





ULTRACAPACITORS

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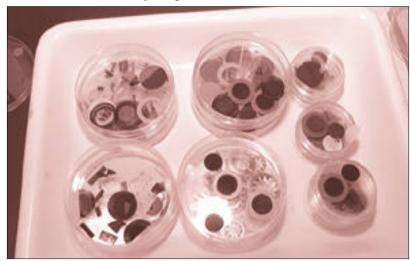
CALIFORNIA

UNIVERSITY

IMAGINING THE FUTURE OF POWER

I magine a battery-like device the size of a dime capable of being recharged millions of times and delivering as much power in each discharge as a battery 10 times its size. A recent discovery at Los Alamos has brought such devices closer to reality.

These ultracapacitors, as they are being called, have the potential to impact nearly every area of electrical energy use, from transportation to communications to computing.



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These ultracapacitors are a new generation of power sources that will have widespread impact on energy use.

DATELINE: LOS ALAMOS

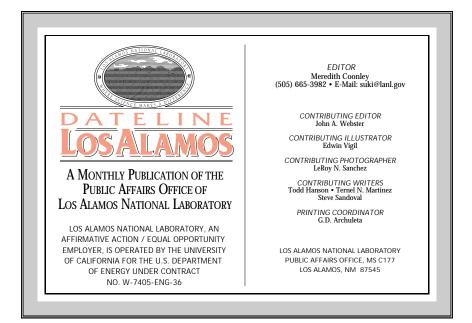
Their ability to replace conventional batteries or capacitors in various applications, or to be coupled with batteries in other applications, makes them part of a new generation of power sources with combined highenergy and high-power densities. This means they can hold substantial energy and power in a small volume.

Researchers in the Laboratory's Electronic and Electrochemical Materials and Devices Group built on a patent granted to the Laboratory in 1996 for discovery of a family of conducting polymers that act as highly effective charge storage materials.

The researchers have created a new single-cell ultracapacitor by electroplating the unique conducting polymer material onto microscopic carbon fibers woven into the form of a paper-thin disk. The polymer-coated carbon paper disk is covered with a porous separator, and electrolytic solution is added before sealing the device.

Using these unique materials and morphology, the Los Alamos researchers were able to achieve 2.7 million charge/discharge cycles for a single ultracapacitor device. Quite a feat, considering a typical battery attains an average of several hundred to several thousand charge/discharge cycles in its lifetime.

In terms of power source properties, ultracapacitors lie somewhere between a battery and a capacitor. Conventional batteries provide stored





energy for extended periods of time, but have peak-power and cycling limitations. They produce and cycle energy using chemical reactions. Because of the chemical reactions that occur within the battery, they have limited ability to charge and discharge energy repeatedly and quickly.

Conventional capacitors are capable of repeatedly providing high levels of power, but can hold very little energy. As a result, they often cannot discharge this power for more than a few microseconds.

Ultracapacitors combine the best of both worlds. They store high levels of energy in a small volume and then release that energy in power

bursts. In an automobile application, for example, a vehicle might use this burst of power to accelerate or climb a hill.

Because ultracapacitors move electrical charges between conducting materials, rather than perform any chemistry, they maintain an ability to cycle far longer than batteries. Ultracapacitors, by their very design, are lighter and smaller than batteries with comparable peak-power levels.

The advantage of the Los Alamos ultracapacitor over



other ultracapacitors currently in development or on the market is the conducting polymer's open molecular structure and the electrode's open microstructure. Together they create a large surface area and allow for higher electronic and ionic connectivity to all charging sites in the conducting polymer.

The group's latest successes with ultracapacitors are only the beginning of the story. The current amount of conducting polymer in the ultracapacitor is a mere 10 percent of the total weight, but the group's near future goal is to reach 25 percent. Reaching this goal, as well as additional planned device structural improvements, could increase the ultracapacitor's energy density to four or five times its current level.

If this happens, either the ultracapacitors of the future could be made even smaller while maintaining equivalent power output levels, or far

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Researcher Steven Shi tests an ultracapacitor cell in a glovebox.



more powerful ultracapacitors could be built that are the same size as current ultracapacitors.

Each of these directions shows significant promise. A smaller equivalent-power ultracapacitor could help miniaturize many areas of conventional electronics and a large, powerful capacitor could find many industrial and transportation applications.

The conducting polymers used in the Los Alamos ultracapacitor are the result of a steady collaboration with chemical researchers at the University of Texas in Dallas who continue to create the starting material, or monomer, for the conducting polymer used in the heart of the ultracapacitor.

The original Los Alamos research into conducting polymers began as part of the Laboratory Directed Research and Development program back in the late 1980s. The success of this LDRD project led to funding from the Department of Energy's Office of Transportation Advanced Industrial Materials. The Central Intelligence Agency provides current funding for the program.



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Steven Shi fabricates an ultracapacitor.



A JOURNEY FROM IMPURITY TO ADDITIVE

Over the past few years, the starting materials, or monomers, provided by John Ferraris' team at the University of Texas in Dallas for making conducting polymer active materials for ultracapacitors have been of the highest quality.

The University of Texas team's expertise in organic chemistry literally provided the foundation for the development of the ultracapacitor, yet it was an impurity in one particular batch of monomers that led to a breakthrough in ultracapacitor research.

Last summer, Los Alamos researcher Steven Shi was fabricating an ultracapacitor using conducting polymer as the electrode active material. The conducting polymer was electropolymerized from its monomer solution onto a carbon paper disk bonded to a current collector.

When Shi used up one batch of the monomer and started with a fresh batch — subsequently named the "April batch" — the conducting-polymer-coated carbon paper disk displayed a rusty red color, rather than the usual black. Instead of discarding the material and starting over, Shi decided to investigate. His investigation revealed that this new rusty-red-colored conducting polymer was significantly superior to the original black material in terms of polymer morphology and material stability.

The red material exhibits highly porous, open structure, with polymer grain size in the sub-micron range, while the black material shows a relatively compact structure with polymer grain size in the range of several microns.

The new morphology of the red material provides a large, effective, electrolyte-accessible polymer surface area, leading to fast charge/discharge dynamics. More surprisingly, the red material also helps extend the device cycle life in pulsed discharge mode from 100,000 cycles to 2.7 million cycles.

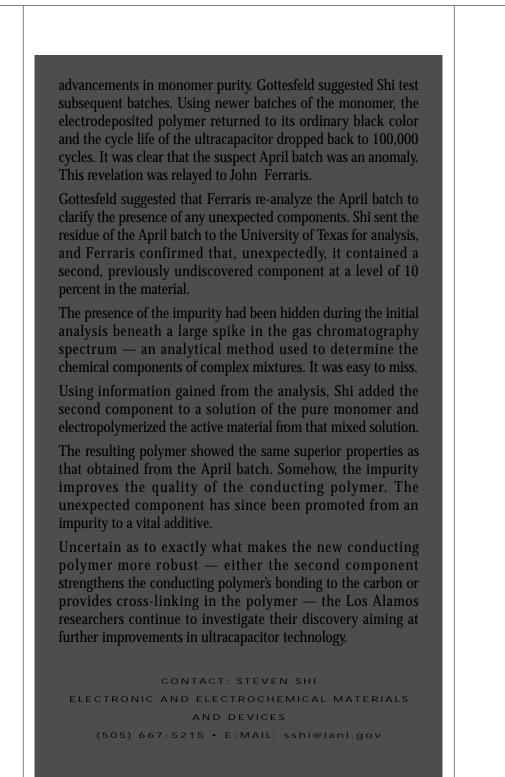
Shi brought this discovery to the attention of Shimshon Gottesfeld, the principal investigator for the project, who thought perhaps the University of Texas team had made



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Steven Shi had a mystery on his hands After the disk Shi holds turned red instead of black, he investigated and discovered that one batch of material included a previously undiscovered component that produced higher energy densities. This impurity has led to a breakthrough in ultracapacitor research.





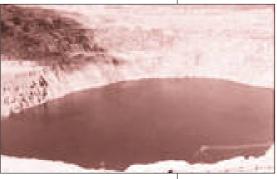


POLLUTION SOLUTION

POLYMER FILTRATION REMOVES TOXIC METAL CONTAMINANTS FROM MINE RUNOFF

S cientists have developed a novel technology capable of removing toxic metal contaminants from acidic mine runoff. The technology provides a potential remedy for some of the world's most challenging environmental problems.

There are thousands of abandoned mine sites in the United States alone. "Some of these abandoned mines, like the Berkeley Pit near Butte, Mont., pose hazards to local aquifers due to acid mine drainage," said Los Alamos researcher Tom Robison. "To address this problem, we developed a technology to remove toxic metal contaminants such as lead from acid



mine drainage and, in the process, recover the economically valuable metals, like silver, copper and zinc. Typically these metals are lost in conventional remediation processes."

An EPA Superfund site, the Berkeley Pit is an abandoned open-pit copper mine containing more than 20 billion gallons of tainted water.

Known as polymer filtration, the patented Los Alamos technology couples unique water-soluble polymers with a process known as ultrafiltration. Scientists use a homogeneous polymer solution that binds with metal ions in the wastewater. After the polymer binds to the metal ions, the polymer-metal combination is filtered and concentrated using ultrafiltration.

At process end, clean water is discharged and the metals are recovered for disposal or refining when the pH of the polymer solution is changed and the metal ions come unbound.

Since the polymers are recycled back into the polymer filtration system, there is no secondary waste or sludge stream — unlike that produced by hydroxide precipitation wastewater treatments. Perhaps most importantly, instead of working with individual batches, the technology is designed to be an in-line treatment so it can rapidly and continuously

The Berkeley Pit Mine in Montana.

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process mine wastewater. Polymer filtration operates at low pressure and low temperature. It is more efficient than conventional ion-exchange resin processes.

In tests conducted on water samples taken from the Berkeley Pit as part of a proof-of-principle experiment, the polymer-filtration process began working immediately after researchers added a dilute solution of basic polymer to the samples. The addition of the polymer decreased acidity in the water causing the precipitation of nearly all the iron and aluminum in the samples. The samples were then treated with another polymer and ultrafiltered.

Tests of this treated Berkeley Pit water showed traces of copper, aluminum and iron, fewer than 10 parts per billion of zinc and fewer than 3 ppb of nickel, chromium, lead and cadmium — all far below current EPA discharge limits.

The polymer-filtration technology is based on Laboratory-Directed Research and Development-funded work conducted at Los Alamos in this area since 1992. Prior successes included actinide removal from aqueous streams and electroplating process waste minimization. The technology, as it was adapted for the electroplating industry, received an R&D Magazine R&D 100 Award in 1995.

To facilitate the continued diffusion and advancement of the polymerfiltration technology, Los Alamos has created a user facility in the Separation Science and Technology Technical Deployment Center and is actively seeking interested industrial mining partners to establish the technology.

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SUPERCOMPUTING CHALLENGE

LOS ALAMOS ASSISTS HIGH SCHOOL STUDENTS IN SCIENTIFIC COMPUTING

N early 500 students from 43 schools spent the last year researching scientific problems and writing programs to solve them on supercomputers at Los Alamos

as part of the New Mexico High School Supercomputing Challenge. A team from Albuquerque Academy took first prize for "The Evolution of Hive Intelligence Using Genetic Programming," which ran on an SGI Origin 2000.

The goal of the supercomputing challenge is to increase knowledge of science and computing, expose students and teachers to computers and applied mathematics, and instill enthusiasm for science in high school students, their families and communities. Any New Mexico high school student in grades 9-12 may enter.

The challenge was conceived in 1990 by former Los Alamos Director Sig Hecker and Tom Thornhill, president of New Mexico Technet Inc., a nonprofit company that in 1985 set up a computer network to link the state's national laboratories, universities, state government and some private companies.

U.S. Sen. Pete Domenici, R-N.M., and John Rollwagen, then chairman and chief executive officer of Cray Research Inc., added their support.

The challenge is sponsored by the Laboratory and New Mexico Technet Inc.

Benefactors include CISCO Systems Inc.; DP Signal; Intel Corp.;



First-prize winners (from left) Ryan Davies, Kevin Oishi, Tom Widland and Alex Feuchter each took home a \$1,000 savings bond and a computer loaded with software for their teacher's classroom. Ryan Dureay also was part of the winning team, but was unable to attend the April 28 ceremony in Los Alamos.

Kinko's; and Microsoft Corp. Patrons include Sandia National Laboratories; University of New Mexico; New Mexico State University; New Mexico Institute of Mining and Technology; Albuquerque Tribune; SGI; Council for High Education Computing Services (CHECS Inc.); Eastern New Mexico University; New Mexico Highlands University; New Mexico Department of Education; San Juan College; Santa Fe Community College; and the Air Force Research Lab.

Visit the challenge web site at http://www.challenge.nm.org

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ROCKY FLATS CLEANUP

LOS ALAMOS DEVELOPS TECHNOLOGIES TO HELP DECONTAMINATE DOE SITE

 \mathbf{F} or nearly 40 years, the Rocky Flats Nuclear Weapons Plant was the main U.S. site for manufacturing plutonium pits — the heart of nuclear weapons — and other weapon components for the nation's nuclear stockpile. With its defense mission long since past, the entire site currently is undergoing decontamination and decommissioning.

Los Alamos researchers also are playing a vital role in the massive cleanup effort, which is headed by Kaiser Hill, LLC, of Denver. Specifically, the researchers are helping Kaiser Hill identify and solve urgent, unanticipated technical problems encountered during the cleanup work.

The task of cleaning up the Department of Energy-owned site is a daunting, technologically challenging one to say the least. Located about 15 miles from downtown Denver, what is now known as the Rocky Flats Environmental Technology Site has more than 100 buildings spread out over more than 6,500 acres. About 170 contaminated areas have been identified.



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A view of the Rocky Flats site outside of Denver.



Moreover, Rocky Flats' current inventory includes 50,000 containers of transuranic and low-level radioactive waste — destined either for the recently opened Waste Isolation Pilot Plant in Carlsbad, N.M., the Nevada Test Site Waste Repository or the Envirotech Waste Repository in Utah — and about 14 tons of plutonium, more than any other DOE manufacturing facility.

The goal is to raze all buildings and clean up the site to where it can be used for residential or other industrial purposes, if desired. Thus all existing wastes and residues must be disposed of properly, meaning the waste must be stabilized, possibly repackaged and certified for acceptance at the appropriate disposal sites.

Kaiser-Hill also is aiming at a new closure date of 2006, four years earlier than the original 10-year plan baseline date. If successful, this will save a substantial amount of money from the original plan's baseline cost, estimated at \$7 billion.

Various types of nondestructive assay, or NDA, technologies are used to examine drums and containers and their contents to ensure that they meet safeguards requirements and repository acceptance criteria. Insufficient NDA capability or capacity delays cleanup activities and increases costs.

A joint Los Alamos/Rocky Flats team was formed to provide the NDA technical support necessary to successfully meet the NDA challenges at Rocky Flats. It is through this mechanism that Los Alamos is providing technical expertise and designing, fabricating and deploying several world-class NDA systems.

One Los Alamos technology currently being used at Rocky Flats is the mobile Tomographic Gamma Scanner, a 4-foot by 6-foot device that performs gamma-ray tomographic scans of waste containers. Developed originally to assay waste in 2-foot by 1-foot boxes, 30- and 55-gallon drums and 83-gallon overpacks, the versatile TGS provides quick assays of low, medium and high-density waste in both cans and drums.

This mobile system can be taken directly to the waste drum storage location, which significantly reduces the transportation costs associated with transporting waste to an assay facility for characterization.

Initial TGS results show that radioactive material is located in the bottom portion of many drums. If this holds true, the unit may provide a database of information that could help minimize waste in the future.

The TGS outperformed 15 other NDA systems for superior assaying capability during a DOE-sponsored performance demonstration

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program. Indeed, Los Alamos technology has passed every one of the PDP test cycles to date and usually are the best performers of all equipment tested.

Los Alamos also built a skid-mounted TGS — an improved version of an earlier TGS system — that is being used at the glove-box line at Rocky Flats. Of particular note is that the Los Alamos researchers designed, tested and deployed this world-class system in only six months, or half the time it normally takes for such an endeavor.



Also under construction at Los Alamos is the Standard Waste Box Counter (also known as the super Highefficiency Neutron Counter, or superHENC), a device that analyzes the amount and arrival times of neutrons from fissioning nuclear materials. This trailer-mounted NDA system is designed to measure transuranic waste low-level and waste packages in standard waste boxes. The SWB Counter is scheduled for delivery to Rocky Flats next February.

Another Los Alamos technology being used in support of all assay systems is the Fixed-energy Response

Analysis of Multiple energies, or FRAM, isotopic system. This technology determines the ratio of plutonium and other isotopes to total plutonium, which is necessary to accurately compute the total nuclear material in any given sample.

Los Alamos also is helping Rocky Flats upgrade its calorimeters and improve assay speeds. Calorimeters are devices used for measuring the heat developed from the nuclear decay of isotopes in waste and residue samples. It is the most precise NDA instrument available, but the existing Rocky Flats calorimeters may take up to 27 hours for a single

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Researcher Tom Prettyman makes an adjustment on a skid-mounted TGS. The 30-gallon drum in the center of the device shows where a sample would be placed to be assayed.



measurement. When complete, the upgraded calorimeters are expected to make the same measurement in about eight hours or less.

Los Alamos first established an office at Rocky Flats in 1989 to provide defense-related technical support to the site as part of the Laboratory's Nuclear Materials and Stockpile Management Program. The office now is part of the Laboratory's Environmental Management Programs Office, and is collaborating with the Safeguards Science and Technology and Environmental Science and Waste Technology groups at Los Alamos to provide technical support to Kaiser Hill.

The Safeguards Science and Technology Group is providing the various NDA technologies, while the Environmental Science and Waste Technology Group tests and certifies those technologies before they are shipped to the Denver site. Los Alamos researchers also make sure the systems operate as designed at Rocky Flats. Approximately 50 Laboratory staff members are involved in the Accelerating Cleanup Plan.

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MUSEUM COLLABORATION

LOS ALAMOS SCIENTISTS ASSIST AMERICAN MUSEUM OF NATURAL HISTORY WITH FIVE EXHIBITS IN THE NEW EARTH SCIENCES FACILITY

E arth scientists and computer scientists from Los Alamos contributed their expertise to five computer/video exhibits in the new Hall of Planet Earth at the American Museum of Natural History in New York City.

The earth sciences facility, Hall of Planet Earth, opened in June at the AMNH, the largest natural history museum in the world. The two other parts of the museum's new Earth and Space Center, the Hayden Planetarium and the Hall of the Universe, will open next year.

The exhibits in which Los Alamos was involved feature atmospheric dynamics, subsurface water flow, ocean dynamics, the Earth's magnetic field and convection in Earth's mantle. Like other exhibits in the new hall, they focus on the processes that have shaped the Earth, rather than the history of the planet.

The videos, which run for a few minutes each, show animations of the physical processes, Lab scientists talking about their research and



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The 8-foot Dynamic Earth Globe is suspended from the ceiling in the Hall of Planet Earth at the American Museum of Natural History in New York City.

Illustration courtesy of the American Museum of Natural History



visualizations of their computer simulations. The computational "number-crunching" required to handle the vast amounts of data in the models is illustrated by equations and programming code that scroll up the screen.

Chick Keller, director of the Institute of Geophysics and Planetary Physics at Los Alamos and coordinator of the Lab's involvement in the project, views the collaboration as an exciting opportunity for scientists to communicate with the general public.

"One thing that's hard to communicate is the result of these enormous computer runs in simple, easy to understand ways. We don't necessarily do it very well at the Lab, but the museum staff excels at it," Keller said. "So this collaboration has become an excellent way to tell the public quickly what scientists are doing, how they're doing it and what results they're seeing and for the Lab to gain expertise in doing this."

The use of computer models as learning tools is an important element of the museum exhibits. "These models are so detailed that ... they allow you to go where you can't go," said Keller. "You can actually explore places on Earth that can't be observed and watch changes in time over millions of years."

"We're doing something that I don't think has ever been done in a natural history museum before, and that's trying to explain the nature of computer modeling and its bearing on modern science," said Ed Mathez, chair of the museum's Department of Earth and Planetary Sciences. "The kind of numerical modeling that Los Alamos is explaining has become a very important approach to explaining science in just the past few years."

The new 8,830-square-foot hall includes a suspended 8-foot hemisphere with an internal projection system that shows how Earth looks from space, complete with cloud and ocean formation. Other exhibits include sulfide chimneys, called "black smokers," from the ocean floor, an ice core containing a climate record dating back 115,000 years and an "Earth Event Wall" displaying events such as earthquakes, volcanic eruptions and major storms as they occur.

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DATELINE: LOS ALAMOS

SCIENCE DIGEST

KNOCKING ON ETHYL'S DOOR



A Los Alamos scientist has patented a new portable device for quickly and accurately determining the octane rating of gasoline. The octane rating, developed in 1926 by the Ethyl Corp., is a number indicating the amount of engine knocking caused by a fuel under standard test conditions. Current tests for octane require gasoline samples be run through a knock-test engine. This cumbersome and timeconsuming process does little to guarantee a given fuel supply's actual octane content. The solid-state Los Alamos device is

roughly the size of a hand-held calculator and has no moving parts. It operates on the principle of acoustic resonance. The device tests fuel for octane content by transmitting sound waves into the fuel container from the outside and then measuring the speed of the sound waves through the container. Correlating the speed of sound through the container to speeds through fuels with various octane contents determines the octane content of the fuel in the container. The test process takes only a few seconds and can be used for continuous fuel monitoring.

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WHERE IN THE BODY?

Researchers at Los Alamos have developed a technology for the noninvasive measurement of drug concentrations in tissue. The fiberoptic instrument uses optical spectroscopy to detect changes in tissue in real time and with site specificity. New computational methods allow determination of the path lengths of photons in tissue based on tissue scattering properties. The analysis of the optical spectra reflected from the tissue enables a determination of the compound or drug concentrations. The system is also being tested to perform pharmacokinetic measurements on tumors following drug administration in animals. Researchers have successfully demonstrated the ability to differentiate



between tumor cells and normal cells in bladder, colon and breast cancers. CONTACT: IRVING BIGIO, (505) 667-7748, E-MAIL: ijb@lanl.gov

A METEORIC SPRITE

Los Alamos scientists have advanced a theory that a meteor passing through the upper atmosphere can precondition the air for formation of columniform sprites, a specific type of high-altitude electrical discharges that recently have been recorded with video cameras. Meteors leave a trail of ions and aerosols in their wakes, and these particles affect the conductivity of the upper air for about 12 minutes. If during this time a storm cloud discharges a lightning stroke to the ground, the resulting electric field can both drive conventional air breakdown processes within the meteor trail — creating brief columns of light, the observed sprites — and start a runaway electron cascade at the cloud top. The

passage of the runaway electron beam through the meteor trail extinguishes the discharge. Computer simulations show good agreement between this model and observations of columniform sprites, though the researchers point to additional work that's needed. The frequency of meteor showers implies the atmosphere is continually being preconditioned



for this process. They suggest coordinating observations of high-altitude discharges with known meteor showers during thunderstorm season. CONTACT: EUGENE SYMBALISTY, (505) 667-9670, E-MAIL: esymbalisty@lanl.gov

"THE NAME'S BOND, ION IMPLANTATION BOND"

Los Alamos and Arizona State University researchers recently received a patent for a process to improve bone growth around prosthetic devices such as hip and knee implants, thereby increasing the life of the prosthetics. Many doctors today use titanium implants that are plasma spray-coated with a mineral called hydroxylapatite, or HA. Bone is living material composed of 75 percent HA and therefore interfaces well with the coating. But HA does not interface well with titanium, which





can result in implant failure. The new patented process uses an ion implantation beam — ideal for implants of any shape — to effectively mix the first layer of HA coating to the implant's metal surface and strengthen the bond.

Next, the implant is dipped into an HA solution filled with ceramic particles, then heated to form a hardened coating around the initial ionimplanted coating. By reducing the temperature for each successive coating, the layers (as many as 100) become decreasingly dense. The bone easily grows into the outer, porous HA layer and progressively slows with each denser HA layer it encounters. In essence, the HA coatings are custom-tailored to the bone and implant and greatly reduce the risk of implant failure. The researchers are looking for funding to conduct proof-of-principle experiments for the newly patented process.



ENERGY AND THE ENVIRONMENT

LOS ALAMOS TO WORK WITH FOSSIL ENERGY RESEARCH ORGANIZATION TO DEVELOP TECHNOLOGICAL SOLUTIONS

L os Alamos and the nation's largest fossil energy research organization have pooled their scientific and technological resources to collaborate on a broad range of energy and environmental issues.

A recently signed five-year memorandum of understanding calls for the Laboratory and the Federal Energy Technology Center to work together in developing technological solutions in such areas as carbon management and sequestration, environmental remediation, power grid adequacy and reliability, global climate change and water resource planning and analysis.

FETC is a field office of the Department of Energy's Office of Fossil Energy. Its mission is to solve national energy and environmental problems through partnerships with private industry, universities, nonprofit organizations, national laboratories and other government agencies. FETC manages more than 600 research, development and demonstration projects in all 50 states and in 16 countries.

Areas of potential collaboration between Los Alamos and the FETC include:

• developing science-based options for managing carbon dioxide produced by fossil fuel power generation

• assessing issues related to the development and deployment of carbon management and sequestration approaches

• analyzing the impact of current restructuring initiatives (essentially any federal or state utility deregulation initiatives that could impact the power system infrastructure), pending pollution regulations and global climate change concerns on the power system infrastructure

• developing and applying more effective, representative integrated watershed models to aid in planning and analyzing regional water resources

• developing and applying cost-effective, scientifically based environmental restoration methodologies, using appropriate sites as testbeds

• conducting workshops, meetings and other forms of outreach to promote and improve stakeholders' understanding of the issues involved and disseminate results of the collaboration

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BRIEFLY ...

NEW MEXICO HIGH SCHOOL STUDENTS JOINED STUDENTS FROM CALIFORNIA AND WASHINGTON STATE IN THE FIFTH CRITICAL ISSUES FORUM, sponsored last month by the Laboratory's Education Programs Office. This year's topic, "Nonproliferation vs. Proliferation in the Nuclear Age," challenged students and teachers to examine the issues confronting our nation's scientists and other leaders as they seek to manage nuclear technology without being controlled by it. Laboratory volunteers and online mentors assist the teams by answering questions and suggesting areas for further study and research. Previous forums have dealt with the loss of rain forests, terrorism, the global nuclear vision and the thorny question of what to do with excess nuclear materials worldwide. The conference included presentations of posters and World Wide Web pages the student teams developed, as well as concurrent discussion sessions on student research. More information about the student poster sessions and the forum is available at http://set.lanl.gov/programs/cif/CIF99 online.

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LOS ALAMOS NATIONAL LABORATORY

