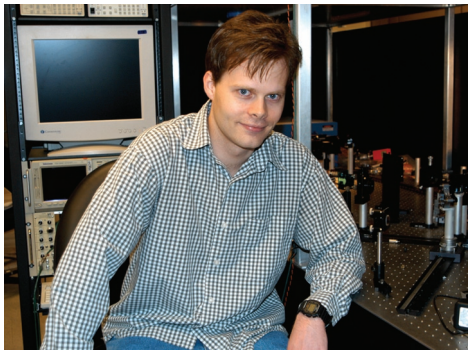

A. Moser


D. Shoemaker

Postdoc Profile
Jonathan Crowhurst

CMS postdoc **Jonathan Crowhurst** grew up in South Africa and received his Ph.D. in physics from the University of the Witwatersrand in Johannesburg. Although Jonathan knew of Livermore's reputation as a world-class scientific institution, he never imagined that he would one day have the opportunity to conduct basic science research using the Laboratory's sophisticated equipment.

However, in 1999, Jonathan attended AIRAPT-17, a conference sponsored by the International Association for the Advancement of High Pressure Science and Technology, and met CMS scientist **Joe Zaug**. The two discovered that Jonathan's dissertation work on applying Brillouin spectroscopy to opaque materials at high pressures in the diamond anvil cell (DAC) overlapped with Joe's research on impulsive stimulated light scattering (ISLS). A connection was made, and Jonathan subsequently joined CMS in February 2002.



CMS postdoc **Jonathan Crowhurst** with the impulsive stimulated light scattering equipment.

The primary goal of Jonathan's research has been to determine the elastic properties of metals under high pressure using ISLS. He and Joe are also using the technique to determine the equations of state of transparent fluids that are suspected to be products of detonation. This information is needed to refine the thermochemical code CHEETAH. In addition, Jonathan is carrying out measurements to determine the yield strengths of metals under ultrahigh pressure in the DAC.

Jonathan and **Alexander Goncharov** are also collaborating with the Geophysical Laboratory in Washington, D.C. to study the behavior of the high-critical-temperature superconductor MgB_2 under simultaneous conditions of low temperature and pressure via Raman scattering.

In the future, Jonathan plans to extend ISLS to higher temperatures and pressures. He also intends to use ISLS to measure the thermal-transport properties of materials under extreme conditions. ■

CMS Postdoctoral Symposium

The annual CMS Postdoctoral Symposium will take place on Wednesday, July 16, in the Gold Room and lobby of Building 235. The symposium will showcase the research accomplishments of our postdoctoral researchers through a series of talks and poster sessions.

Two awards will be presented at the symposium: the second annual Hal Graboske Postdoctoral Award to the postdoc with the most outstanding contribution to our directorate and the Laboratory and an award for the best poster presentation of the symposium.

All are invited to join us in what promises to be an exciting day of science. Contact **Tom Arsenlis** (ext. 4-2584), director of the CMS Postdoctoral Program, for more information.

Postdoc People News

- Please welcome our new CMS postdocs: **Scott McCall** (MSTD) and **Nir Goldman** (CChED).
- **Julie Perkins** is the new deputy director for the CMS Postdoctoral Program.
- **Jennifer Young** has been named a CChED postdoc omsbud.
- **Andrea Hodge** has replaced **Tony Esposito** as the CMS postdoc liaison.

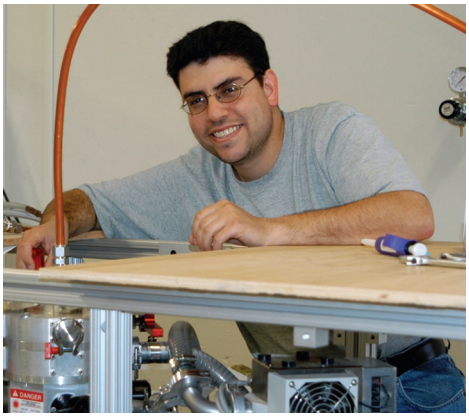
Postdoc Profile
David Fergenson

A trip to northernmost Quebec to see the aurora borealis, or northern lights, changed **David Fergenson's** career path, eventually leading him to become a CMS postdoc in the BioSecurity and Nanosciences Laboratory (BSNL).

At the time, David was a premed, creative-writing major. As he and his brother drove north, they arrived at Chisasibi, a Cree village near James Bay, and saw villagers stricken by mercury poisoning. The poisoning had been traced to the construction of a nearby dam. For years, plants had taken up mercury from the soil and had converted it to methyl mercury. The flooding caused by the dam released methyl mercury into the water, contaminating the fish—the Cree's primary food source.

Upon learning that the Cree's suffering could have been averted if chemical analyses had been conducted to assess the environmental effects of the dam, David decided to become a chemist.

David earned his Ph.D. in chemistry from UC Riverside, where he helped develop a portable aerosol mass spectrometer. While at Riverside, David worked with a postdoc named **Eric Gard**, who later recruited David to CMS. Impressed by the quality of people and facilities at the Laboratory, David was also drawn by the chance to serve our nation with his research.



CMS postdoc **David Fergenson** with the bioaerosol mass spectrometer that he helped develop at the BioSecurity and Nanosciences Laboratory.

Three weeks after David's arrival at Livermore, 9/11 occurred, followed by the spate of anthrax attacks. In collaboration with BSNL colleagues, David accelerated efforts to develop bioaerosol mass spectrometry (BAMS), a pattern recognition method for identifying *Bacillus* spores in real time. He was then deployed to Florida, where he used BAMS to sample the U.S. mail for anthrax.

Since returning to Livermore, David has helped organize the BAMS research program and is gathering a team to improve the analysis of BAMS data. David also plans to develop BAMS for use in detecting nuclear materials. ■

May Director's Review Committee
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applied to critical explosives safety issues. Al's work is of great value to the Laboratory.

Larry Fried described recent advances in the CHEETAH code. This code has been a continuing success both inside and outside the Laboratory. The extensions of the model to include more detailed chemistry and physics are exceptionally valuable.

Jonathan Crowhurst discussed the use of impulsive stimulated light scattering under extreme conditions. An elegant set of experiments was presented for measuring the elasticity of materials under high pressure in a diamond anvil cell. The data he presented indicate that this essentially surface-wave technique can determine bulk elastic properties to high accuracy. His research also demonstrated that measurements of elastic constants of iron can be made without a liquid interface, thus offering the opportunity for very important measurements on other materials.

Alexander Goncharov described the use of vibrational spectroscopy in the diamond anvil cell to examine the chemistry of detonation products at high temperatures and pressures. Raman and IR spectroscopy are being used to answer fundamental questions in chemistry under extreme conditions.

Larry Fried presented advances in the path-integral Monte Carlo method that can greatly speed up CHEETAH/hydro simulations. As a result, thermochemical properties of molecules at high temperatures now can be computed. In addition, simulations on the time scale of experiments can now be performed.

Posters

George Overturf described the determination of variations in the composition and the density of LX-17, as well as the measurements and detection of voids in the explosive. George's work is highly valued.

Rick Gee presented work applying molecular dynamics methods to elucidate nucleation events in polymer crystallization. His results capture the onset of crystallization at realistic temperatures and show evidence of both entangled and unentangled chain dynamics.

Alex Gash showed excellent exploratory work examining the use of nanocomposites of inorganic fuel and oxidizer materials in the engineering of high explosives. The synthesis, formulation, and processing of several different energetic nanocomposites with versatile properties were described.

Jon Maienschein presented work that is predicting the response of weapons to abnormal stimuli. The Livermore program has integrated a number of unique Laboratory computational capabilities in terms of thermal, mechanical, and chemical codes (ALE3D), as well as experiments in burning rates, shock response, and thermal explosion.

Al Nichols and **Craig Tarver** provided details about a new physical-chemistry-based model for the shock initiation and detonation of solid high explosives. This updated model of the initiation hot-spot scenario is a significant improvement over the previous model.

John Molitoris described two projects conducted in support of the recent conflicts in Afghanistan and Iraq. The first involved designing a weapon for attacking targets in tunnels, while the second investigated developing a weapon for defeating biological agents. John's work shows how the Laboratory can rapidly respond to national needs.

Rob Schmidt presented both a talk and a poster describing his work as a member of the United Nations inspection teams in Iraq. Rob is commended for his commitment and skill.

Concluding Session

Al Moser described CMS operations, including many initiatives that have been undertaken to facilitate the CMS focus on science and technology. His talk was followed by tours of the newly opened Building 155, as well as three new facilities that house research using our new secondary ionization mass spectrometer (the NanoSIMS), nuclear magnetic resonance, and aerosol science.

Finally, **Dave Shoemaker** kindly completed a talk on the Counterproliferation Analysis and Planning System (CAPS) Program that was started but not finished during the February DRC meeting. Dave described the work conducted in CAPS to analyze the weapons-of-mass-destruction capabilities of other countries. ■

Interview With...
Continued from page 2

Ali Argon at MIT. Vasily, who received his Ph.D. in the physics and mechanics of materials from the Academy of Sciences, USSR, in 1986, had won a prestigious postdoctoral fellowship sponsored by the Kaiser Foundation. The fellowship targeted young, promising scientists from behind the Iron Curtain, offering them one year of funding at the U.S. university of their choice.

In 1991, Vasily's fellowship was coming to an end, so his wife and children returned to Moscow. Vasily planned to wrap up his research and then rejoin his family in the Soviet Union. However, an anti-Gorbachev coup took place in the Russian government, leading Vasily to fear that he would never see his family again. Fortunately, order was restored in a few days, but the coup had an unintended effect: MIT offered Vasily a research scientist position. Vasily took the job and eventually brought his family back to the United States.

Vasily is pleased to be at Livermore and especially values the Laboratory's ability to sustain and fund long-term basic science research, something he finds lacking in academia and industry efforts. As the co–principal investigator for CMS of the Laboratory's Dynamics of Metals Program, Vasily is excited to be part of a large, cross-directorate effort to predict materials strength from first principles and is helping to develop codes that can model materials behavior and strength. The performance of one modeling code, DD3D, is already 2 orders of magnitude better than that of all other comparable codes.

As Vasily looks ahead, he believes that the success of the Dynamics of Metals Program lies in continued development of ultrasmart algorithms that are based on the fundamental understanding of the physics of material strength and that take advantage of the superpowerful computers in the Laboratory's Advanced Simulation and Computing (ASCI) Program. ■

Message from the Associate Director

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minds of many people outside—cast a doubtful shadow over our ability to execute our national-security mission.

In response to the most recent event, Laboratory Director **Michael Anastasio** stated, "People understand that in an organization of this size, things can happen. The real question is when those things happen, do we handle them promptly and appropriately?"

Effective communication is key to our overall success. I believe that we in CMS are good at communicating. But we can always be better, and we are taking decisive steps to prevent potential communication failures. In particular, I have made it clear to all CMS managers that they are responsible for listening to any concerns identified by our staff, ensuring that appropriate action is taken to address these concerns, and promptly communicating any such actions back to the staff.

Each division recently conducted all-hands and group meetings to ensure that everyone in CMS has an unambiguous understanding of his or her communication pathway up and down the reporting line. This information is also available via our internal Web site at http://cmsonly.llnl.gov/mgt_comm.html.

We have received many constructive suggestions from these meetings for actions that we can immediately implement to strengthen our ongoing communications. Examples include providing frequent feedback to anyone who raises issues and additional classification review training, to name a few.

I want to thank all of you for your suggestions. In the near future, I will be communicating with you regarding what actions we will take to follow up on your recommendations.

Cheers,
Tomás ■

Corner on Science

Continued from page 1

capability of the TEM to measure the electron energy loss at specific points in the Pu structure, each with a clearly determined crystal structure. Examples of their energy-loss spectra, shown as plots of intensity as a function of energy loss, are provided in Fig. 2.

The energy-loss curves for α′- and δ-Pu were distinct and agreed with XAS measurements of polycrystalline samples at the Advanced Light Source in Berkeley. These results mean that electron energy loss spectroscopy can be used to interrogate the Pu phases present in a given sample. This new phase-identification method will enable Pu researchers to direct their efforts toward conducting experiments, such as those in support of the Laboratory's Stockpile Stewardship Program, rather than on preparing single-crystalline Pu samples.

Moore et al. also discovered that the Pu energy-loss curves lacked the prepeak found in the α-Th and α-U curves. This finding provides direct evidence of j-j coupling in the Pu 5f electronic structure and highlights the need for new Pu electronic-structure models that are based on j-j coupling instead of on Russell–Saunders coupling, as is true for most existing models.

Related Publication

Moore, K. T. et al. Failure of Russell–Saunders Coupling in the 5f States of Plutonium. *Phys. Rev. Lett.* **90**, 196404 (2003). Available at http://link.aps.org/abstract/PRL/v90/e196404. ■

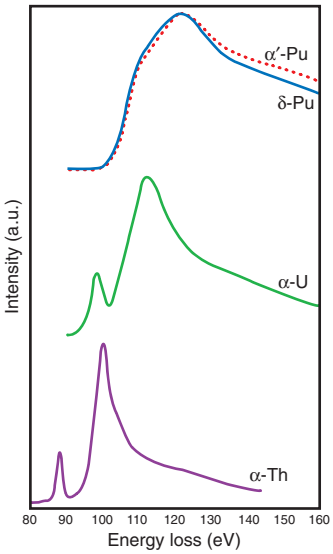

Fig. 2. A comparison of intensity as a function of energy-loss spectra for α′-Pu, δ-Pu, α-U, and α-Th. The absence of a prepeak in the Pu curves provides direct evidence for a Pu 5f electronic-structure model that is based on j-j coupling.

A color PDF of this newsletter can be downloaded from the Chemistry and Materials Science Directorate Web site: http://www-cms.llnl.gov/news/newsletter.html.