MPA material matters

October 2006

Newsletter of the Materials Physics and Applications Division

Discovery offers possibility of less expensive fuel cell

New class of catalysts could conquer obstacles to commercial hydrogen fuel cell development

MPA-11 scientists Rajesh Bashyam and Piotr Zelenay have developed a new class of hydrogen fuel cell catalysts that exhibit promising activity and stability. The catalysts are made of low-cost nonprecious metals entrapped in something called a heteroatomic-polymer structure, instead of platinum materials typically used in fuel cells.

In research published recently in the scientific journal *Nature* (*Nature*, **443,** 63 2006), Bashyam and Zelenay describe tests conducted on a cobalt-polypyrrole-carbon (Co-PPY-XC72) composite. The composite, consisting of cobalt, polymer and carbon, was developed in research aimed at developing low-cost non-platinum catalysts for the polymer electrolyte fuel-cell (PEFC) cathode.

While the electrical energy producing activity of the catalyst is lower than that of platinum-based catalysts used in polymer electrolyte fuel cells, the new material shows exceptional performance stability for over one hundred hours of continuous testing, a result never before obtained with non-precious metal catalysts in PEFCs.

"Besides being made of inexpensive and environmentally benign materials," said Zelenay, "the chief advantage of these composite catalysts for oxygen reduction is that they can operate in the acidic environment of the polymer electrolyte fuel cell."

Piotr Zelenay and Rajesh Bashyam, MPA-11, discuss the advances detailed in their recent *Nature* paper "A class of non-precious metal composite catalysts for fuel cells."

Bashyam and Zelenay are investigating the nature of catalysts in a variety of composites. They are also part of a larger Laboratory effort aimed at developing new catalyst and electrode structures that could increase the current output from fuel cells.

According to Ken Stroh, program manager for the Laboratory's fuel-cell effort, "The two biggest obstacles in making a commercially viable fuel cell have traditionally been high cost and inadequate durability. Our focus at Los Alamos is to attack those obstacles as

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Magnet laboratory renewal submitted to National Science Foundation

The National High Magnetic Field Laboratory recently submitted to the National Science Foundation a $200 million renewal proposal for funding from 2008-2012.

The proposal requests funding for the magnet laboratories' three sites, with approximately $40 million intended for Los Alamos' Pulsed Field Facility. Los Alamos' facility is one of three branches of the magnet laboratory, which also has laboratories in Tallahassee and Gainesville, Florida.

The proposal, submitted Sept. 29, was prepared and written in response to the National Academies' report on "Opportunities in High Magnetic Field Science."

In April, The National Science Foundation, with the approval from the National Science Board, agreed to accept a renewal proposal from the National High Magnetic Field Laboratory rather than hold a national competition for operation of the nation's magnet lab.

The unanimous NSF panel decision was based on reasons such as "science remains fertile...infrastructure is magnificent, and outstanding performance by present management."

The NHMFL grant renewal is "in the best interests of science and engineering."

From John's desk

Materials Physics and Applications: Happy New Year

Welcome to the first edition of *MPA Material Matters* for fiscal year 2007. As an organization, we've survived our first fiscal year, completed our first cycle of performance and salary management, launched FY07, and we continue to make important technical and programmatic accomplishments. It's certainly worth taking a moment to congratulate yourself on these many achievements. I'm quite proud of all of you and the many things that you accomplish on behalf of MPA and the Laboratory.

Among many recent accomplishments, there are two I would like to highlight this month. MPA-NHMFL successfully commissioned the world's first non-destructive, multi-shot 100 Tesla Magnet. This is the culmination of nearly a decade's work by a large team of dedicated scientists, engineers, and technicians to produce a unique experimental capability. It follows closely on the heels of the 60 Tesla Long Pulse Magnet that was also recently commissioned. And, just in time: the three-site NHMFL (Los Alamos, Florida State, and University of Florida) recently submitted its renewal proposal to the National Science Foundation for another five years of operations.

Also recently, MPA produced its first publication in *Nature*: Rajesh Bashyam and Piotr Zelenay of MPA-11 reported the discovery of a new class of non-precious-metal catalysts. Replacing platinum is one of the grand challenge problems in fuel cell research, and by exploiting novel materials chemistry, Piotr and Rajesh have demonstrated promising catalytic action using cobalt in a novel molecular matrix. (*Read more in this month's issue..)*

Hopefully, you're already aware of the Grand Challenge Workshops coming up the last week of October. As Terry Wallace has articulated and as I've mentioned in other e-mails, this is an important part of our overall institutional science strategy. While I know there's some skepticism regarding the overall process, I'm personally spending a large fraction of my time on this effort and am fully committed to its success. If you haven't already, please give some thought to how your work fits within the Laboratory's grand challenge framework and participate in the process by attending one of the discussion sessions in your area(s) of interest. Many details can be found at http://int.lanl.gov/conferences/challenges/.

Finally, especially at this time of year, it's impossible not to talk about money. I'm sure you're all aware of the status of the Laboratory's overall budget and the impact that may have on contractor staffing levels. Locally, within MPA our budget looks strong. Nevertheless, I want to encourage you to be as frugal and cost-effective as possible, especially for discretionary expenses such as travel and materials and supplies, and where you see examples of potential waste or inefficiency to pass this along to your group leaders or to me. Protecting our most important asset, our people, while we continue to deliver on our mission is our highest priority.

We've managed to lower our directorate overhead rate for FY07. This has the very positive benefit of lowering the cost we charge our direct customers; it also means we'll have to do more with less, especially in our group and division offices. I'm confident that if we all collectively re-commit to working together effectively and efficiently, the future for MPA is quite bright.

— John Sarrao, MPA Division Leader

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Celebrating service

MPA-STC's long carbon nanotube array singled out for "great commercial promise"

MPA-STC's long carbon nanotube array has been chosen as the invention disclosure with the "greatest commercial promise" in the IDEAS contest sponsored by Technology Transfer Division.

For their invention, "long carbon nanotube arrays for fiber spinning," STC's Qingwen Li, Yuntian Zhu, Paul Arendt, Raymond DePaula, and James Groves will receive $25,000 to be spent for research or educational activities in support of technology transfer.

The researchers were presented with their award at a recent ceremony.

According to Zhu, carbon nanotubes (CNTs) are the strongest materials ever known to mankind, being a hundred times stronger than steel, but are less than one sixth the weight, giving them the potential to revolutionize a host of applications.

Ultralong nanotube arrays mean nanotubes can be spun into the long lengths in large quantities necessary for high-strength structures.

Previously, the STC team had made individual four-centimeter-long nanotubes, a world record, but still incapable of being used for high strength structures because of their small quantity.

The project is funded by an LDRD project.

The Laboratory has licensed the CNT technology to Seattle-based CNT Technologies Inc. Within six months the company plans to be making one kilogram per day of the ultrastrong, lightweight carbon-nanotube fiber, branded SuperThread™.

Over the next 15 months, CNT Tech plans to scale up production of the nanotubes in its new laboratory at the Los Alamos Research Park.

State energy and environmental policy official tours Laboratory's energy and materials programs and capabilities

Sarah Cottrell, senior advisor for energy and environmental policy for the Office of the Governor, State of New Mexico, received an overview of the Laboratory's energy and materials programs and capabilities recently.

Cottrell, who began working in the Governor's Office in July, was on site to learn about alignment on energy and environmental issues between Los Alamos and the State. In the Office of the Governor, her duties include advising the Governor on environmental issues and moving forward his initiatives on water quality, climate change, and air quality.

Cottrell toured MPA-11's fuel cell laboratories and CINT's visualization room as well as LANSCE. While here, she was briefed by George Guthrie, SPO-FE, on fossil energy programs and by Bill Tumas, SPO-AEI, on LANL's alternative energy programs. She also discussed energy issues with LANL staff involved in energy programs including MPA-11 group leader Ken Stroh.

General Motors scientists visit MPA-11, discuss Los Alamos fuel cell programs

In September, four senior scientists from General Motors' Fuel Cell Research and Development Center in Honeoye Falls, New York visited MPA-11.

Visitors were Mark Mathias, head of fuel cell research, Fred Wagner, electrocatalyst development, Hubert Gasteiger, electrode development, and Mike Budinski, materials characterization.

Gasteiger and Budinski gave a presentation titled "Open Questions on PEFC (polymer electrolyte fuel cells) Electrode Structure, Performance, and Durability."

In the talk, Gasteiger and Budinski identified electrode-related research issues that they would like to see addressed in order to accelerate PEFC commercialization. The remainder of the day was devoted to discussions of LANL programs and capabilities that might address the issues raised by GM.

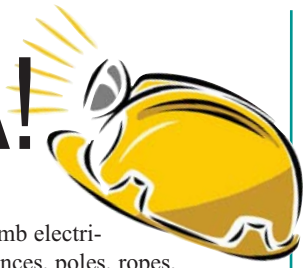
Lei joins MPA-STC as Director's Postdoctoral Fellow

Fu Lei recently joined MPA-STC as a Director's Postdoctoral Fellow.

Lei, who grew up in Wuhan, China, earned his bachelor's degree in chemistry from Wuhan University and his doctorate in physical chemical from Institute of Chemistry, Chinese Academy of Science.

At Los Alamos he will perform photoelectric studies on nanostructured materials for high efficiency solar cell applications.

Heads UP MPA!



Preventing, identifying wiring damage due to rodents

Having signs of rodents in our offices and labs can mean more than just a concern for Hantavirus.

In August, as MPA-STC's Jeff Willis and Paul Dowden were working on upgrading components on experimental apparatus, an inspection of a power cord showed it had been damaged.

Immediately after unplugging the cord from the 110 VAC receptacle, both the plug and equipment end of the cord were cut off so the cord could not be reused.

A closer investigation of the cable under a binocular microscope showed the damage was the result of a rodent or other small animal chewing on the cord.

Both the neutral and the "hot" conductor were exposed, exposing anyone handling the cord to an electrical shock, and while energized, representing a fire hazard.

A rodent victim was not found after a careful search, so it was presumed that the bare conductors had not proved fatal to the culprit. Maybe a tingle had discouraged the beast from further gnawing.

The moral of the story is that when in the lab, and especially if you are changing the wiring configuration of any equipment, check for damage to any of the cords or plugs.

Even when there are no signs of rodents, be aware that damage to cords and cables can result in an electrical shock.

To reduce the likelihood of rodents

- Reduce the amount of food and water available to rodents by keeping food covered or in a refrigerator; promptly cleaning dirty dishes; placing garbage in rodent-proof containers.
- Keep outside entrance doors closed; and routinely perform housekeeping in work spaces and storage areas to minimize the availability of nesting areas.
- Seal, cover, or screen all openings that are large enough for mice to enter (anything over 1/4 inch), including areas where pipes and wires enter buildings.
- Be careful when accessing equipment that has not been accessed for awhile such as equipment that has been in storage.

Mice can

- Run along or climb electrical wires, pipes, fences, poles, ropes, cables, vines, shrubs, and trees to gain entry to a building;
- Climb almost any rough vertical surface, such as wood, brick, concrete, weathered sheet metal, and many plastic products; crawl horizontally along or through pipes, augers, conveyors, conduit, and underground utility and communications lines;
- Gnaw through a variety of materials, including lead and aluminum sheeting, window screens, wood, rubber, vinyl, fiberglass, plastic, and low-quality concrete or concrete block;
- Enter openings larger than 1/4 inch (0.6 cm);
- Jump as high as 18 inches (46 cm) from a floor onto an elevated surface;
- Travel considerable distances crawling upside-down along screen wire;
- Survive and reproduce at a temperature of 24 o F (-4 o C) if adequate food and nesting material are available.

Pressure relief valves

Check valves are often used instead of pressure relief valves here at the Laboratory. However, it's easy to put them in backwards because sometimes the arrow showing the flow direction is hard to see.

While check valves do not strictly satisfy the requirements for pressure safety, they are tolerated for non-ASME-coded pressure systems because they do work if installed properly and have sufficient flow area. Also, there are so many of them already in use at the Laboratory. Still, because they can easily be installed backwards, have them checked—or better yet, replace them with real pressure relief valves.

October is National Ergonomics Month

Ergonomic practices, equipment, and education all contribute to protecting health and improving the quality of work and home life. To learn more about this issue visit http://ergo.lanl.gov.

At this website you can learn about the ergonomic equipment available in the ergonomics demo room (open 1-3 p.m. Tuesdays and Thursdays), sign up for ergonomics classes, request an ergonomics evaluation, and discover how to perform your own ergonomics self-assessment.

Heads UP, MPA! reports on environment, safety, and health, security, and facility-related news and information.

"Fuel cells" *Continued from page 1*

a system in which you simultaneously strive for lower costs and higher durability."

The United States Department of Energy's Office of Hydrogen, Fuel Cells and Infrastructure Technologies funds much of the PEFC fuel cell research at Los Alamos.

— By Todd Hanson

MPA-11 acoustic technique subject of cooperative research agreement

A Cooperative Research and Development Agreement (CRADA) has been executed to verify that the acoustic technique, developed by MPA-11, can indeed quantify the depth and size of defects on the surface of a natural gas pipeline using the acoustic stand-off defect monitoring technique developed by

Los Alamos. MPA-11's Dipen Sinha is the principal investigator

The agreement was executed between the Laboratory and the Northeast Gas Association (NGA) for $60K.

NGA is a regional trade association focusing on education and training, technology research and development, operations, planning, and increasing public awareness of natural gas in the northeastern United States.

Got news?

MPA Material Matters features technical highlights developed each week for the Director's Office.

If you have unclassified news you'd like to see featured, please send it to your group leader to be forwarded to *MPA Material Matters* Editor Karen Kippen.

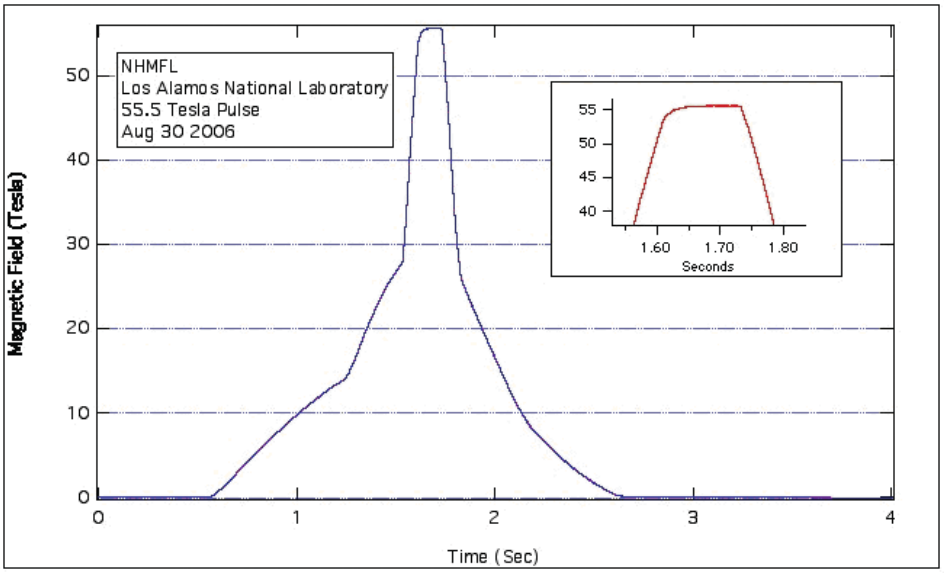
MPA-NHMFL sets new world record with 60 Tesla long-pulse magnet

The National High Magnetic Field Laboratory's Pulsed Field Facility (MPA-NHMFL) recently set yet another world record for high-performance pulsed magnets.

In completing commissioning, researchers pulsed the 60 Tesla (T) long-pulse magnet up to 55.5T, in the process setting a record for field intensity and time, reaching 55.5T for about 100ms.

Instrumental in this achievement were MPA-NHMFL's James Michel, Mike Pacheco, Ernie Serna, and Darrell Roybal for their work in the magnet assembly; Curtt Ammerman, Gretchen Ellis, Ken Hurtle, Mario Manzo, and James Sims of AET-1 for magnet design; and MPA-NHMFL's Mike Gordon, Alan Paris, Jeff Martin, Dwight Rickel, and Joe Schillig for magnet commissioning.

The researchers are now testing the cryogenics and sample environment in preparation for their first experiment.



Field profile of the last shot of the 60T long-pulse magnet. Inset shows profile of record for field intensity and time.

The 60T-LP Project is funded by the National Science Foundation.

Laboratory experts contribute to updated classic on chemistry of the actinide and transactinide elements

Plutonium chapter available as Laboratory publication

A team of international experts, including a substantial number from Los Alamos National Laboratory, has coauthored the third edition of a classic text, "The Chemistry of the Actinide and Transactinide Elements."

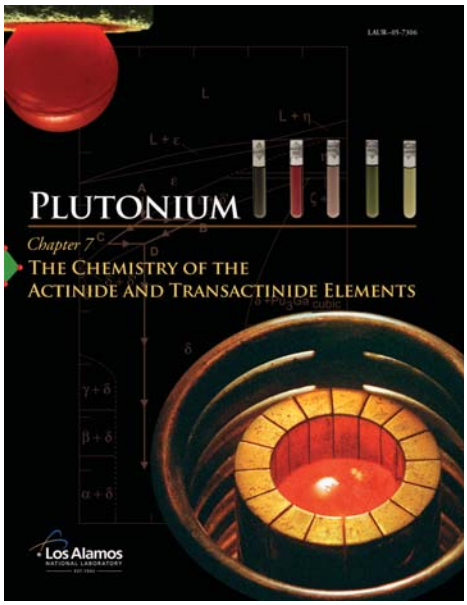
Available from Springer Publishers, the five volume set is critically acclaimed as the most authoritative and comprehensive compilation to date of the chemical properties of the actinide and transactinide elements and is anticipated to be the definitive work on actinides for the next 25 years.

Los Alamos' Seaborg Institute is planning to publish the plutonium chapter of the publication as a Laboratory publication. It can be ordered by sending an email request to Susan Ramsay (ramsay@lanl.gov) .

The first edition of "The Chemistry of the Actinide Elements," edited by Joseph Katz and Glenn Seaborg, was published in 1957 before the discovery of nobelium, lawrencium, and the transactinide elements. The second edition, edited by Katz, Seaborg, and Morss, was published in 1986 by Chapman and Hall.

The third edition contains 31 chapters and includes a contemporary and definitive compilation of the chemical properties of the elements from actinium (atomic number 89) to hassium (atomic number 108). Also included are authoritative review chapters on specialized topics such as thermodynamics, electronic theory, spectroscopy, magnetic properties organoactinide chemistry, coordination chemistry, solution chemistry separations science and technology, environmental science, analysis, and future-element predictions.

Los Alamos authors and the chapters to which they contributed include David L. Clark, ADSMS; Siegfried Hecker, MST-DO; Gordon Jarvinen, ADSMS; and Mary Neu, ADCLES, (Plutonium); Wolfgang Runde, C-IIAC (Americium); Robert Penneman and P. Gary Eller, both retired (Curium); David Hobart, C-AAC (Berkelium); P. Jeffrey Hay, T-12 (Theoretical Studies of the Electronic Structure of Compounds of the Actinide Elements); the late A.J. Arko, and John



Joyce, MPA-10 (The Metallic State of the Actinides); Carol Burns, C-NR (Organoactinide Chemistry: Synthesis and Characterization and Organoactinide Chemistry: Reactivity in Catalytic Processes); and Jerry Stakebake, PMT-1 (Handling, Storage, and Disposition of Uranium and Plutonium).

The complete table of contents and author listing can be found at http://www.springer.com/west/home/generic/search/results?SGWID=4-40109-22-51202286-0.