December 1998

Science & Technology REVIEW

Lawrence Livermore National Laboratory

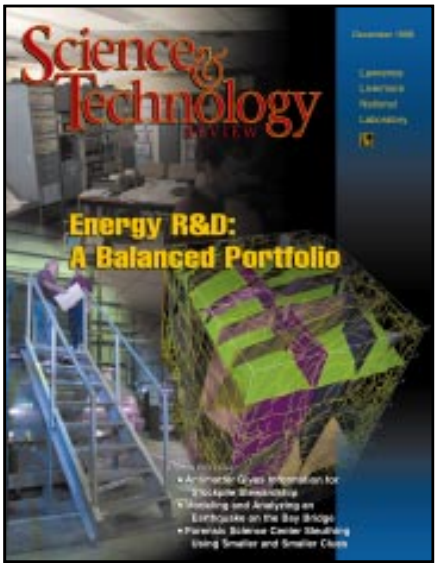
Energy R&D: A Balanced Portfolio

Also in this issue:

- Antimatter Gives Information for Stockpile Stewardship
- Modeling and Analyzing an Earthquake on the Bay Bridge
- Forensic Science Center Sleuthing Using Smaller and Smaller Clues

About the Cover

Livermore's Energy Directorate responds to a variety of energy challenges and meets head-on complex and interrelated energy issues. At left and center on the cover are the control room and test facility for a Livermore collaboration with Toshiba Corporation to test a superconducting magnet energy storage system, a technology that will be useful for leveling electricity usage loads. At right is a model of the rock environment of the proposed nuclear fuel waste respository in Yucca Mountain, Nevada. Livermore researchers have been assisting in the design for the engineered barrier system to isolate spent fuel. The Laboratory undertakes these and other energy research and development programs that offer near-term solutions to complex problems but are beyond the existing capabilities of industry.



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About the Review

Lawrence Livermore National Laboratory is operated by the University of California for the Department of Energy. At Livermore, we focus science and technology on assuring our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published 10 times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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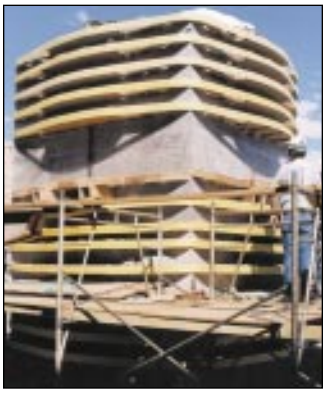

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London to San Francisco in less than two hours

A revolutionary design for a hypersonic aircraft that could fly between any two points on the globe in less than two hours has been developed by a researcher at Lawrence Livermore. HyperSoar could fly at approximately 6,700 mph (Mach 10), while carrying roughly twice the payload of comparable subsonic aircraft. The HyperSoar concept promises less heat buildup on the airframe than previous hypersonic designs—a challenge that has until now limited the development of aircraft.

The key to HyperSoar is the skipping motion of its flight along the edge of the Earth's atmosphere—much like a rock skipping across water. A HyperSoar aircraft would ascend to approximately 130,000 feet—lofting outside the Earth's atmosphere—then turn off its engines and coast back to the surface of the atmosphere. There, it would again fire its air-breathing engines and skip back into space. The craft would repeat this process until it reached its destination.

"We believe the design not only addresses the primary issues in building hypersonic aircraft but does so in a way that creates a number of different uses for HyperSoar, thereby helping offset its development costs," said Livermore aerospace engineer Preston Carter, developer of the concept. Potential applications for HyperSoar include passenger aircraft, air freighters, military aircraft, and space lifts.

Contact: Preston Carter (925) 423-8293 (carter17@llnl.gov).

Livermore interactions help Laughlin win Nobel Prize

Lawrence Livermore extends its congratulations to Robert B. Laughlin, one of three sharing the Nobel Prize for physics in October 1998. Laughlin, a professor of physics at Stanford University, has been associated with the Laboratory for 17 years.

Laughlin credits the Lab's multidisciplinary approach to science as being extremely useful to him in his career. "It is my opinion that the national labs, and Livermore in particular, have tremendous potential for making important scientific contributions," he said.

Laughlin's prize-winning work reveals fundamental insights in quantum mechanics, providing the explanation for the experimental findings of Stormer and Tsui, who discovered the so-called fractional quantum Hall effect. The key surprise of the effect is that collective motions of electrons can behave like a fraction of a given electrical charge for one electron. Previously the only clear example of fractional charges in the laboratory had been quarks.

Contact: Robert B. Laughlin (925) 422-7369 (laughlin1@llnl.gov).

Plutonium experiment successful

In work aimed to further the understanding of the properties and microstructure of plutonium as it ages in the U.S. nuclear stockpile, Livermore scientists conducted an experiment deep in the Nevada desert some 900 feet below ground at the Nevada Test Site, 85 miles north of Las Vegas. The experiment, a year in the making, went off without a hitch.

Four coin-sized disks of plutonium were shocked with explosives into a fine dust. Four clocking devices measured the particles' velocities, while a holographic camera recorded three-dimensional images of the particles in flight, all made possible by a complex array of dozens of lenses directing images to the camera. The data will be used to refine nuclear physics computer models.

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Thwarting terrorists with a new vehicle barrier

Engineers from the Laboratory conducted a successful test of a new roadblock, dubbed a "terrorist vehicle barrier," at the Nevada Test Site, north of Las Vegas. The concept was developed by Livermore consultant Bill Wattenburg in the wake of the truck bombings of U.S. embassies in Kenya and Tanzania. In the experiment, a three-quarter-ton pickup truck loaded with 400 pounds of sand (simulating the weight of explosives) was driven by remote control into the barrier system. Ten ordinary steel pipes—each 24 inches in diameter and weighing 1,300 pounds—were strung together in a U-shaped formation resembling a child's macaroni necklace. Running through the pipes was 1-inch steel cable, anchored at each end with 1,200-pound concrete blocks.

"While the truck did surmount the barrier, it was left totally incapacitated and couldn't have moved another inch," reported project investigator David McCallen. "It was dead on arrival."

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Calling for NIF optics synergy

The National Ignition Facility (NIF) laser under construction at Lawrence Livermore will use 22,000 small optics components, a number that inspired NIF project managers to invite optics manufacturers and NIF engineers to a NIF Small Optics Manufacturing Summit in September. Representatives from more than 60 optics manufacturing firms attended the conference.

Participants discussed NIF's technical specifications and manufacturers' capabilities and shared how to meet NIF requirements, form partnerships, and familiarize themselves with the Laboratory's procurement process.

NIF will be the world's largest optical system, a mammoth 192-beam laser facility dedicated to research in national security, energy, and basic science. When complete in 2003, it will contain 33,000 square feet of precision optics—more than in all the telescopes in the world combined.

Strengthening the U.S. Energy Portfolio

THE Department of Energy invests in research and development for a diverse set of energy technologies to meet the nation's—and the world's—needs for environmentally benign, economic, and secure energy supplies. These investments rely on a broad range of scientific and technical expertise for their successful fruition. That expertise is being provided by, among others, Lawrence Livermore National Laboratory.

The system of energy supply, generation, delivery, and utilization is extremely complex. Energy's development and use affect—and are also constrained by—domestic and international politics, economics, the environment, safety, and security. Each energy choice is a tradeoff in efficiency and these other external elements. Successful marketplace penetration by energy systems is influenced by many factors, including expediency, education, economics, government regulations, infrastructure availability, and operations and maintenance characteristics.

The complexity of energy issues requires us to have a broad point of view about them. We cannot hope to answer energy problems with any single technology, no matter how innovative. Rather, we must look at the problem from a systems perspective and develop an integrated viewpoint that encompasses all of energy's interrelationships.

A systems perspective and multidisciplinary research and development are Livermore's approach. We take advantage of the Laboratory's extensive multidisciplinary capabilities, from advanced computations to materials science to environmental science, to pursue advances. Our unique facilities support programs to meet national energy needs, and through cross-communication of activities among Laboratory projects, we are able to see the bigger picture of our mutual goals and realize opportunities for synergism. Livermore provides an ideal community for scientific cooperation—among research programs within the Laboratory and with other labs, universities, and industry.

As the article beginning on p. 4 indicates, we are developing a range of significant technologies that contribute to the U.S. energy portfolio. Some of this work leads to technologies or energy resources that are more economical and therefore more attractive to the marketplace. Other work mitigates or reduces the impact of energy development on the environment. Our focus is on meeting national energy needs, while keeping a watchful eye on the implications and ramifications of energy production and use on a global scale. Our work in the broad arena of carbon management addresses the global issue of possible climate change as a result of fossil fuel use. Efforts both domestically and internationally address operational, security, and nonproliferation issues associated with continued nuclear energy development and use.

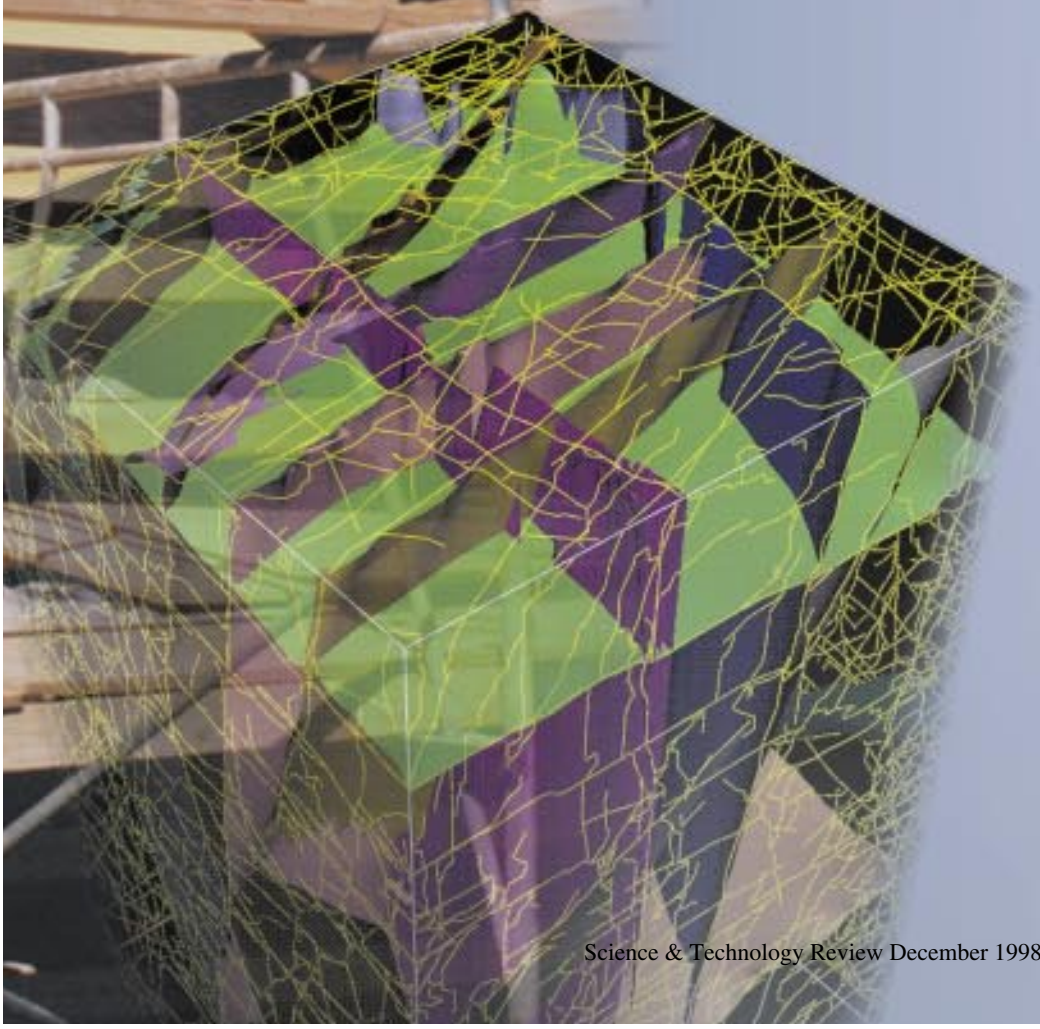
At this national laboratory, we undertake work in areas that are high-risk or long-range and thus are beyond the immediate scope of industry. In areas where we have special capabilities, we also do research that can have near-term impact. Such work includes developing fuel cells, energy-efficient manufacturing processes, and the disposal of radioactive waste. For longer-term needs, we are pursuing research to develop next-generation nuclear fission reactors. Looking still further ahead, we are developing alternative concepts for fusion energy, a new magnetic levitation concept, and ways to sequester the carbon dioxide from fossil fuel emissions.

Energy may be plentiful and cheap now, but that situation could change quickly over coming decades because of political or economic developments elsewhere in the world. The lead time for the development and successful penetration of new technologies into the marketplace can be so long as to require significant investment many years before the need becomes immediate. Thus, the balanced energy R&D portfolio requires funding now in order to develop new technologies and resources for the long term. Livermore is making meaningful contributions in energy research and development to ensure that these technologies will be available to meet this nation's energy needs in the next century.

■ Terry Surles is Associate Director, Energy.

Energy to Keep Everything Running

A nuclear waste repository. Thin-film solid-oxide fuel cells. A superconducting magnet energy storage device. Carbon management technology. The Laboratory's Energy Directorate works in diverse ways to keep U.S. energy available, safe, clean, and inexpensive.



TO the unknowing eye, the energy chart produced by Livermore's Energy Directorate is just a tangle of lines, patterns, and colors (Figure 1). But to Energy staffers, it provides useful information about energy flow for a given year in the United States, from source to use.

Beyond its numbers, the chart portrays the complexities and interrelationships of the energy systems needed to support the quality of life and economic stability of the U.S. and, by inference, of any developed economy. It also points to substantial inefficiencies in converting energy into usable forms and transmitting, distributing, and using it.

Reducing these inefficiencies is one of the challenges that the Department of Energy faces in ensuring that U.S. energy needs can continue to be met. Energy availability is also threatened by other factors. The emergence of developing economies puts increasing pressure on world energy supplies. U.S.

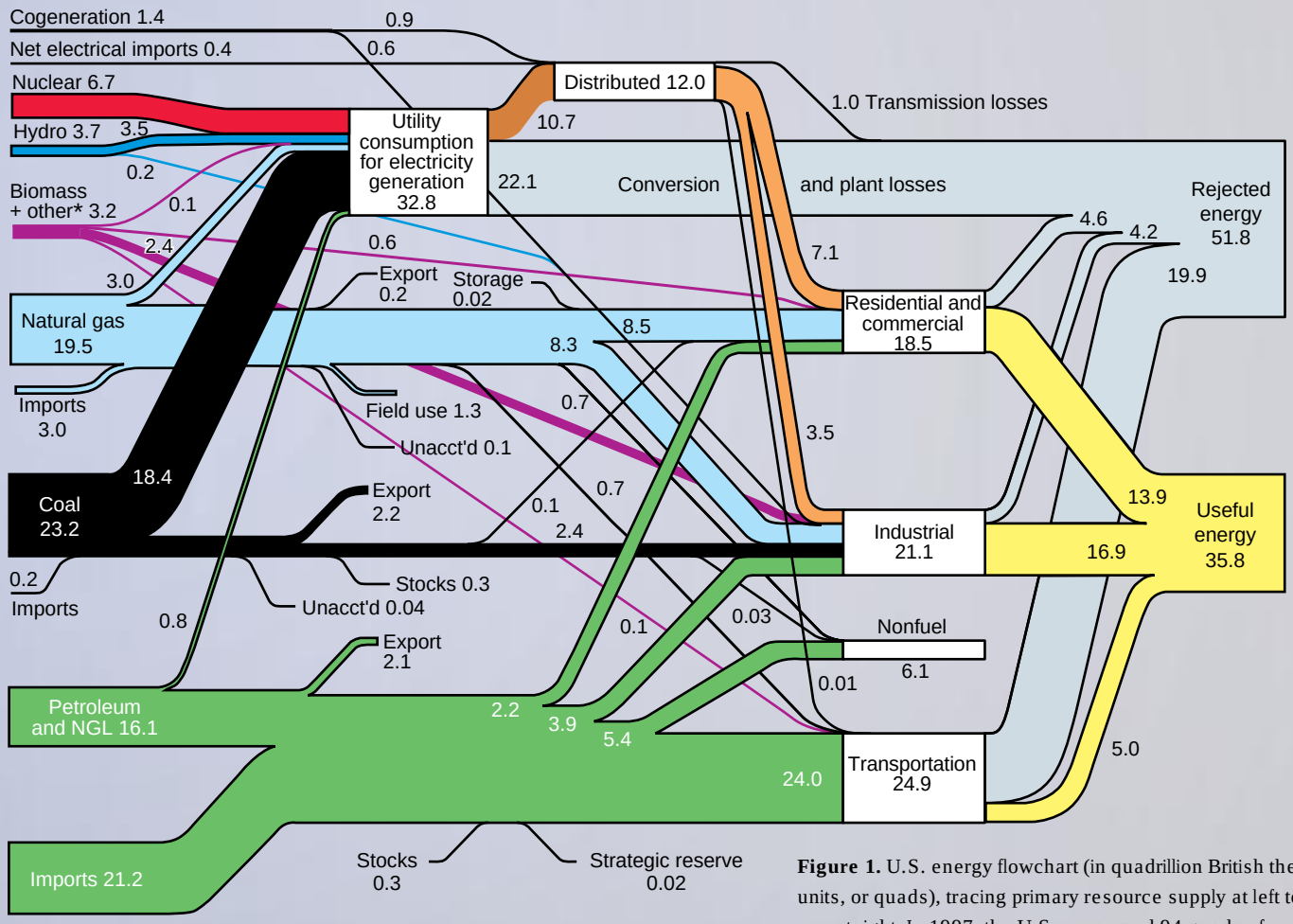
dependence on foreign oil means that political disputes can result in energy crunches. The possibility of global climate change caused by burning fossil fuel is stimulating some rethinking about energy resources and energy production. In addition, the continuing concern about nonproliferation and nuclear waste disposal may limit nuclear energy options.

Pursuing Integration

Lawrence Livermore's Energy Directorate is helping DOE address some of these large energy issues. Not only is Livermore innovating technologies for energy production, storage, and distribution, it is assessing the risks and feasibility of various alternative energy resources and investigating transitions to other forms of energy.

The Laboratory continues to develop better ways to ensure the safety and reliability of nuclear power by addressing the technical problems of the nuclear fuel cycle from supply, fuel storage, and transport issues to waste storage, safety, and security issues. Livermore nuclear specialists are working with other national laboratories, private industry, and universities to propose the development of next-generation, small-scale fission reactors that improve reactor safety, economics, waste management, and proliferation resistance.

In the meantime, magnetic fusion energy researchers are experimenting with new fusion reactor configurations—such as a spheromak—not only to meet the scientific goals and requirements for achieving fusion, but also to make fusion power economically feasible. Feasibility will largely depend on finding more compact and less complex fusion



*Other: geothermal, solar, wind, waste

Figure 1. U.S. energy flowchart (in quadrillion British thermal units, or quads), tracing primary resource supply at left to end use at right. In 1997, the U.S. consumed 94 quads of net primary energy resources.

schemes. The spheromak generates its own magnetic fields by an internal dynamo and thus does not require as many magnets as fusion devices such as the tokamak, which in turn leads to engineering simplicity. By using a combination of theory, experiments, and advanced computational simulations, researchers are working to make the spheromak an attractive fusion reactor.

The breadth of the energy R&D landscape could lead to seemingly disparate research. However, Terry Surles, the new Associate Director for Energy, urges his scientific and technological experts to provide "big picture" thinking, which will create opportunities to solve complex national and international energy problems and do it better (see box below). He also directs effort toward developing new ways to use resident expertise to enlarge problem-solving capabilities, achieve synergies, and leverage Laboratory talent.

Because energy use is complex, research topics naturally are diverse. Surles encourages researchers to leverage their projects to reach a worthy objective: speed up the development of innovative technologies and ease their commercialization so the public can benefit from them sooner.

Livermore expertise can cut a wide swath through energy research and technology development needs, he says, "provided there is careful thinking about technology development—to identify the program areas most appropriate for Livermore—and the best integration of Livermore disciplines."

At the same time, Surles demonstrates how energy projects are less dispersed than they seem, because they can be organized into what he calls "a technology portfolio based on technology-specific 'bins' such as conversion and storage, carbon management, or the nuclear fuel cycle."

Keeping Nuclear Energy Viable

Although 20 percent of the country's electrical energy is supplied by nuclear power plants, challenges remain for this source of power. After the experience with Three Mile Island and Chernobyl, concerns continue about the safety and proper waste management of this source of relatively clean electricity.

One issue continuing to concern the public has been the disposal of hazardous nuclear waste generated by nuclear reactors. Thousands of metric tons of spent fuel from commercial nuclear power plants are being stored, temporarily, at facilities that are almost at capacity. A permanent disposal site is crucial, not only for safety and environmental reasons, but also for continuing nuclear power plant operation. Work to provide such a site has been progressing, with Lawrence Livermore involved in a key part of it.

The work on the Yucca Mountain Nuclear Waste Repository is now entering the viability assessment phase, which means that Congress will soon decide whether the Yucca Mountain site is suitable for nuclear waste disposal and whether to seek licensing by the Nuclear Regulatory Commission (NRC). Arriving at this decision point has taken over 20 years.

This considerable effort is required because the project is unique as well as important. No one has had experience in completely isolating stored nuclear waste materials for 1,000 years, which is the capability the NRC is requiring for the repository. After the 1,000-year mark, the nuclear waste releases cannot exceed more than 1 part in 100,000 of its remaining radionuclide inventory, and that rate must hold for at least 10,000 years. This means that repository scientists and engineers must predict how nuclear waste, subject to initially high temperatures as well as radiation, will behave in and interact with its engineered barrier system and the geologic environment for thousands of years.

Lawrence Livermore, one of many organizations working on Yucca Mountain, is responsible for the engineered barrier system to keep the waste contained (see *S&TR*, March 1996). The work to develop this system includes designing different waste packaging concepts to accommodate spent nuclear fuel and high-level waste, assisting in the design of the containers into which the waste packages will be placed, and studying the interactions of the waste and the waste packaging with the immediate repository environment.

Bridging Scientific Disciplines

Recent issues of *Science & Technology Review* have highlighted many Livermore energy projects, including:

- Induct95, software for simulating plasma-assisted manufacturing, October 1998
- Magnetically levitated train concept, June 1998
- Simulations of physics processes in magnetic fusion energy, May 1998
- Argus computerized security system, April 1998
- Software protection systems, March 1998
- Precision engineering, January/February 1998
- Oil-field tiltmeter, October 1997
- Nuclear power safety, July/August 1997
- Unitized regenerative fuel cell, May 1997

The goal—repository licensability—will be achieved only if high confidence in the long-term safety of the repository is demonstrated. Livermore's work toward this goal is being accomplished by a multidisciplinary team. A wide range of expertise is needed for conducting the detailed investigations of the material behavior and geologic conditions of an engineered barrier system and for developing models that will describe the system's long-term behavior and overall performance. Work performed by Livermore researchers has included a variety of tests to understand corrosion effects on candidate waste packaging materials; detailed measurements of actual blocks of Yucca Mountain rock to understand its thermal, hydrologic, and geochemical characteristics (Figure 2); and testing in the actual repository environment (carried out in onsite laboratories deep within Yucca Mountain) to determine the site's hydrologic and geochemical characteristics.

As the project moves closer to licensing application, which is slated for 2002, Bill Clarke, project leader for engineered barrier system materials, says the project is stepping up its quality assurance (QA) program and checking, certifying, and qualifying all project documentation.

"QA documentation," says Clarke, "provides the basis for scientists and engineers, the regulators, the government, and the public to engage in a process of understanding each other's point of view." The supporting facts and figures in QA documents also allow scientific assessments of repository performance to be defended in licensing hearings.

Clarke says that quality assurance will continue to be important through the long life of the repository because "future researchers without any actual experience on the project will need to understand the threads and progression of this work as they are evaluating repository performance."

One major component of the QA effort deals with the qualification of project software, specifically the large set of numerical models used to simulate repository processes to predict repository performance for tens of thousands of years into the future.

The demands on these models are unprecedented, and development has been challenging because data have been difficult to obtain. For instance, much of the information on how chemical processes affect rocks and other materials over very long times

Figure 2. (a) Rock was cut out of Yucca Mountain in Nevada and (b) tested to determine hydrologic and geochemical characteristics.

cannot be ascertained by accelerating the change processes in the laboratory. Rather, this information must be obtained from analogs—concrete in civil structures of known ages or very old relics excavated from geologic areas with characteristics relevant to Yucca Mountain geology (Figure 3).

The unique models are undergoing a highly structured qualification process that will provide documents describing the purpose, lifecycle, methodologies, and usage of the software. One important component of the documentation is the verification and validation plan, which provides for comparisons of modeling results with other codes, problems, and expert judgment.

Fusion Spinoff: Quality Power

Computer users know that surge suppressors are important for protecting sensitive electronics. Similarly, this kind of protection is even more desirable for expensive industrial equipment and electronic controls because their failure could shut down critical operations or an entire plant. When a momentary surge of power, sagging voltage, or other power-supply problem occurs and affects loads connected to a regional transmission system, a momentary supply of local "clean power" is needed.

Such a supply could come in the form of stored energy augmenting or substituting for incoming power. Energy storage technologies currently pursued by Livermore's Energy Directorate may prove useful for this purpose. These include the modern battery, flywheel, and superconducting magnetic energy storage (SMES) systems. Although batteries deliver hundreds of watts, and flywheels can store some tens of kilowatts, SMES systems can deliver multimegawatts and more.

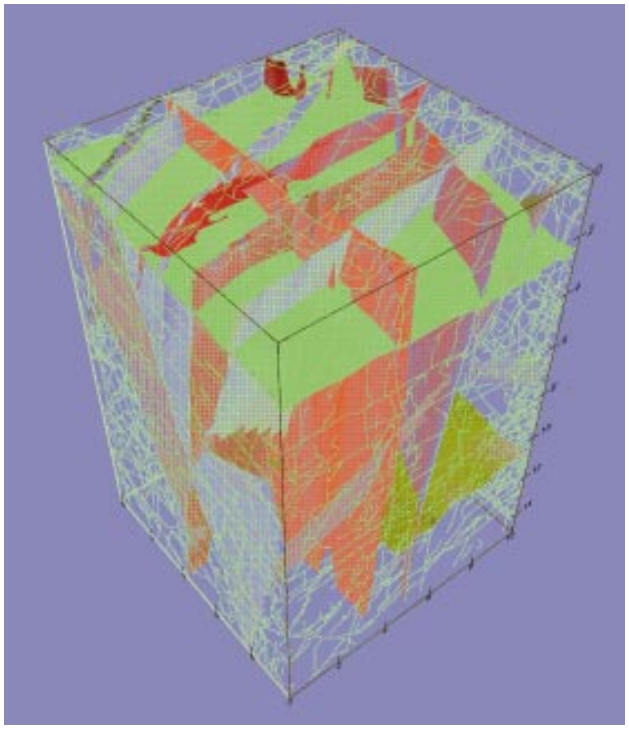


Figure 3. Chemical processes from the rock tests (see Figure 2b) and other data are being integrated into a model of the immediate environment of the proposed Yucca Mountain nuclear waste repository.

Superconducting magnets of the specific type useful for a SMES system have been in continuous development in magnetic fusion energy programs throughout the world. Specifically, the conductor for these magnets, consisting of superconducting cable inside a conduit with liquid helium flowing under high pressure, is a major development. This kind of conductor must exhibit little loss when stored energy is extracted from the magnet.

Livermore's superconducting magnet experts have been collaborating in a national effort to build a model superconducting coil for the International Thermonuclear Experimental Reactor. In addition, Livermore has a high-field, high-current magnet test facility—one of only a few similar testing facilities in the world. The combination of expertise and facility proved attractive to the International Superconductivity Technology Center of Japan and led to a contract to test the Toshiba Corporation's SMES developmental coil, which is part of a Japanese national project.

At the Laboratory, the 3.5-meter-diameter Toshiba SMES coil has been installed in a 4-meter-diameter vacuum vessel (Figure 4). A crew of mechanical and electrical engineers and technicians has been busily getting the superconducting magnet testing facility online after it had been mothballed for three years.

In the facility's control room, engineers Jon Zbasnik and Nicolai Martovetsky have been planning the tests and performing system checkouts with several Toshiba engineers. Tests will provide information such as how well the coils' superconducting material performs, how well the coils can cycle without excessive energy loss, and how many cycles can be run before maintenance is needed.

Toshiba envisions a pilot SMES plant using a toroidal magnet system to store up to 480 megajoules. Ray Smith, engineering group leader for Energy, says that SMES devices, when fully developed, will have several uses. For example, in addition to providing emergency power in critical facilities where electrical power loss could cause big problems, SMES devices may be used to create an immense network of distributed storage systems that could radically alter the energy infrastructure in a deregulated system.

Figure 4. The Laboratory is testing (a) Toshiba Corporation's developmental superconducting coils at (b) Livermore's Superconducting Magnet Test Facility. Such magnet coils would be used as energy storage devices for emergency power.

Improving Generating Efficiency

Most combustion processes that generate electricity use fossil fuel and create pollution. A fuel cell, which converts the chemical energy in fuels directly into usable electricity without combustion, is highly efficient and far less polluting. Lawrence Livermore scientists have studied a variety of fuel cells—zinc–air, proton exchange membranes, and solid-oxide—for transportation and stationary power applications.

Solid-oxide fuel cells (SOFCs) have emerged as the Livermore fuel cell technology with the greatest potential. Livermore's materials-science expertise has led to new concepts in thin-film deposition and multilayer technologies that are being used to improve the cells' power density, reduce their operating temperatures, and lower their fabrication costs.

SOFCs consume fuel and an oxidant that are combined at elevated temperatures to produce electrical current. A fuel cell consists of three electrochemical components: a cathode that electrochemically reduces oxygen from air, an electrolyte that ensures the transport of oxygen ions, and an anode where fuel (hydrogen or another combustible gas) is oxidized by combining with the oxygen ions

transported through the electrolyte. A single fuel cell generates a low voltage (about 1volt), so many fuel cells must be connected in series (a fuel cell stack) to obtain higher voltage. An electrical interconnect provides contact between cells (Figure 5).

A fuel cell can be made more efficient when its electrolyte layer is made thinner, thus reducing its resistance losses. Livermore has developed fuel cells that use thin films of yttria-stabilized zirconia to reduce electrolyte thicknesses as well as fuel-cell operating temperatures by at least 200°C (Figure 6).

The world leader in developing SOFCs, Westinghouse, uses a tubular geometry for the anode-electrolyte-cathode trilayer. Commercializing the SOFC, however, has been slow partly because the method for depositing the thin-film electrolyte in this configuration proved to be a delicate, time-intensive, and expensive operation. Livermore has been performing work to get around this problem.

In a Laboratory Directed Research and Development project to improve the thin-film technology used for SOFC manufacturing and to increase power density, materials scientist Quoc Pham is leading a team to develop a new thin-film deposition technique that may pave the way to commercializing SOFCs. The technique is based on colloidal processing, in which a substrate is repeatedly dipped in a colloidal solution. Pham's team modified this well-known process to a single coating that ranges from 1 to 80 micrometers thick. The new technique can be applied to a variety of substrate geometries. Prototype planar fuel cells fabricated with this deposition technology were tested and found to produce very promising power densities. Pham and the team are now modifying the technique for tubular substrates.

The team is also experimenting with a compositionally graded fuel-cell structure, which starts out at one edge as a pure material (the anode), progressively changes to another material (zirconia, the electrolyte), and finally transitions into the pure cathode material. The graded structure serves two purposes. It alleviates problems with chemical incompatibility between materials, and it alleviates the stress that arises from differences in thermal expansion coefficients that often exist between two pure materials. Stress usually leads to cracking at the interface during thermal cycling.

In separately funded work, the team's thin-film processing technique will be spun off to develop high-temperature steam electrolyzers that can produce hydrogen from water electrolysis. Hydrogen is an important reactant in the chemical processing industry and potentially an important, nonpolluting transportation fuel. Water electrolysis is a simple technology for producing hydrogen, simpler than more commonly used methods such as steam reforming of natural gas or coal gasification. However, water electrolysis has not been cost effective because it consumes large amounts of electricity. The Livermore technology can be used to fabricate steam electrolyzers that are cost competitive and ideal for small-scale use as well as large industrial applications.

The novel chemical and thin-film deposition processes will spin off in numerous other ways, according to Bob Glass, program leader for Energy Storage and Conversion Systems. They will be particularly useful for applications where a robust coating of oxide materials is needed or where planar as well as complex substrates must be coated. As the team is developing next-generation fuel cells, it is also helping private industry lower manufacturing costs and thus hasten commercialization of current SOFC designs.

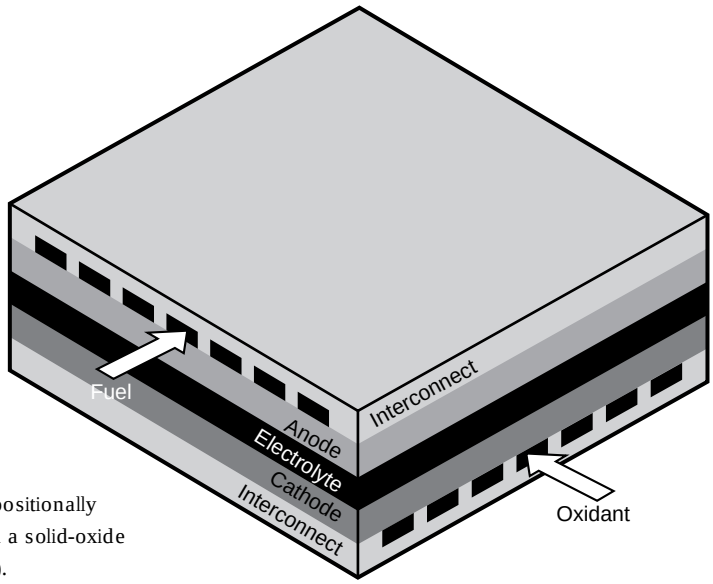


Figure 5. Compositionally graded layers in a solid-oxide fuel cell (SOFC).

Ahead: Sequestering Carbon

One important goal of Livermore's energy research is to find ways of mitigating the potentially adverse environmental effects of burning fossil fuels. Of major concern are the greenhouse gases (primarily carbon dioxide) that are emitted to the atmosphere from burning fossil fuels and that may be contributing to global climate change.

Carbon management is the umbrella term for three mitigation approaches: (1) reduction of carbon emissions through increasing various efficiencies (fossil-fuel-fired power plants and manufacturing process technologies); (2) decarbonization of the energy mix by using energy resources that involve no carbon (fission, fusion, or hydrogen and renewable energy resources) or less carbon (natural gas combined-cycle power plants); and (3) carbon sequestration, the capture and destruction or storage of carbon for geologic time periods.

Research in carbon sequestration technology is a natural extension of climate research work being carried out in the Laboratory's Earth and Environmental Sciences Directorate. A large component of that work is devoted to understanding the carbon cycle in nature (see *S&TR*, March 1998, pp. 14–20). When technologists began looking at the option of injecting CO_2 into the ocean for storage, Livermore's carbon cycle modeling experts found they could contribute their expertise to evaluate the feasibility, costs, and risks of this idea.

CO_2 is absorbed into the ocean by a number of ongoing but very slow natural processes. The ocean's capacity for CO_2 is quite large. However, important questions must be answered before CO_2 sequestration in the ocean can be deemed viable. For example, given the natural cycling of carbon, how long would the CO_2 stay put in the ocean?

Ocean modeler Ken Caldeira attempted to answer this question by simulating the injection of CO_2 into the ocean off Cape Hatteras, North Carolina. The simulations revealed that most of the injected CO_2 slowly returned to the atmosphere, but the length of time it remained in the ocean depended on how deeply it had been injected. Simulations of injections to 410 meters showed the carbon remained in the ocean for over 100 years, and injections to 1,720 meters remained for over 450 years.

Although the modeling results look promising for ocean injection and storage of CO_2, the fact that storage is not permanent led Caldeira and colleague Greg Rau to look at other ocean processes controlling the carbon cycle, including some that occur over thousands to hundreds of thousands of years. Among the most important of these natural processes is one in which the CO_2 in seawater forms carbonic acid and dissolves carbonate sediments, typically the shells of ancient organisms. This "rock weathering" phenomenon is commonly observed by geologists; it is one of nature's ways of depleting CO_2.

Recently, Rau and Caldeira came up with a new concept to mimic this weathering chemical process in reaction vessels and use it for human control of CO_2. The approach converts aqueous carbon dioxide—one of the products of dissolving CO_2 in water and the form that eventually cycles back to the atmosphere—into a bicarbonate, which does not interact with the atmosphere and therefore fixes carbon in the ocean.

The reaction vessel Rau and Caldeira designed for the process holds inside it a bed, pile, slurry, suspension, or aerosol of metal carbonate mineral (Figure 7) such as that found in limestone. Carbon dioxide, which may come from the waste stream of a power plant, enters from one side, comes into contact with water, and becomes hydrated to form carbonic acid, a chemical that can dissolve limestone and other carbonate minerals. When the carbonic acid dissolves the metal carbonate inside the vessel, it reacts the CO_2 to form bicarbonates in solution, effectively sequestering the CO_2 from the atmosphere. Waste streams exiting the reaction vessel comprise a gas stream depleted of CO_2 and an aqueous

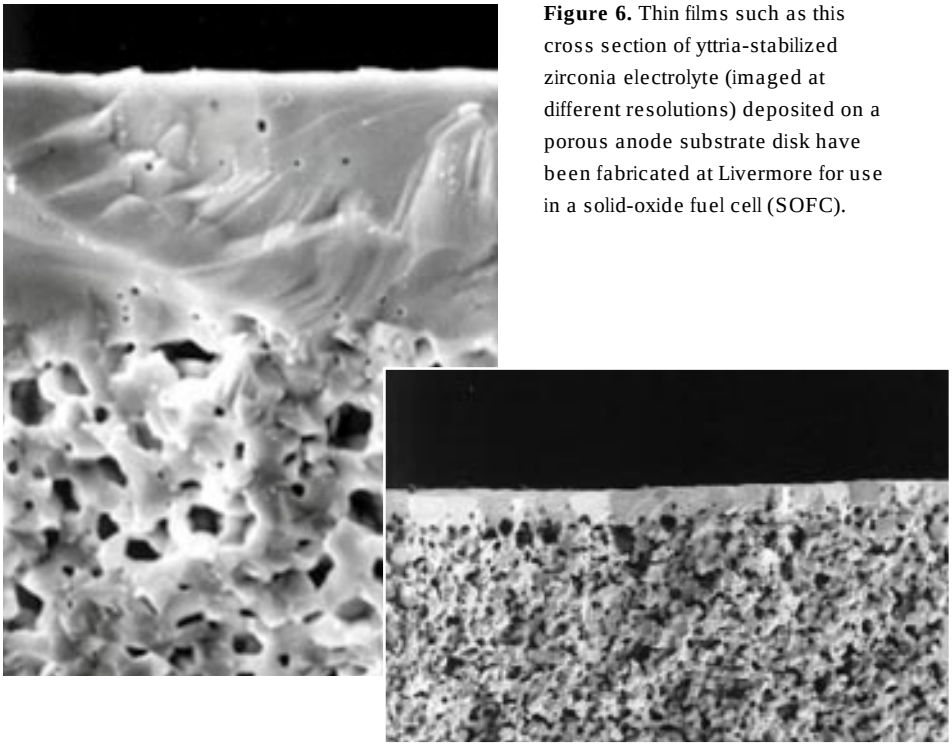


Figure 6. Thin films such as this cross section of yttria-stabilized zirconia electrolyte (imaged at different resolutions) deposited on a porous anode substrate disk have been fabricated at Livermore for use in a solid-oxide fuel cell (SOFC).

solution of metal ions and bicarbonate that can then be injected into the ocean.

Rau and Caldeira are the first to propose accelerating natural carbon mineral weathering reactions to sequester carbon dioxide in the ocean in the form of bicarbonate. Their reaction vessel is still in the design stage but is envisioned for use wherever there is waste gas containing CO_2. Many processes produce such waste streams: the combustion or processing of coal, petroleum, natural gas, or other fossil fuel; the combustion, processing, or metabolism of wood, peat, plant products, or organic compounds derived from them; and the decarbonation of limestone in the production of lime, cement, and gypsum. Caldeira says, "This device may be a cheap and easy first fix to control carbon dioxide, if the global warming issue comes to be taken seriously."

Contributing Pieces to a Portfolio

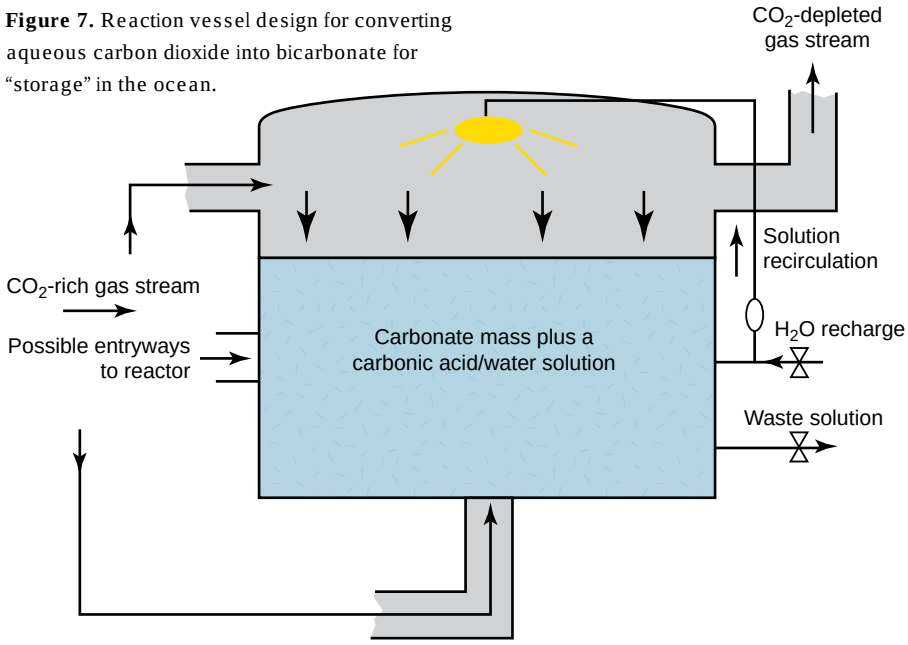
A wide spectrum of energy technologies will be needed to meet the long-term energy needs of the U.S. and the world. Lawrence Livermore is doing its part to assure a viable energy portfolio for the future, and the Energy Directorate is charting a course to make sure the Laboratory's contribution to that portfolio provides an integrated perspective.

— Gloria Wilt

Key Words: carbon sequestration, energy, fuel cell, global warming, nuclear waste repository, ocean model, quality assurance (QA), solid-oxide fuel cell (SOFC), superconducting magnetic energy storage (SMES), thin films, Yucca Mountain.

For further information contact Mark Strauch (925) 422-1469 (strauch1@llnl.gov).

Figure 7. Reaction vessel design for converting aqueous carbon dioxide into bicarbonate for "storage" in the ocean.

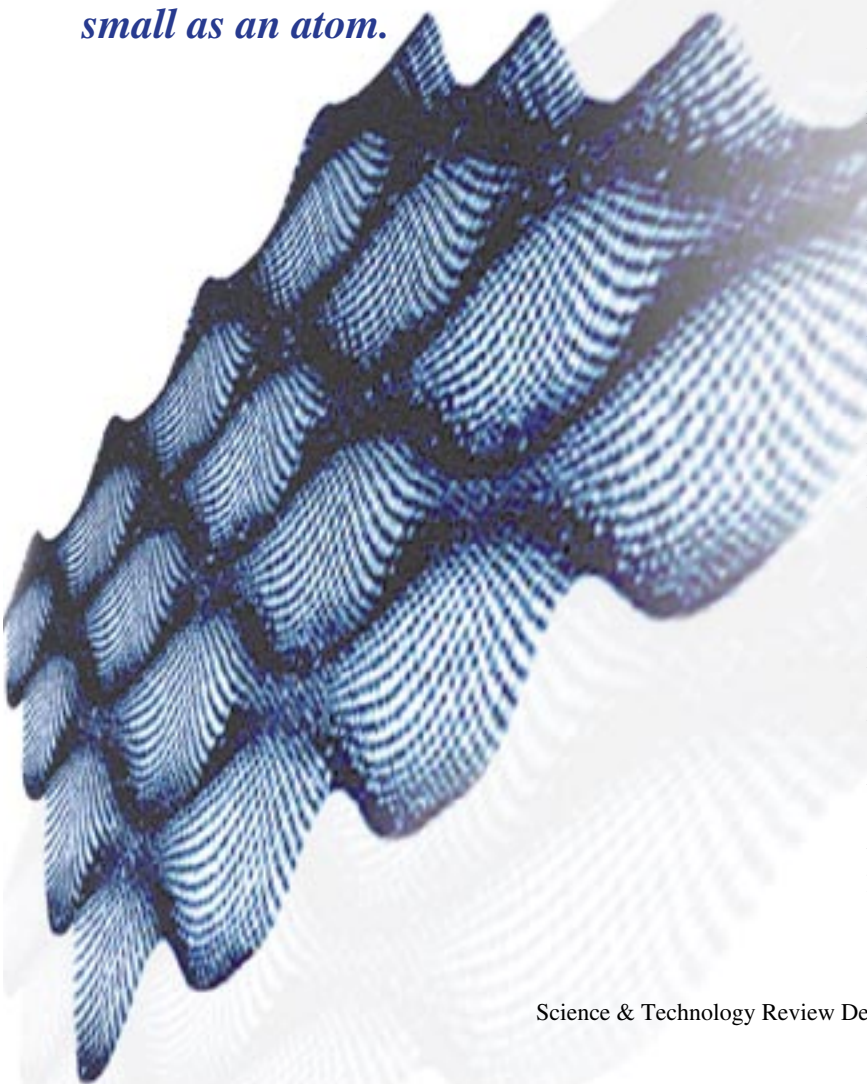


About the Engineer

MARK STRAUCH came to Lawrence Livermore from the University of Michigan, where he received his B.S. and M.S. in electrical engineering in 1976 and 1978. An electrical engineer, he joined the Electronics Engineering Department to work on the Magnetic Fusion Energy Program. Since then, he has also supported the weapons program and O Division and was a group leader and division leader in the Engineering Directorate. He became deputy program leader of the Fission Energy and Systems Safety Program and assistant deputy associate director in the Energy Directorate five years ago. Strauch is an active member of the Institute of Electrical and Electronics Engineers.

Antimatter Helps to Protect Our Nuclear Stockpile

Livermore's new positron microprobe will increase scientists' ability to detect material defects to a resolution as small as an atom.



IN an underground accelerator in a corner of Lawrence Livermore National Laboratory, scientists are systematically creating antimatter and have been for years. They do this to study electrons, negatively charged particles that exist in all atoms and thus in all matter.

In the presence of electrons, the antimatter—positively charged particles called positrons, the "anti-particles" of electrons—exists for only a split second. When a positron and an electron come in contact, they annihilate one another, creating energy in accordance with the famous equation $E = mc^2$. Energy is released in the form of electromagnetic radiation, or gamma rays. By characterizing the gamma rays through spectroscopy, scientists can determine the properties of the electrons. The annihilation rate gives them the density of the electrons, and the energy and angle of the annihilation supply information about electron momentum.

Solid-state physicists have used this spectroscopy technique for over 20 years to study the properties of many metals and alloys. Scientists have also discovered that measurement of positron annihilation is an excellent tool for studying the structure of microscopic defects on and inside metals and other materials. With the increasing use of exceedingly small electronic devices and thin films in the semiconductor and polymer industries has come the challenge of detecting proportionately small material defects. A void as small as several atoms can render a microdevice defective.

If positrons are directed at material that contains voids or other open-volume defects, they wander around the material—for all of a nanosecond—and tend to be trapped at the defects. A void means no atoms and hence fewer electrons, so the positrons live longer than they would in a defect-free material. Positron lifetime spectroscopy is an excellent tool for

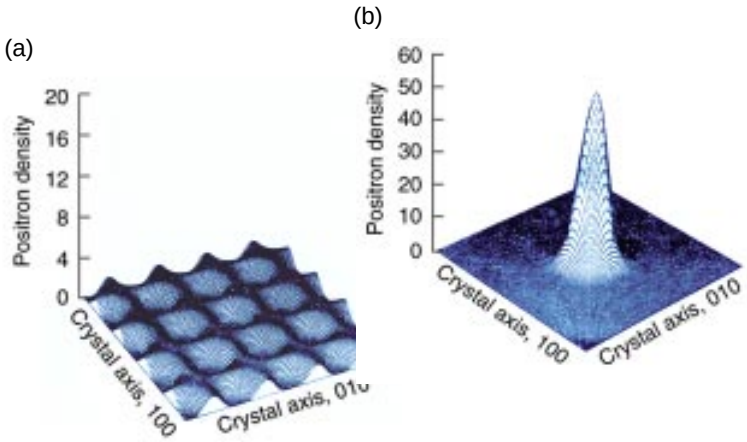


Figure 1. Images based on modeling calculations show how positrons are distributed in (a) defect-free material and (b) material with a defect. Positrons can migrate to defects as small as a single atom. The length of a positron's life is an indicator of the size of the defect.

nondestructive evaluation of defects as small as an atom (Figure 1).

Defects affect much of a material's behavior. They evolve from changes in temperature and pressure or over long periods of time, affecting the ultimate strength of the whole system. Livermore researchers have studied many problems caused by defects, including defect species in high-temperature superconductors, defects active during oxygen transport in uranium corrosion, and radiation damage in metals. Optical microscopy, neutron scattering, transmission electron microscopy, scanning tunneling microscopy, atomic force microscopy, and x-ray scattering are methods that have been developed to find vacancies, voids, and other defects in materials. Each technique is useful at specific depths for certain defect sizes and concentrations, and each has found its niche in appropriate research or manufacturing activities (Figure 2). But positron annihilation lifetime spectroscopy is the best of the lot for finding the smallest defects and a range of defect concentrations at virtually any depth in metals, semiconductors, and molecular or organic compounds.

As part of the Department of Energy's science-based Stockpile Stewardship Program, researchers at Livermore's Positron Facility, under the leadership of physicist Richard Howell, are enhancing current capabilities as well as developing new ones to detect changes in weapons materials. Livermore's new three-dimensional (3D) positron microprobe is scheduled to come online in the fall of 1999. Its pulsed positron beam with a radius of less than a micrometer will have the highest spatial resolution of any positron analysis system in the world.

Positron lifetime analysis can detect the size, location, and concentration of defects that result from stress, strain, radiation damage, fatigue, corrosion, delamination, and embrittlement. Says Howell, "Early detection is important because defects on the atomic level may ultimately evolve into mechanical failure."

He adds, "The new microprobe and its positron beam will aid stockpile stewardship and other projects at the Laboratory. Material scientists from other national laboratories, universities, and industry are interested in using them, too. The microprobe and our other positron facilities are enormously valuable for studying a variety of materials."

The development of the microprobe builds on Livermore's 20 years of experience with positron experiments related to magnetic fusion, superconductors, plasmas, high explosives, encapsulated plutonium, and aircraft composite materials.

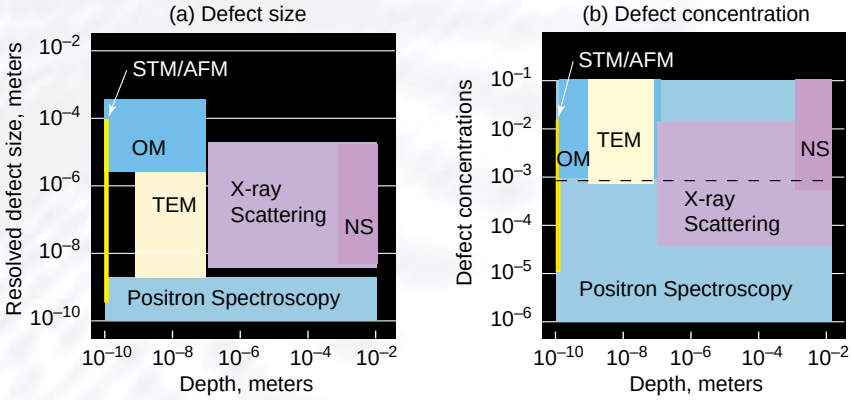


Figure 2. Of several methods for detecting defects in materials, positron spectroscopy can locate (a) the smallest defects and (b) the smallest defect concentrations at various depths. (STM = scanning tunneling microscopy; AFM = atomic force microscopy; NS = neutron scattering; OM = optical microscopy; TEM = transmission electron microscopy.)

Creating Positrons

Positrons are formed through naturally occurring radioactivity called beta (+) decay. When a radioactive nucleus decays via beta (+) decay, a positron is produced. Positron annihilation spectroscopy traditionally has been performed by placing a sample material in proximity to a radioactive

source such as sodium-22. With the radioactive source inside an accelerator and the positron beam passing through a lens, the energy and direction of the positrons can be controlled. Livermore's high-energy Pelletron Accelerator uses this method of creating a beam of megaelectronvolt positrons.

Another process, known as pair production, can be used to create a high-current beam, or one with a high number of positrons, in the range of tens of billions of positrons per second. An electron beam from a linear accelerator (linac) hits a thick tungsten target and generates a high-energy photon beam. As the photons traverse the target, each is converted into an electron and a positron. All high-current positron beams, including Livermore's new 3D microprobe, use this method as their source of kiloelectronvolt positrons.

High Energies Go Deeper

Livermore's high-energy positron beam comes from a 3-megaelectronvolt Pelletron Accelerator, one of just two such sources in the world (Figure 3). The beam is derived from a sodium-22 source moderated by a tungsten foil positioned at the high-energy end of the accelerator. Both the moderated positrons and positrons directly emitted from the source are captured and accelerated. They produce a beam with a current of 850,000 positrons per second.

To measure positron lifetimes, the time at which the positrons are implanted in the sample is determined as each positron passes through a scintillator. Annihilation gamma rays from the implanted positrons are then detected by a barium fluoride detector. The annihilation lifetime is calculated from the time difference between the two detectors to a system resolution of about 250 picoseconds. Positrons leave the implantation detector with an average energy of 2.6 megaelectronvolts and a beam diameter of 1 centimeter directed at a sample placed 4 centimeters downstream. At this high energy level, positrons are implanted from millimeters to centimeters deep, depending on the density of the sample.

Says Howell, "We use the high-energy beam to analyze thick samples. The beam can even pass through thin windows before implanting positrons into a sample, allowing nondestructive *in situ* measurements in controlled environments." Up to 50 samples a day can be analyzed with this system.

This high-energy beam has been used to determine aging effects in aircraft components made of carbon fiber resin composites. Howell and his team measured the changes in hole volume brought on by accelerated aging at elevated temperatures and in hostile atmospheres. These data were correlated with infrared spectroscopy and mechanical tests to provide a complete description of the changes during aging.

For the DOE's Enhanced Surveillance Program, which is part of its Stockpile Stewardship Program, the high-energy beam is helping to determine the effects of self-irradiation on plutonium. Data from these experiments are used to validate Livermore models that predict the time scale of void swelling, embrittlement, and related radiation effects.

One experiment compared two samples of plutonium: a 21-year-old sample and one that had recently been cast. Positron lifetime spectroscopy revealed that most vacancies in both samples were filled with helium, which is produced naturally when plutonium decays. Despite high concentrations of these vacancies, which are a necessary precondition for void growth and swelling, no voids were found. The results of this experiment were good news for our stockpile.

3D with the Microprobe

The team uses the Positron Facility's 100-megaelectronvolt electron linac for its 3D scanning positron microprobe. The linac's electron beam produces

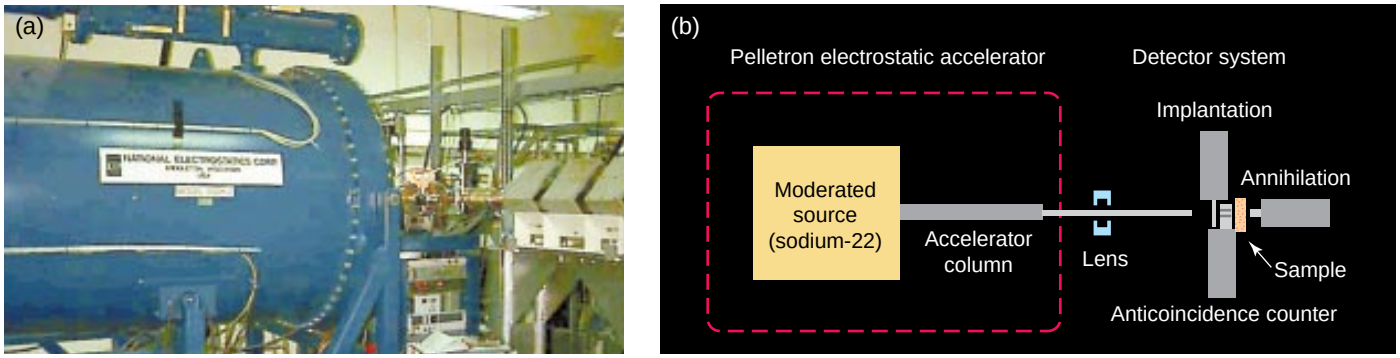


Figure 3. (a) Photo and (b) schematic of Livermore's high-energy positron annihilation lifetime system. Decay of sodium-22 produces positrons in the accelerator. Instrumentation near the sample measures when positrons are implanted in the sample and detects gamma rays produced when positrons annihilate with electrons in the sample. This system is used to study samples from millimeters to centimeters thick.

positrons through pair production for the highest current positron beam in the world. The electron beam has been upgraded to produce an even higher current beam of up to 10 billion (10^{10}) positrons per second.

Enormous numbers of positrons are necessary to produce the tightly focused beam that the microprobe needs for 3D mapping of defects with high spatial resolution. A pulsed beam and variable positron output energies in the range of 1 to 50 kiloelectronvolts are also required. Many individual features of this new system are found in other systems, but Livermore's positron microprobe system is the first to integrate all of them.

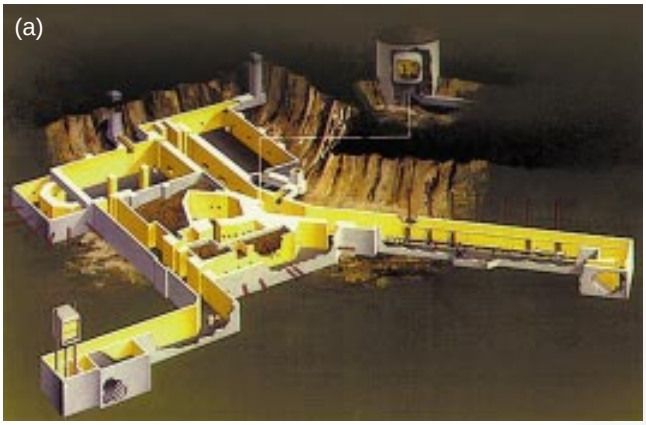
The microprobe is most similar to a scanning electron microscope, in which a tightly focused continuous electron beam scans small regions of a sample and detects defects. However, the scanning electron microscope cannot detect defects on the atomic scale, information that Livermore needs for stockpile stewardship and other applications. With the fast-pulsed, tightly focused beam of Livermore's new microprobe, positron lifetime annihilation spectroscopy will have spatial resolution at the atomic level.

Figure 4 shows a rendering of key elements of the 3D microprobe. As the initial high-current positron beam races through the system, its pulse is shortened and its diameter is focused to less than 1 micrometer. With the small spot size comes some loss of current, although the team has succeeded in keeping those losses to a minimum.[1]

By controlling the implantation location and energy of the microprobe's beam, the team will be able to detect and identify depth-dependent concentrations of vacancies, voids, gas-filled voids, and other negatively charged defects to a depth of a few micrometers. Typical depth and lateral resolution will be less than 0.2 micrometer. Maximum depth for implanting positrons with this beam will be 10 micrometers, which makes this mapping method ideal for very thin materials. The location of buried features can be identified with high precision by sweeping the energy and location of the positron beam in small steps.

The microprobe will give an entirely new view of defects in materials, and it will give scientists their first detailed look at defects around microscopic cracks. The microprobe will also supply valuable new information about defects at grain boundaries, which is important for stockpile stewardship studies of aging and stressed plutonium. It will give the closest look yet at electromigration, a defect caused by electrical current passing through a material. Electromigration is a major concern for the semiconductor industry because it can damage microcircuitry.

Data from positron beam experiments (Figure 5) are already serving to validate Livermore's



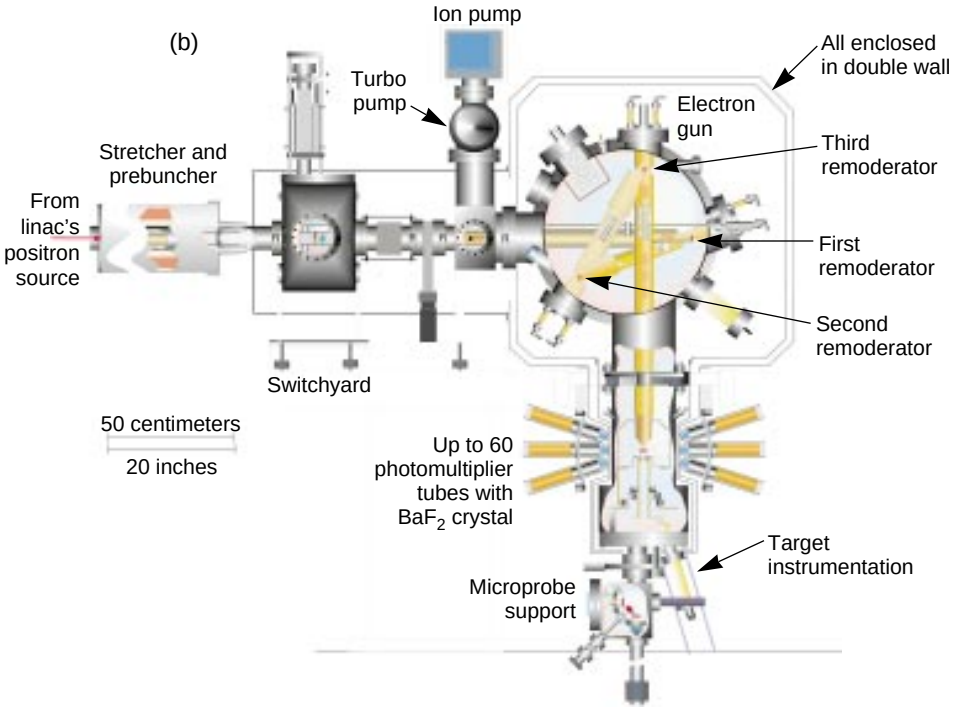


Figure 4. (a) Livermore's linear accelerator and (b) positron microprobe already produce the highest-energy positron beam in the world. The schematic shows the basic components of the technology. The Livermore facility is being upgraded to offer the best spatial resolution for detecting atomic-scale material defects.

modeling calculations for material defects and their effects. Spatially resolved data from the microprobe will provide a new level of detail for input to materials models as well as for further validation of Livermore calculations.

Defect Analysis Is Key

The Livermore system's upgraded high-current beam can be used without the microprobe to perform other forms of spectroscopy. Notes Howell, "The new beam will be very attractive to scientists outside Livermore who have no other access to such a high-current positron beam."

As so many products in our world shrink yet become more powerful, the ability to perform nondestructive analysis of these small devices at the atomic level is critical. Positron lifetime analysis is a particularly effective tool for defect identification and quantification, leading to smaller and better electronic devices, more effective polymeric coatings, and stronger and more corrosion-resistant metals and alloys. With newly upgraded positron experimental facilities, Livermore researchers will be positioned to break new ground in the analysis of material defects.

— *Katie Walter*

Key Words: electrons, linear accelerator, materials science, nondestructive analysis, Pelletron electrostatic accelerator, positron annihilation lifetime spectroscopy, positron microprobe, DOE Stockpile Stewardship Program.

For further information contact Richard Howell (925) 422-1977 (howell5@llnl.gov).
Livermore's Electron-Positron Beams Facility Internet address is **http://www-phys.llnl.gov/H_Div/Positrons/**.

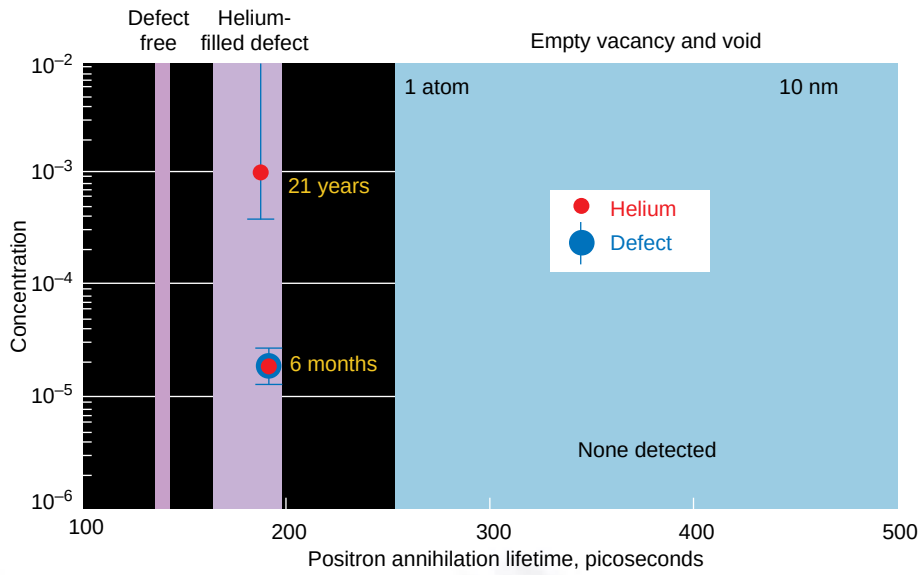


Figure 5. Shaded areas show modeling calculations for positron lifetimes in plutonium that is free of defects, has helium-filled defects, and has empty defects. (As plutonium decays, it produces helium atoms, so helium-filled defects are expected. Empty defects, on the other hand, are more problematic.) Data from experiments on 21-year-old plutonium and a recently cast sample gathered by Livermore's high-energy positron system fall within predictions for helium-filled vacancies and reveal no voids among the defects.

About the Scientist

RICHARD HOWELL received a B.A. in physics from Miami University in 1965 and a Ph.D. in physics from Michigan State University in 1972. When he joined Lawrence Livermore in 1972, he was a member of the Special Projects Division. Since 1974, Howell has been a member of the H Division in the Physics and Space Technology Directorate. Howell has performed basic physics and materials analysis with positrons for over 20 years, publishing over 130 articles on his work.

Reference

1. For more information about the positron microprobe, see Richard H. Howell et al., "Positron Beam Lifetime Spectroscopy at Lawrence Livermore National Laboratory," *Application of Accelerators in Research and Industry*, J. L. Duggan and I. L. Morgan, Eds., New York: AIP Press, 1997.

A Shaker Exercise for the Bay Bridge

CALIFORNIANS know this about earthquakes: they are bound to happen. Everyone knows that any number of seismic faults could produce The Big One, and most experts predict a large earthquake will occur in the San Francisco Bay Area within the next 30 years. We would like to be assured that construction codes for seismic safety are adequate and that buildings, roads, bridges, and other structures can stand up to any future earthquake. Unfortunately, that's just not so.

Confidence in public safety will grow if a group of scientists from Lawrence Livermore and the University of California (UC) at Berkeley has anything to do about it. Working in a campus–laboratory collaboration, they have been performing cross-disciplinary studies on earthquake hazards and are now performing computer simulations of the San Francisco Bay Bridge to find out how the bridge would respond to an earthquake along the nearby Hayward fault.

A site-specific analysis is requisite to confidence in predicting an earthquake's behavior and how a structure will respond to it. The Bay Bridge–Hayward fault project is the first step toward fuller delineations of earthquake risk so appropriate seismic safety measures for public structures can be implemented.

This particular simulation is also of interest because the Bay Bridge is a crucial transportation link in northern California. It carries the highest daily volume of traffic of any bridge in the U.S., and its long spans embody many seismic concerns. One span came undone in the 1989 Loma Prieta earthquake, prompting an overall seismic retrofit, soon to begin. In addition, the Hayward fault, located in a densely populated area and having a 50% probability of rupturing in a 30-year time frame, is considered the most dangerous of Bay Area faults. Seismologists think it could cause death and destruction comparable to that of the 1995 earthquake in Kobe, Japan, which resulted in 6,000 fatalities and over $100 billion in damage. The Bay Bridge is particularly vulnerable to the Hayward fault, located a mere 14 kilometers away.

The simulation is large and complex, requiring advanced numerical techniques, gigantic amounts of computational power, and the coupling of earth sciences and engineering know-how. Researchers can look forward to more massive computational power from the DOE Accelerated Strategic Computing Initiative's computers, which are used primarily to support stockpile stewardship and will enable even larger simulations.

Simulating the Earthquake

Before the bridge's response can be simulated, the rupturing of an earthquake fault must be simulated to generate ground motion information. A rupture of the Hayward fault was simulated with the powerful E3D seismic code developed by Livermore computer scientist and geophysicist Shawn Larsen. The code incorporates three-dimensional (3D) information about propagation of seismic waves: how they are radiated from the earthquake's source to the surface, at what velocities they propagate, and how they interact with the geology and topography in their path. Because the simulation involves distances to several hundred kilometers and depths to 50 kilometers, accurately predicting the strength and geographic distribution of seismic waves demands robust computing.

E3D integrates seismic information through a complex 3D geologic model of the San Francisco Bay Area, which was developed at UC Berkeley by Professor Doug Dreger and graduate student Christiane Stidham with funding from the U.S. Geological Survey. The model contains representations of large sedimentary basins (such as the San Pablo Basin, Santa Clara Valley, and Livermore Valley), deep crustal and mantle structures, near-surface alluvium and very low-velocity bay mud, high-velocity zones (such as Mt. Diablo), and seismic velocity contrasts across major faults in the region.

E3D has many advanced computational enhancements that allow it to run approximately a hundred times faster than other computational codes. In addition, it has been implemented on a variety of high-performance computers, including massively parallel processors.

E3D's simulations of the Hayward fault represent the largest seismic simulation done anywhere in the world, with 45 million nodes of calculations. These three-dimensional

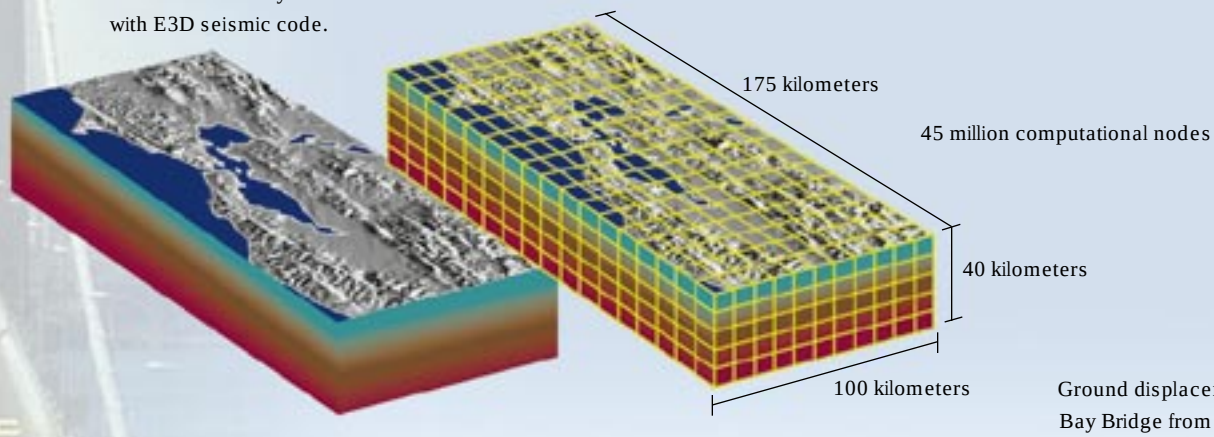
calculations model the response of an entire seismogenic zone at the resolution needed to assess ground motion effects and the resulting earthquake hazards (see figure below).

The Bay Bridge in an Earthquake

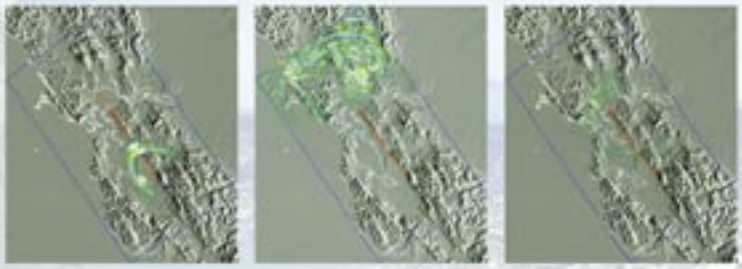
The ground motion predictions from E3D are fed into SUSPNDRS, the code for simulating long-span bridge dynamics. A bridge's numerous interacting parts and connections can act and react differently to each other, resulting in structural changes and effects that are out of proportion to their causes.

SUSPNDRS, a finite-element code developed by Livermore's David McCallen and UC Berkeley's Abolhassan Astaneh-Asl, incorporates algorithms that accommodate the nonlinearities in bridge geometry and material properties. The code also uses an efficient bridge model that represents the bridge structure through five components (towers, deck system, cable system, deck impacts, and piers) with reduced

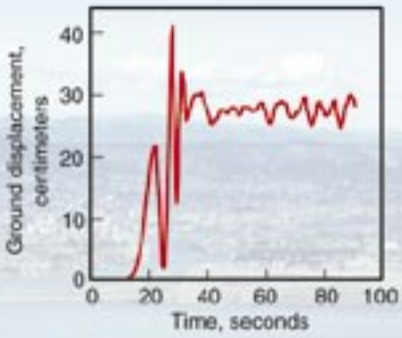
San Francisco Bay Area modeled with E3D seismic code.



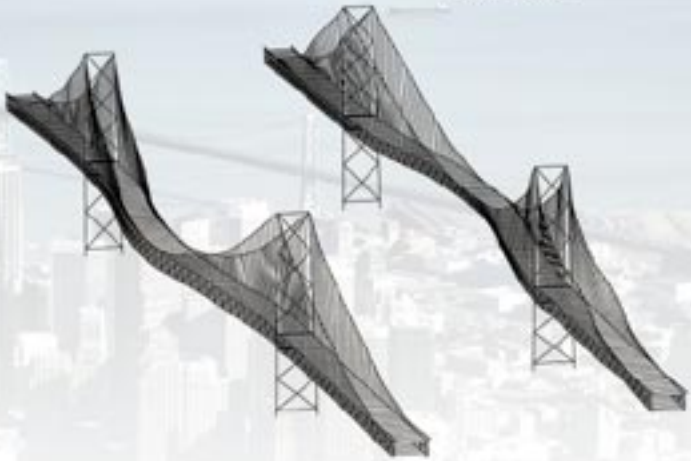
E3D simulations of an earthquake on the Hayward fault.



Ground displacement under the Bay Bridge from an earthquake on the Hayward fault.



SUSPNDRS code simulation of the Bay Bridge's dynamics.



degrees of freedom to save computational time without sacrificing essential bridge dynamics. SUSPNDRS efficiently performs calculations in three dimensions in a matter of three to four hours instead of the days or weeks required for such calculations in the past.

One unique feature of SUSPNDRS is the way its calculations are sequenced. By having the code emulate the construction sequence of the bridge components, McCallen and Astaneh-Asl could make the model calculations match actual forces and loads in key elements of the structure. They referred to construction drawings and historical construction documents to make their code calculations approximate the order of construction: towers erected, cables spun into place, stiffening trusses for the deck lifted segmentally into place, deck steel added, and finally the deck joints rigidly connected. The specific construction sequence has a significant effect on the final bridge deck member forces, so the computational model must reflect the same physical forces.

The figure on p. 19 also shows the bridge model where responses were simulated. The simulation results are now being validated. One validation method compares SUSPNDRS results with the first ambient measurements of bridge vibrations, collected in the 1930s with a vibrometer and documented in the *Bulletin of the Seismological Society of America*.

As bridge simulations progress, the work will focus on three seismic safety issues specific to long-span bridges: (1) the effect of a series of seismic waves on the bridge structure if, instead of propagating singly, they combine into one large-amplitude wave; (2) the effects caused by waves arriving at different times at different points of a structure; and (3) permanent ground deformations occurring near the ruptured fault that would affect the nearby bridge structure. Because few measurements exist of this important near-field phenomenon, large-scale simulations are providing new understanding for seismologists and engineers.

The long-term results of this campus–laboratory collaboration will enhance seismic safety in California. In the interim, the Bay Bridge results may benefit retrofit efforts for one of the Bay Area's most important long-span bridges.

— *Gloria Wilt*

Key Words: bridge dynamic analysis, campus–laboratory collaboration, E3D, earthquake simulation, earthquake risk assessment, Hayward fault, hazard assessment, San Francisco Bay Bridge, seismic safety, SUSPNDRS.

For further information contact Shawn Larsen (925) 423-9617 (larsen8@llnl.gov) or David McCallen (925) 423-1219 (mccallen2@llnl.gov). Internet address: www-ep.es.llnl.gov/www-ep/ghp/Larsen/Hayward/hayward.html

Forensic Science Sleuthing

LIKE high-tech colleagues of Sherlock Holmes, experts from Lawrence Livermore's Forensic Science Center develop sophisticated analytical equipment for combatting terrorism and the proliferation of weapons of mass destruction, supporting stockpile stewardship efforts, and responding to law-enforcement requests. Using center-developed prototypes, these experts in organic, inorganic, biological, and nuclear chemistry can determine the composition and often the source of the most minute samples of evidence. The sophistication of their sleuthing is beyond the wildest dreams of even Mr. Holmes and Dr. Watson.

Past issues of this publication have detailed the techniques of the center (*E&TR*, March 1994, pp. 1–8; and *S&TR*, August 1995, pp. 24–26). Some of the systems and methods have now "come of age" and are used in the field for remote analyses and real-time results.

This summer in Cape Cod, Massachusetts, the center first used its portable thin-layer chromatography system in the field for the first time. This system interrogated the interior of more than a thousand munitions dating back to World War II. The center also placed modern solid-phase microextraction (SPME) sampling tools at a Department of Energy weapons plant to monitor the safety and efficacy of the current nuclear stockpile. In the law-enforcement arena, the center is a key participant in the new partnership between the Federal Bureau of Investigation (FBI) and Lawrence Livermore (see the box on p. 22).

Blast from the Past

During an environmental cleanup operation at the Massachusetts Military Reservation in the spring of 1998, Army personnel discovered a suspicious depression in an area once used for training. The depression turned out to be the "burial ground" for mortars and ordnance that had been used during target practice exercises (Figure 1). Three questions needed answers: How many of the munitions were "live"? How should they be rendered safe? What was the best way to dispose of them?

Brian Andresen, director of the Laboratory's Forensic Science Center, assessed the situation at the request of the Defense Ammunition Center. His initial samples indicated that approximately one munition out of ten was live, while the rest were dummies of wax and plaster of paris. Although they couldn't explode, the dummies did have live fuses, and some of the rounds—the exact quantity unknown at that point—could have contained appreciable quantities of high explosive (HE).

Figure 1. When the Army unearthed more than a thousand mortar rounds dating from a World War II training area, they enlisted the Laboratory's Forensic Science Center to determine which were live munitions and which were dummies.

Andresen recommended cutting each of the thousand-plus mortars in half and sampling them for HE. The Army agreed, so in July 1998 Livermore's Jeff Haas and Greg Klunder packed up sampling kits and analysis equipment and headed east.

The project was an ideal test case for the center's thin-layer chromatography (TLC) screening system, which was originally developed as a field-portable propellant analysis system for the Department of Defense. Propellants (essentially HE) require stabilizers (such as diphenylamine) to prevent spontaneous ignition. Because stabilizers are depleted by extended exposures to high temperatures, the military needed a way to quickly determine the safety of large numbers of bulk propellants. The TLC system screened the Army site for explosive compounds. Sensitive and fast, the system required only 50-milligram samples of explosive, instead of the gram quantities required by other methods, and 15 minutes for each group of 20 samples.

Haas and Klunder analyzed 1,236 mortar rounds in two days (Figure 2). With the real and dummy munitions identified, the Army sent the dummy pieces to a military salvage yard and safely disposed of the remaining live shells. In the past, normal protocol was to group the mortars—live ones and dummies together—in piles of 100 and to explode them all, but that solution is no longer considered environmentally acceptable.

The nearby town of Borne also gained peace of mind from the center's analysis. The work demonstrated that the HE

amounts were insignificant and that environmental contamination did not occur while the munitions were buried.

Back to the Future for the Stockpile

In 1998, center staff also developed methods for verifying the safety of the weapons systems in the U.S. nuclear stockpile.

"Our task was to provide a way of determining the condition of a nuclear weapon's internal components without using either electricity or light and without disturbing the weapon's internal geometry," said Andresen.

The materials in a modern nuclear weapon include highly sensitive and reactive components, such as plutonium and uranium, as well as organic materials. These organic materials include the HE that initiates the nuclear fission reaction as well as structural materials and adhesives that maintain precise internal alignments. Such materials are stable polymers with small diffusion coefficients (10^{-11} to 10^{-5} square centimeters per second). However, in the weapon environment—over a period of many years, at elevated temperatures, in a hermetically sealed radioactive environment—certain systems may outgas at detectable levels. When outgassing, these organic materials release compounds that can indicate problems such as corroded metals, degrade components that affect the overall integrity of other warhead materials, and generally signal decomposition of materials within the warhead. By monitoring these chemicals, experts are alerted to problems that may be developing inside the weapon.

Figure 2. Livermore's Jeff Haas sampled over 1,200 mortars in two days using the center's unique thin-layer chromatography screening system.

Recipe for Safety: Yellow Cake and Simple Green

In the summer of 1998, Secretary of Energy Bill Richardson announced a new partnership between the Federal Bureau of Investigation (FBI) and Lawrence Livermore to combat international terrorism with high technology. This formal partnership affirms the role the Forensic Science Center plays in supporting forensic investigations.

Two recent incidents—both with happy endings—demonstrate the speed and efficiency with which the center responds to urgent requests from law-enforcement agencies and nuclear regulators.

The first incident involved unknown material in a coffee can obtained by a high school student at a local swap meet. The material—a light yellow, very fine powder—was confiscated by the school. The material was discovered to be radioactive, and the center was called in by DOE.

Nuclear chemist Ken Moody performed the analysis and relayed the results back to DOE within 16 hours of receiving the material. "Since everyone was anxious to get immediate results, we expedited nuclear counting techniques and assayed the material with gamma-ray spectrometry and alpha-particle spectroscopy. We measured no radionuclides above background other than unperturbed isotopes of uranium. The material was naturally occurring uranium, or yellow cake, not an enriched or otherwise processed uranium compound."

The second incident occurred as FBI agents searched the Los Angeles home of a man arrested for stealing military weapons. Among an arsenal of assault rifles, hand guns, explosives, and heavy-duty flak vests, they found a jar of green liquid labeled "poison." Concerned that the liquid might be a chemical warfare agent, the FBI contacted the center.

"Rich Whipple and I conducted field sampling within an FBI-controlled area," explained Pat Grant, deputy director of the center. "We put the sample—which had been well packaged by a hazardous materials team—into a containment glovebag inside a field-portable hood. Using the solid-phase microextraction (SPME) technique, we exposed two microfibers, one at a time, to the liquid and then repackaged the jar. We transported the SPME fibers to the center in O-ring-sealed metal containers. Armando Alcaraz performed gas chromatography–mass spectrometry (GC–MS) analyses, we analyzed and interpreted the data, and the results were reported to the FBI just two-and-a-half hours after the start of our investigation."

Good news. The green substance turned out to be a nontoxic cleaning solution. In fact, the next day Whipple brought in a commercial "simple green" household cleanser and ran a SPME GC–MS analysis of the fluid. The chemical signatures of the commercial product and the suspect solution were virtually identical.

The techniques and analytic protocols rely on center-developed solid-phase microextraction (SPME), which allows rapid and efficient environmental sampling and processing. The key to microextraction is a minuscule fiber inside a syringe needle (Figure 3). The fiber is coated with an adsorbant that, when exposed to the ambient environment, collects the molecules of a suitable sample.

Five types of fiber with specialty polymer coatings are available commercially. For example, one fiber picks up acids in preference to bases; another extracts alcohol more efficiently than hydrocarbons. Each SPME fiber coating can collect thousands of different compounds of a specific class after only a few seconds of sampling time. Before the development of this technique, it took weeks to collect and characterize only a few tens of unknown compounds from warhead materials.

In the SPME project, chemists David Chambers and Heather King are identifying the gas-phase chemicals in a weapon's primary headspace and studying their time histories. "In the first phase of this project, we're identifying what chemicals, if any, are emitted by weapon components," said Chambers, the project's principal investigator. "So far, we've characterized weapons-material components as well as HE associated with two weapons systems."

The most recent stockpile stewardship application of the SPME technique involves monitoring the headspace of individual warheads. For instance, at the Pantex Plant in Amarillo, Texas, SPME is being used with other types of nondestructive surveillance to monitor 10 weapons.

The Future of Forensic Analysis

The term "forensic science" used to apply only to the scientific analysis of evidence in the context of civil or criminal law. Increasingly, forensic analyses are used to monitor or verify compliance with international treaties and agreements—particularly those involving weapons of mass destruction—and for stockpile stewardship.

A busy future of forensic science was recently underscored by DOE Secretary Bill Richardson in his August 1998 visit to Lawrence Livermore, when he announced that the Laboratory was the first in a "network of premier laboratories around the country that will give the FBI next-generation crime-fighting capacity."

Holmes and Watson would be proud!

— Ann Parker

Key Words: Federal Bureau of Investigation (FBI), Forensic Science Center, gas chromatograph–mass spectrometer (GC–MS), solid-phase microextraction (SPME), thin-layer chromatography (TLC).

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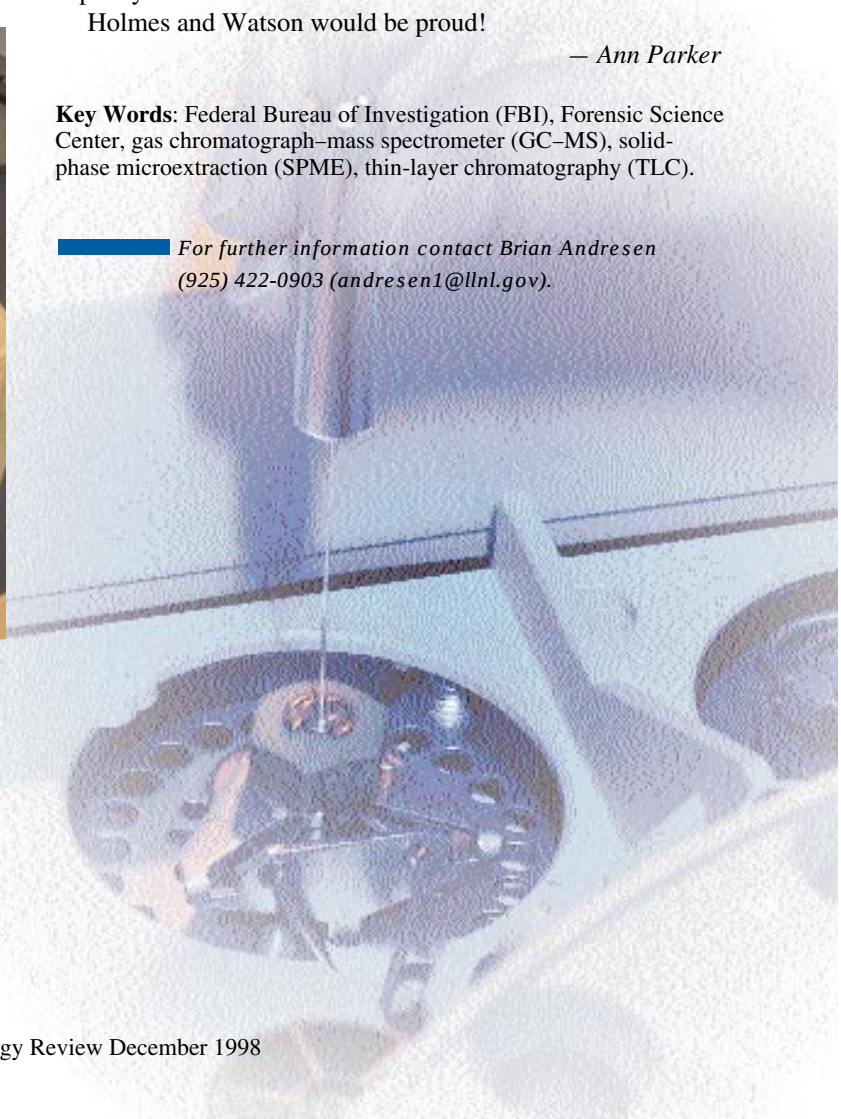

Figure 3. (above) Heather King and David Chambers demonstrate Livermore's solid-phase microextraction (SPME) sampling technique. The microfiber inside the syringe is coated with a special polymer that collects molecules of gas-phase chemicals. (right) The fiber is then desorbed in the injection port of a gas chromatograph–mass spectrometer, which identifies the compounds and measures their amounts.

Patents

Each month in this space we report on the patents issued to and/or the awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Joseph Neev Luiz B. Da Silva Dennis L. Matthews Michael E. Glinsky Brent C. Stuart Michael D. Perry Michael D. Feit Alexander M. Rubenchik	**Ultrashort Pulse High Repetition Rate Laser System for Biological Tissue Processing** U.S. Patent 5,720,894 February 24, 1998	A method and apparatus for fast, efficient, precise, and damage-free biological tissue removal using an ultrashort-pulse laser system operating at high pulse-repetition rates. The duration of each laser pulse ranges from 1 fs to 50 ps, such that energy deposition is localized and occurs before significant collateral damage can take place. The depth of material removed per pulse is about 1 micrometer, and the minimal thermal and mechanical effects associated with this ablation method allow for high-repetition-rate operation to over 1,000 Hz, which achieves high material removal rates.
Alan M. Frank Ronald S. Lee	**Precision Flyer Initiator** U.S. Patent 5,756,925 May 26, 1998	A precision flyer initiator forming a substantially spherical detonation wave in a high explosive (HE) pellet. An explosive driver—e.g., detonating cord, wire bridge circuit, small explosive—is detonated. A flyer material is sandwiched between the explosive driver and the end of a barrel that contains an inner channel. A projectile, or flyer, is sheared from the flyer material by the force of the explosive driver and projected through the inner channel. The flyer then strikes the HE pellet, which is supported above a second end of the barrel by a spacer ring. A gap of shock-decoupling material delays the shock wave in the barrel from predetonating the HE pellet before the flyer. A spherical detonation wave is formed in the HE pellet. Thus, a shock wave traveling through the barrel fails to reach the HE pellet before the flyer strikes the HE pellet. The precision flyer initiator can be used in mining, well-drilling, and antitank devices.
Donald A. Bender Thomas C. Kuklo	**Separators for Flywheel Rotors** U.S. Patent 5,775,176 July 7, 1998	A separator that forms a connection between the rotors of a concentric rotor assembly of a high-performance flywheel energy storage system. This separator allows for the relatively free expansion of outer rotors away from inner rotors while providing a connection between the rotors that is strong enough to prevent disassembly. This combination of inner flywheel ring, separator, and outer flywheel ring may be nested to include an arbitrary number of concentric rings. The separator may be a segmented or continuous ring that abuts the ends of the inner rotor and the inner bore of the outer rotor. It is supported against centrifugal loads by the outer rotor and is affixed to the outer rotor. It is made of a material that has a modulus of elasticity lower than that of the rotors.
Eric H. Silver Mark Legros Norm W. Madden Fred Goulding Don Landis	**Broadband High Resolution X-Ray Spectral Analyzer** U.S. Patent 5,777,336 July 7, 1998	A superior-performance, broad-bandwidth, high-resolution, x-ray-fluorescence spectrometer. It consists of an array of four large-area microcalorimeters with 95% quantum efficiency at 6 keV, and it produces x-ray spectra between 0.2 and 7 keV with an energy resolution of 7 to 10 eV. The resolution is obtained at input count rates per array element of 10 to 50 Hz in real time, with analog pulse processing and thermal pile-up rejection. The detectors are incorporated into a compact, portable, cryogenic system that is ready for use in analytical spectroscopy as a tool for x-ray microanalysis or other research applications.
Richard F. Post Charles S. Vann	**Mechanical Beam Isolator for High-Power Laser Systems** U.S. Patent 5,777,775 July 7, 1998	A mechanical beam isolator that uses rod-shaped elements having a Gaussian configuration to interrupt the path of a beam of photons or particles when the time scale of the needed interruption is a microsecond or less. One or more of these rods are mounted transversely to, and penetrate through, a rotating shaft supported by bearings. The rods can withstand much higher rotation speeds than rods having any other geometrical shape. This invention is a means for isolating the optical amplifier elements of high-power pulsed laser systems from the deleterious effects of light reflected back from elements such as targets.

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Scott E. Groves Steven J. Deteresa	**Interlayer Toughening of Fiber Composite Flywheel Rotors** U.S. Patent 5,778,735 July 14, 1998	An interlayer toughening mechanism to mitigate the growth of damage in fiber-composite flywheel rotors over a long lifespan. The interlayer toughening mechanism may comprise one or more tough layers of high-elongation, high-strength fibers arranged in a woven pattern at a range from 0 to 90° to the rotor axis and bound by a ductile matrix material that adheres to and is compatible with the materials used for the bulk of the rotor. The number and spacing of the tough interlayers are a function of the design requirements and expected lifetime of the rotor. The mechanism has particular application in uninterruptible power supplies, electrical power-grid reservoirs, compulsators for electric guns, and electromechanical batteries for vehicles.
George P. Sutton	**Stepped Nozzle** U.S. Patent 5,779,151 July 14, 1998	An insert that allows a supersonic nozzle of a rocket propulsion system to operate at two or more different nozzle area ratios, resulting in improved vehicle flight performance or increased payload. The insert, temporarily fastened by a simple retaining mechanism to the aft end of the diverging segment of the nozzle, provides for a multistep variation of nozzle area ratio. When mounted in place, the insert provides the nozzle with a low nozzle-area ratio. During flight, the retaining mechanism is released, and the insert is ejected, thereby providing a high nozzle-area ratio in the diverging nozzle segment.
William J. Benett Peter A. Krulevitch Abraham P. Lee Milton A. Northrup James A. Folta	**Fabrication Method for Miniature Plastic Gripper** U.S. Patent 5,783,130 July 21, 1998	A miniature plastic gripper actuated by inflation of a miniature balloon and a method of fabricating same. The gripper is constructed of either heat-shrinkable or heat-expandable plastic tubing, formed around a mandrel, and cut to form gripper prongs or jaws. Then the mandrel is removed. The gripper is connected at one end with a catheter or tube having an actuating balloon at its tip, whereby the gripper is opened or closed by inflation or deflation of the balloon. The gripper is designed to retain a member to which is connected a quantity of medicine, plugs, or microcomponents. The inexpensive miniature plastic gripper can be used for gripping, sorting, or placing micrometer-scale particles for analysis.
Alison Chaiken Richard P. Michel	**Growth of Oxide Exchange Bias Layers** U.S. Patent 5,783,262 July 21, 1998	An oxide (NiO, CoO, NiCoO) antiferromagnetic exchange bias layer produced by ion-beam sputtering of an oxide target in pure argon sputtering gas, with no oxygen gas introduced into the system. Antiferromagnetic oxide layers are used, for example, in magnetoresistive read-back heads to shift the hysteresis loops of ferromagnetic films away from the zero field axis. The present invention is a simpler process of producing oxide exchange bias layers.
Nicholas J. Colella Howard L. Davidson John A. Kerns Daniel M. Makowiecki	**Composite Material Having High Thermal Conductivity and Process for Fabricating Same** U.S. Patent 5,783,316 July 21, 1998	A process for fabricating a composite material with high thermal conductivity for applications such as heat sinks or heat spreaders for high-density integrated circuits. The composite material produced by this process has a thermal conductivity between that of diamond and copper, consisting of coated diamond particles dispersed in a high-conductivity metal, such as copper. The composite material can be fabricated in small or relatively large sizes using inexpensive materials. The process uses a sputter-coating diamond powder with several elements (including a carbide-forming element and a brazable material), compacts them into a porous body, and infiltrates the porous body with a suitable braze material, such as copper–silver alloy, to produce a dense, diamond–copper composite material with a thermal conductivity comparable to synthetic diamond films at a fraction of the cost. The present invention can be used for integrated circuits, particularly copper–diamond heat sinks, and for copper–diamond composite material, such as that having high thermal conductivity for fabricating composite materials.

(continued on page 26)

(continued from page 25)

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Joe N. Lucas Tore Straume Kenneth T. Bogen	**Method for Identifying and Quantifying Nucleic Acid Sequence Aberrations** U.S. Patent 5,783,387 July 21, 1998	A method for detecting nucleic-acid sequence aberration by detecting sequences having both a first and a second sequence type. The presence of the first and second sequence type on the same nucleic-acid sequence indicates the presence of a sequence aberration. The method uses one hybridization probe that includes a nucleic-acid sequence that is complementary to a first sequence type and a first complexing agent capable of attaching to a second complexing agent and a second hybridization probe that includes a nucleic-acid sequence that selectively hybridizes to the second sequence type over the first sequence type and includes a detectable marker for detecting the second hybridization probe. The method of the present invention increases by severalfold the sensitivity, precision, and speed of detecting randomly occurring nucleic-acid sequence aberrations (such as chromosome translocations) over current detection methods including FISH assays. The method of the present invention may also be readily adapted for the diagnosis of diseases.
Richard F. Post	**Self-Adjusting Magnetic Bearing Systems** U.S. Patent 5,783,885 July 21, 1998	A self-adjusting magnetic bearing that automatically adjusts parameters of an axially unstable magnetic bearing such that its force balance is maintained near the point of metastable equilibrium. Complete stabilization in an electromechanical battery can be obtained with the application of weak restoring forces either from a mechanical bearing (running at near-zero load, thus with reduced wear) or from the action of residual eddy currents in a snubber bearing. In one embodiment, a torque is generated by the approach of a slotted pole to a conducting plate. The torque actuates an assembly that varies the position of a magnetic shunt to change the force exerted by the bearing. Another embodiment achieves axial stabilization by sensing vertical displacements in a suspended bearing element and uses this information in an electrical servo system. In a third embodiment, a rotating eddy current exciter approaches a stationary bearing and heats a thermostat that actuates an assembly to weaken the attractive force between the two bearing elements.
James L. Kaschmitter Steven T. Mayer Richard W. Pekala	**Process for Producing Carbon Foams for Energy Storage Devices** U.S. Patent 5,789,338 August 4, 1998	A high-energy-density capacitor incorporating a variety of carbon-foam electrodes. The foams, derived from the pyrolysis of resorcinol-formaldehyde and related polymers, are high-density (0.1–1.0 cm^3) and electrically conductive and have high surface areas (400–1000 cm^3). Capacitances on the order of several tens of farad per gram of electrode are achieved.

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Energy to Keep Everything Running

Lawrence Livermore's Energy Directorate provides an array of scientific and technological expertise to help the Department of Energy meet its commitment of providing low-cost energy to sustain the U.S. quality of life and economic stability. The directorate's projects look to future trends and requirements in energy sources and uses. Energy's research, which ranges from short- to long-term work, is unlikely to be performed by commercial entities but is in keeping with Laboratory missions and expertise. The innovative work described in the article includes a nuclear waste repository that will be applying for its license in 2002; a thin-film, solid-oxide fuel cell that efficiently generates electricity yet produces little pollution; tests of a superconducting magnet energy storage system useful for leveling electricity usage loads; and a carbon sequestration technology to mitigate the adverse effects of fossil fuel use.

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Antimatter Helps to Protect Our Nuclear Stockpile

To study the properties of metals and alloys, Livermore scientists use positron spectroscopy, which is a powerful tool for locating the smallest defects. Increasingly smaller devices and thin films in the semiconductor and polymer industries increase the challenge of detecting proportionately smaller defects. A void as small as several atoms can render a microdevice defective. Using a process called pair production, Livermore's linear accelerator and positron microscope now provide the world's most intense kiloelectronvolt positron source. Livermore's new positron microprobe, the facility's upgrade that will be completed in 1999, will offer 3D images faster and at better resolution than currently possible and will detect material defects at the atomic level.

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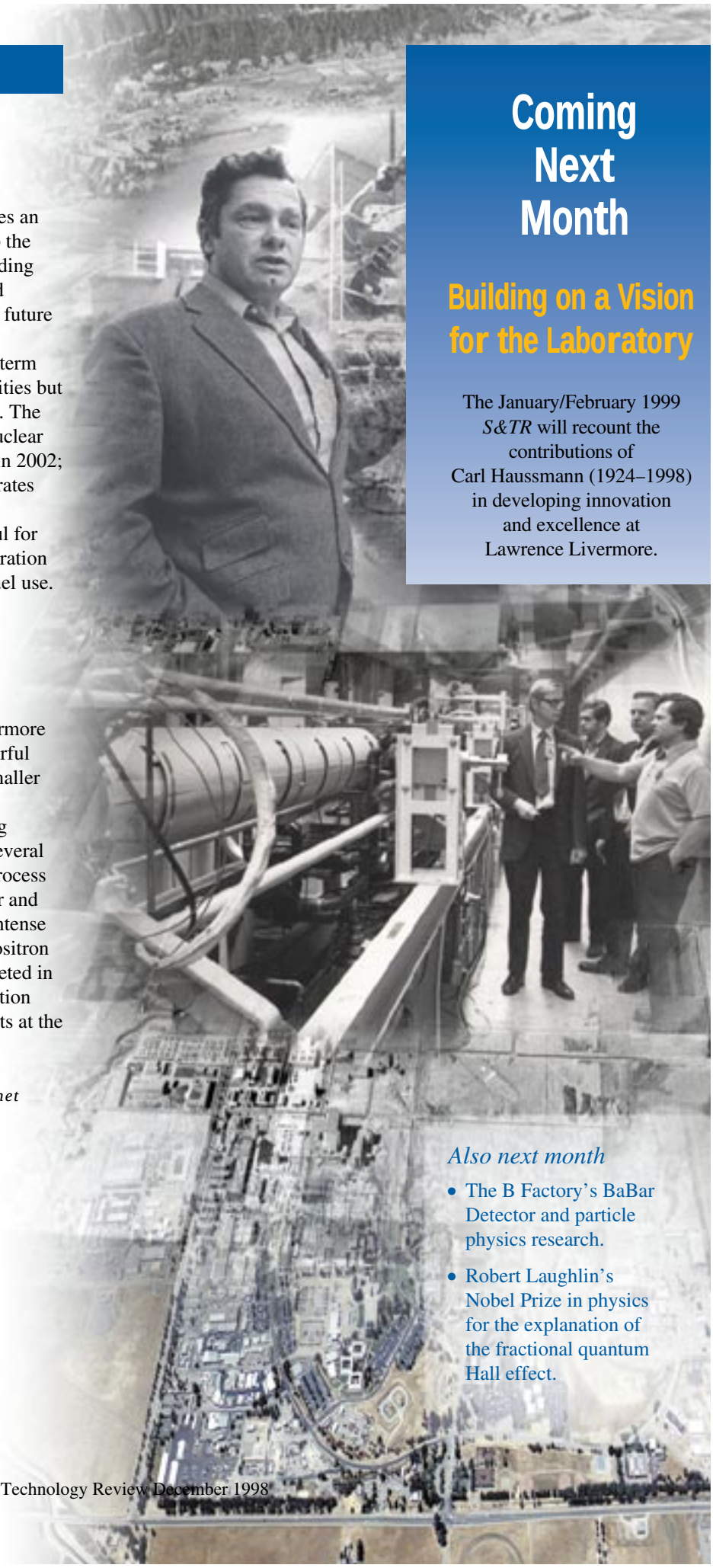
U.S. Government Printing Office: 1998/783-046-80003



Coming Next Month

Building on a Vision for the Laboratory

The January/February 1999 *S&TR* will recount the contributions of Carl Haussmann (1924–1998) in developing innovation and excellence at Lawrence Livermore.

Also next month

- The B Factory's BaBar Detector and particle physics research.
- Robert Laughlin's Nobel Prize in physics for the explanation of the fractional quantum Hall effect.

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