March 2012

Longer Life for the W78

Also in this issue:

Retirement Tribute to George Miller New Techniques for Designing Microstructures **Microbe-Based Energy Generation Chemical Detection without Batteries**

About the Cover

In July 2010, the National Nuclear Security Administration assigned Livermore to lead a lifeextension program (LEP) on the W78 warhead. As described in the article beginning on p. 6, stockpile stewards at Lawrence Livermore and Sandia national laboratories will explore the technical challenges and manufacturing issues of various options for prolonging the warhead's service life and enhancing its safety and security. LEPs also help the national security laboratories maintain a knowledge pipeline of scientists, engineers, and technicians with the expertise required for maintaining the nation's nuclear deterrent. On the cover, Livermore technicians (from left) Brad Wong, Brian Cracchiola, and Raul Garza prepare an experiment at the Laboratory's High Explosives Applications Facility. The background shows several Mark 12A reentry vehicles, which enclose the W78 warheads deployed on Minuteman III intercontinental ballistic missiles.



About S&TR

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure 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 eight 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.

The Laboratory is operated by Lawrence Livermore National Security, LLC (LLNS), for the Department of Energy's National Nuclear Security Administration. LLNS is a partnership involving Bechtel National, University of California, Babcock & Wilcox, Washington Division of URS Corporation, and Battelle in affiliation with Texas A&M University. More information about LLNS is available online at www.llnsllc.com.

Please address any correspondence (including name and address changes) to *S&TR*, Mail Stop L-664, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, or telephone (925) 423-3432. Our e-mail address is str-mail@llnl.gov. *S&TR* is available on the Web at str.llnl.gov.

© 2012. Lawrence Livermore National Security, LLC. All rights reserved. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. To request permission to use any material contained in this document, please submit your request in writing to Public Affairs Office, Lawrence Livermore National Laboratory, Mail Stop L-3, P.O. Box 808, Livermore, California 94551, or to our e-mail address str-mail@llnl.gov.

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.



Prepared by LLNL under contract DE-AC52-07NA27344

Science Technology

March 2012

Lawrence Livermore National Laboratory

Contents

Features

- 2 Honoring a Legacy of Service to the Nation The nation pays tribute to George Miller, who retired in December 2011 as the Laboratory's tenth director.
- 5 Life-Extension Programs Encompass All Our Expertise Commentary by Bruce T. Goodwin
- 6 Extending the Life of an Aging Weapon Stockpile stewards have begun work on a multiyear effort to extend the service life of the aging W78 warhead by 30 years.

14 Materials by Design

Material microstructures go three-dimensional with improved additive manufacturing techniques developed at Livermore.

Research Highlights

21 Friendly Microbes Power Energy-Producing Devices

Livermore researchers are demonstrating how electrogenic bacteria and microbial fuel cell technologies can produce clean, renewable energy and purify water.

24 Chemical Sensor Is All Wires, No Batteries Livermore's "batteryless" nanowire sensor could benefit

applications in diverse fields such as homeland security and medicine.

Departments

- 4 The Laboratory in the News
- 27 Patents and Awards
- 29 Abstracts

S&TR Staff

SCIENTIFIC EDITOR Rebecca J. Nikolic

Managing Editor Ray Marazzi

PUBLICATION EDITORS Carolin Middleton and Caryn Meissner

WRITERS Monica Friedlander, Arnie Heller, Caryn Meissner, and Ann Parker

ART DIRECTOR AND DESIGNER Daniel S. Moore

DESIGNER George A. Kitrinos

PROOFREADER Pamela MacGregor

PRINT COORDINATOR Charlie M. Arteago, Jr.

S&TR, a Director's Office publication, is produced by the Technical Information Department under the direction of the Office of Planning and Special Studies.

S&TR is available on the Web at str.llnl.gov

Printed in the United States of America

Available from National Technical Information Service U.S. Department of Commerce 5285 Port Royal Road Springfield, Virginia 22161

UCRL-TR-52000-12-3 Distribution Category UC-99 March 2012

Honoring a Legacy of Service

EORGE H. Miller, the tenth director of Lawrence Livermore and a Laboratory legend, retired in December 2011 after 39 years of service to the nation. He also stepped down as president of Lawrence Livermore National Security, LLC (LLNS), which manages the Laboratory for the Department of Energy's National Nuclear Security Administration (NNSA).

Miller joined the Laboratory in 1972 and throughout his career was a critical force in strengthening U.S. nuclear security. As a nuclear weapons designer and project leader, he made important contributions to the development of modern nuclear weapons such as the B83 strategic bomb and the W84 warhead, which the U.S. Air Force deployed on its ground-launched cruise missiles. He rose from group leader to project manager for the W84 warhead (1978-1980), to division leader for thermonuclear design (1980–1984), to deputy associate director for nuclear design (1984–1985).

In 1985, Miller was selected as associate director for Livermore's weapons program. Anticipating that nuclear weapons testing would be limited in the future, he led the program toward a focus on high-performance computing and acquiring a more fundamental understanding of nuclear weapons performance.

From 1989 to 1990, he served in Washington, DC, as special scientific advisor on weapons activities to Admiral James Watkins, then Secretary of Energy, and Undersecretary John C. Tuck. During this time, Miller made important contributions in studying the transformation of the nuclear weapons complex, including how to dismantle weapons in a safe and secure manner.

Miller returned to Livermore to lead the Laboratory's nuclear weapons program as the Cold War was ending. He was instrumental in helping to formulate the Stockpile Stewardship Program, which was designed to sustain confidence in the safety, security, and performance of the nation's nuclear deterrence in the absence of nuclear testing. Stockpile stewardship required bold advances in computational and experimental capabilities. Under Miller's leadership, the Laboratory brought into operation the world's most powerful parallel computers, initiated the first successfully completed life-extension program (for the W87

to the Nation

warhead), and launched the effort to construct the National Ignition Facility (NIF). Miller also helped advance Laboratory programs in nonproliferation and arms control and in Department of Defenserelated research.

Throughout his career, Miller tackled a variety of management and scientific challenges in support of national security. In 1999, when he became associate director for NIF, Miller assembled a new management team whose goal was to implement a revised project execution plan that put the facility's construction on track for completion in 2009.

Miller began his term as Laboratory director in March 2006. During his tenure, he led the institution through another significant transition when its management contract was transferred from the University of California to LLNS. Under Miller's leadership, as both Laboratory director and LLNS president, Livermore employees continued to deliver exceptional science and engineering while significantly improving the Laboratory's business and operations functions.

Miller also represented the Laboratory's national security programs to decision makers, not only in the Departments of Energy and Defense but also in other agencies of the executive branch as well as the U.S. Congress. He currently provides advice to the commander of the United States Strategic Command as a member of the USSTRATCOM Strategic Advisory Group and serves as chairman of the group's Science and Technology Panel.

Expressions of Gratitude and Thanks

On December 8, 2011, current Laboratory Director Parney Albright hosted a special tribute to honor Miller's contributions during his long and distinguished career—an event described as "celebrating a commitment to the Laboratory and to the nation." During the tribute, government officials and long-time colleagues,

Past and present directors of Lawrence Livermore and Los Alamos national laboratories attended the retirement celebration for George Miller (from left): Johnny Foster, Mike May, Miller, Mike Anastasio, John Nuckolls, Bruce Tarter, Sig Hecker, Parney Albright, and Charles MacMillan.



speaking in person or as part of a videotaped presentation, offered their thanks and gratitude to Miller.

Donald Cook, deputy administrator for NNSA Defense Programs, presented Miller with the NNSA Administrator's gold medal for "distinguished service in the national security of the United States" and a glass globe representing the global importance of Miller's contributions. Cook read a message from Secretary of Energy Stephen Chu. "Our nation is safer and more secure due to your outstanding leadership," Chu wrote. Miller also received a crystal bowl from the University of California in honor of his service to the university and the nation.

University of California vice president Bruce Darling said, "George brings that E. O. Lawrence focus to the Laboratory. So everything is not about the Laboratory. It's not about George. It's not about programs at the Laboratory. It's about how the Laboratory can use outstanding scientists and engineers, the capabilities that they bring, all to put solely in the interests of the nation."

Ed Moses, principal associate director for NIF and Photon Science, said, "Everywhere he's been at the Lab, whether it was in the weapons program, or the laser program, or as the Director, the Lab has flourished. And he's always brought in when times are hard. When NIF was in trouble, who did the Lab turn to? George. And when we had to go through the contract renegotiation, who did the Lab turn to? George. And whenever there's a hard problem, George is the one we go to. And that's because of all his natural virtues and good judgment, and kindness, and I think, love he has for our Laboratory and for the country."

Former Secretary of State George Shultz said, "When George briefs you on something, what comes through is tremendous knowledge and complete credibility. You know what he is saying is true, or he wouldn't say it. And if he thinks there are question marks, he will tell you. There's that sense of total credibility."

Former Laboratory director Johnny Foster said, "I have the greatest respect for George Miller. He is an excellent scientist, engineer, and manager. And yes, he took charge of NIF, changed the management, and put that superb national facility on track for successful completion. He has dedicated his career to our national security, to this Laboratory, and to job one: the maintenance of a credible, reliable, and secure nuclear security future."

Paul Hommert, director of Sandia National Laboratories, said, "What I see from George is a really unique combination of passion, knowledge, experience . . . an approach to getting to the bottom line, to the essence of an issue."

Phil Coyle, former Livermore associate director and currently a senior advisor to the Center for Defense Information, described Miller as "a wonderful director and manager at the Lab and a fabulous colleague, but he's also, and always has been, a real scientist. In other institutions, the CEO might not know anything at all about the detailed work that scientists were doing. At Lawrence Livermore, the Lab director has always known in detail what the Lab employees were doing, and George has exemplified that like nobody else before him." Tom Gioconda, Livermore deputy director, said, "Thanks to George's leadership, we have a really great future ahead of us. Difficult. Challenging. No question about it. But we're in a very strong position today."

Ellen Tauscher, undersecretary of state for Arms Control and International Security, noted that public service is "about moving from me to we" and commended Miller for exemplifying the humility and selflessness that comes from a career dedicated to service to the nation.

California Senator Dianne Feinstein, said, "George and I may not have always shared the same viewpoint, but I always knew he would speak his mind. I always knew him as a straight shooter. And that's a quality I value tremendously. So George Miller, thank you for all you've done for our nation: four decades of public service is truly something of which to be proud. And I wish you the very best of luck in your next chapter in this great thing called life."

A Rewarding Career

In his remarks, Miller said the most rewarding aspects of his career are the accomplishments of employees and the Laboratory. "You are the soul and spirit of this Laboratory," he said, "and what has allowed it to accomplish so much in the service of our country. It's that sense of service that is in each and every one of you and that has come from our founders Ernest Lawrence, Edward Teller, and the University of California.

"This Laboratory has always embraced big ideas and big challenges. We were founded with two bold missions in mind: providing nuclear deterrence to secure the free world from a determined adversary and providing the world with a limitless source of energy—fusion. Both of these are still a work in progress in my view, and I look forward to your bringing them to fruition." —Arnie Heller

For further information contact Kinnon Ernst (925) 422-9327 (ernst3@llnl.gov).

Planets Orbiting Stars Is the Milky Way Standard

An international collaboration involving Livermore astrophysicist Kem Cook has found that planetary systems resemble our solar system more often than they differ. The team's research results also indicate that, on average, every star in the Milky Way hosts one or more planets in an orbital-distance range of 0.5 to 10 times the distance between the Sun and Earth.

For this project, researchers analyzed microlensing data collected between 2002 and 2007 by the Optical Gravitational Lensing Experiment and the Probing Lensing Anomalies Network. Gravitational microlensing occurs when light from a source star is bent and focused by gravity as a second object (called the lens star) passes between the source star and an observer on Earth. A planet rotating around the lens star will produce an additional deviation in the microlensing.

Over the past 16 years, astronomers have detected more than 700 confirmed extrasolar planets. Most of these planets, discovered using the Doppler-shift technique, are gas giants similar to Jupiter and Saturn, and their parent stars are much closer to them than the Sun is to Earth. Although microlensing events are rare, they allow researchers to probe planets with greater orbital-distance ranges.

According to Cook, the team's measurements confirm that low-mass planets are very common. Approximately 17 percent of the Milky Way's stars host Jupiter-mass planets. Cool, Neptunetype planets and super-Earths are even more prevalent, occurring 52 percent and 62 percent of the time, respectively. The team also found that the number of planets increases with decreasing planet mass, in agreement with predictions of the core-accretion scenario for planet formation. Says Cook, "Planets around stars in our galaxy appear to be the rule rather than the exception." Results from the team's research appeared in the January 12, 2012, edition of *Nature*. **Contact: Anne Stark (925) 423-9799 (stark8@llnl.gov).**

Livermore System Monitors Mars Launch

When the Mars Science Laboratory lifted into space on November 26, 2011, a comprehensive radiological emergency preparedness system monitored the launch from the ground. The Livermoredesigned system uses environmental continuous air monitors (ECAMs) to collect samples and analyze suspended particles for radioactivity that might result in the unlikely event of a launch accident.

Onboard the spacecraft is the largest, most advanced rover ever sent to another planet. Named Curiosity, the rover (above) relies on a radioisotope thermoelectric generator essentially a nuclear battery with 4.8 kilograms of plutonium-238 dioxide that converts heat into electricity. The battery powers the rover and keeps its internal systems warm during frigid Martian nights, where temperatures can dip as low as -150° C.

Prior to the launch, the National Aeronautics and Space Administration installed 30 ECAMs on and around the Kennedy Space Center. The monitors send real-time data via satellite to the Kennedy Space Center's Radiological Control Center and to the National Atmospheric Release Advisory Center (NARAC) at Livermore. NARAC scientists then quickly combine the ECAM data with weather, wind, and other information to develop detailed plume models for radiological contingency planning. Two Laboratory scientists, Steve Homann and Ron Baskett, were deployed to the Kennedy Space Center for the launch.

Curiosity will visit regions of Mars not previously explored to collect and analyze rock samples. Its mission is to study the geologic record on Mars and help determine whether conditions are or have ever been favorable for microbial life. More information about the Mars Science Laboratory is available online at www.nasa.gov/msl.

Contact: Steve Homann (925) 423-4962 (shomann@llnl.gov).

Researcher Clarifies Water's Ionic Conductivity

Livermore scientist Sebastien Hamel and collaborators from the Institut für Physik at Universität Rostock in Germany have resolved a long-standing problem in using quantum molecular-dynamics simulations to calculate ionic conductivity in fluids. The researchers combined two well-established techniques—density functional theory molecular-dynamics simulations and polarization theory to determine electrical conductivity directly, without making assumptions about the effective charge transported by protons. Quantum simulations have provided insight into the dynamics

of proton transport at the microscopic level, including how the involved molecular and ionic species interact. For example,

simulations revealed that as pressure and temperature

in water increase, molecules dissociate, allowing more protons to contribute to charge

transport and thus increasing conductivity. The team's simulations with the combined techniques indicate that the effective charge of protons fluctuates on a femtosecond $(10^{-15}$ -second) timescale and is crucial to charge transport in water. The new approach can now be applied to study the ionic conductivities of electronically

insulating materials of arbitrary composition, such as complex molecular mixtures under the extreme

conditions deep inside giant planets. Results from the team's research appeared in the October 25, 2011, issue of *Physical Review Letters*.

Contact: Sebastien Hamel (925) 423-8048 (hamel2@llnl.gov).

Commentary by Bruce T. Goodwin



Life-Extension Programs Encompass All Our Expertise

WHEN the weapons comprising our nuclear forces of deterrence were originally designed decades ago, scientists knew the warheads could not remain safe, secure, and reliable indefinitely. Over time, components and materials deteriorate as the weapons age. As a result, the nuclear design laboratories—Lawrence Livermore, Los Alamos, and Sandia national laboratories—continually assess the health of the stockpile and determine whether a particular weapon type needs to undergo a life-extension program (LEP).

LEP efforts include identifying and correcting potential technical issues by refurbishing or replacing certain components. LEPs also allow us to strengthen existing safety systems, for example, by introducing insensitive high explosives, which are more resistant than conventional high explosives to detonation from fire or accident.

LEPs are an important tool that allows us to seamlessly sustain the nation's nuclear weapons. In effect, LEPs are triumphs of the National Nuclear Security Administration's (NNSA's) Stockpile Stewardship Program, which was launched at the end of the Cold War to maintain our weapons without nuclear testing. Advances in science, engineering, and computing—representing everything we have learned about nuclear reactions and materials science for the past 70 years—are incorporated into LEP efforts to ensure the devices remain safer, more secure, more reliable, longer-lived, and more maintainable than ever.

In 2004, Lawrence Livermore scientists, engineers, and technicians completed the very first LEP without nuclear testing, which was for the W87 warhead. Today, we stand ready to repeat this challenging and exacting endeavor to design, test, and certify components in the life-extended W78 warheads for the Minuteman III intercontinental ballistic missile. For every W78 component, we will choose from among several design and material options while keeping an eye on ways to minimize costs and environmentally sensitive materials and processes.

As the article beginning on p. 6 describes, the W78 LEP effort affords an uncommon opportunity to offer the next generation priceless experience: Livermore's hands-on physics, chemistry, materials science, and engineering know-how of the Laboratory's stockpile stewards. There is no replacement for on-the-job training to learn how to design, build, and test critical components and ensure their integration into exceedingly complex devices of such importance to national security. The W78 LEP also allows us to take advantage of new test and diagnostic instruments, laboratories, and major research facilities across the nuclear security enterprise. For example, we are assembling the first components of the Laboratory's Sequoia supercomputer. This 20-petaflops (20 quadrillion floating-point operations per second) system will be the world's most powerful supercomputer and will perform unprecedented simulations of nuclear reactions. Sequoia will also support scientific discoveries that will inevitably strengthen stockpile stewardship in the years ahead.

We also have new capabilities, such as fiber optic photonic Doppler velocimetry for diagnosing hydrodynamic tests at the Contained Firing Facility (the largest indoor firing facility in the world) at our remote Site 300. The Joint Actinide Shock Physics Experimental Research gas gun at the Nevada National Security Site allows us to investigate the properties of a key metal plutonium—at extremely high pressures and temperatures. And the Dual-Axis Radiographic Hydrodynamic Test Facility at Los Alamos uses two large x-ray machines to obtain detailed threedimensional images of implosions.

We're also advancing our understanding of fundamental nuclear processes and nuclear weapon performance. Last year, a decades-long investigation into so-called energy balance resulted in a theoretical breakthrough for a phenomenon that perplexed physicists for decades. Our theoretical explanation and detailed simulation models were validated in 35 experiments on the National Ignition Facility.

Even with advanced facilities and top-flight Livermore people, we know we cannot complete a successful LEP alone. On the W78 LEP, we will work closely with the Project Officers Group, which includes individuals from the Department of Defense and NNSA. And we will collaborate with our colleagues at Los Alamos and Sandia and at the manufacturing and assembly facilities within the weapons complex. I'm confident that, with this team and its exceptional stewardship capabilities, the W78 LEP will continue stockpile stewardship's remarkable record of success.

Bruce T. Goodwin is principal associate director for Weapons and Complex Integration.

Extending the of an

Life Aging Weapon

Stockpile stewards modernize the W78 warhead for the nation's land-based intercontinental ballistic missiles.

OLLOWING the end of the Cold War, the U.S. discontinued design and development of new nuclear warheads and halted underground nuclear experiments. In place of underground testing, the National Nuclear Security Administration (NNSA) pursues stockpile stewardship, a comprehensive set of scientific and engineering activities focused on ensuring that existing U.S. warheads remain reliable, secure, and safe.

The life-extension program (LEP) for the W78 warhead (above left) will evaluate options for refurbishing the nuclear weapon to address issues identified with aging components. The U.S. Air Force deploys the W78 warhead in its Minuteman III intercontinental ballistic missiles (ICBMs), which are dispersed in hardened silos (left) to protect against attack. (Courtesy of Department of Defense.)

By law, the directors of the NNSA weapons laboratories-Lawrence Livermore, Los Alamos, and Sandiaprovide the secretaries of Energy and Defense with an annual assessment of the stockpile. Confidence in these assessments depends on the laboratories' abilities to evaluate the inevitable changes that occur inside nuclear weapons as they age and to effectively deal with any safety or performance issues that may arise from those changes. Stockpile stewardship activities enhance understanding of nuclear weapons and ensure their safety and performance through a combination of theoretical advances, nonnuclear experiments, supercomputer simulations, and stockpile surveillance. When necessary, life-extension programs (LEPs) are approved to prolong the service life of an aging warhead and enhance its safety and security.

LEPs address issues discovered through routine surveillance and annual stockpile assessments. Nuclear weapon components are made from various materials including high explosives, steel, plutonium, uranium, and plastics. Over decades, plastics can break down, metals corrode, and coatings deteriorate. A material's properties may change unpredictably in response to high radiation fields, fluctuating temperatures, and other environmental conditions to which stockpile components are subjected.

In July 2010, NNSA designated Lawrence Livermore the lead nuclear design laboratory to conduct an LEP on the Los Alamos–designed W78 warhead, with Sandia, California, responsible for the warhead's nonnuclear components. The announcement was made in a letter from Don Cook, deputy administrator for NNSA's Defense Programs.

The W78 is used on U.S. Air Force Minuteman III intercontinental ballistic missiles (ICBMs). The Mark 12A reentry vehicle encloses the warhead to protect it from heat as it speeds through the atmosphere. A team of about 30 Livermore physicists, engineers, and chemists are working on an options study in what is currently planned to be a 10-year effort to extend the W78's service life for another 30 years.

In Congressional testimony in 2011, Laboratory Director George Miller (now retired) underscored the importance of the W78 LEP, saying, "The role of any Life Extension Program is to fix issues that impact-or will soon impactoverall system effectiveness and take actions that will extend the stockpile life. Failure to address these issues can have immediate and drastic consequences for the viability of the deterrent our national security strategy relies on. In particular, it is imperative that we begin the study of options for refurbishing the W78 warhead to address evolving issues identified in the annual assessment of this weapon system."

"When the W78 was added to the stockpile in 1979, no one anticipated it would not have been replaced 33 years later," says physicist Hank O'Brien, who leads the W78 LEP for Livermore's Weapons and Complex Integration Principal Directorate. "We are seeing signs of aging among W78 components,



although these changes have yet to impact system reliability. It is important to start the LEP process to prevent this aging issue from becoming a real problem."

The W78 will be the fourth nuclear weapon system to undergo refurbishment. In 2004, Lawrence Livermore successfully completed NNSA's first LEP, refurbishing the W87. That effort enhanced the structural integrity of the warhead and extended its life by 30 years. For the W87, Livermore and Sandia scientists and engineers developed and certified the engineering design and worked closely with NNSA production facilities to ensure a cost-effective design and ease of manufacture. The W87 effort has served as a model for subsequent LEPs, including two being conducted by Los Alamos: the W76 warhead used in Trident II submarine-launched ballistic missiles (SLBMs) and the B61 family of nuclear bombs. (See the table on p. 9.)

LEPs progress through a series of phases labeled 6.X. Phase 6.1 is a concept study, during which scientists and engineers explore options, reviewing each one's performance characteristics, manufacturing issues, and technical challenges; expected improvements in performance margins, safety, and security; and long-term maintenance and surveillance requirements. Livermore stockpile stewards expect the W78's 6.1 phase to conclude this year. It will then be followed by three phases: option selection and detailed design and cost studies (6.2), development engineering (6.3), and production engineering (6.4). First production of the modified warheads (phase 6.5) is scheduled to begin about 2023, followed by full-scale production (phase 6.6).

As part of phase 6.1, Livermore and Sandia researchers are working with NNSA production agencies (Los Alamos,

The Minuteman III ICBM, shown in a flight test, contains the W78 warhead. (Courtesy of Department of Defense.) Y-12 National Security Complex, Kansas City Plant, Pantex Plant, Savannah River Site, and Sandia, New Mexico) as they assess the manufacturability of options for components and systems. In particular, they want to identify manufacturing processes that reduce waste and do not use hazardous materials.

A Project Officers Group, with representatives from the Department of Defense, NNSA, Livermore, Sandia, and Los Alamos, meets regularly to assess progress. At the conclusion of phase 6.1, Livermore managers will present the recommended LEP options to this group. "We are thoroughly analyzing all options to present decision makers with low-risk, cost-efficient alternatives," says O'Brien. "Our findings and recommendations are based solely on our best technical assessments of cost, risk, and ability to meet stockpile goals."

According to O'Brien, U.S. government policy requires LEP design teams to consider options for refurbishing the existing design, reusing components from other stockpiled designs, and implementing nuclear-test-based designs that are not in the current stockpile. The Department of Defense also requires LEP studies to identify and assess options that improve safety and security features and that make the warhead adaptable for deployment on SLBMs as well as ICBMs. No new military capabilities or missions are required. Among the suite of options identified, the stockpile component reuse designs show the most promise to address the LEP requirements cost-effectively and with high confidence in performance.

Looking to Increase Confidence

A modern nuclear explosive package includes nuclear and nonnuclear components that comprise a primary explosive device and a secondary, both enclosed within a case to confine radiation from the primary explosion. Among the options being considered as part of phase 6.1, designers for the primary and secondary are examining ways to increase confidence that the weapon will reliably achieve its predicted energy release, or nuclear yield.

A primary is typically a shell of fissile material—called the pit—that is imploded by a surrounding layer of chemical high explosive (HE). Options that entail changes to the weapon's primary to increase confidence in performance make it possible to accommodate insensitive high explosives (IHEs) and other safety and security components to meet U.S. Air Force requirements. However, says O'Brien, "We can't simply swap out IHE for the conventional HE being used in the W78. The primary design must be modified."

O'Brien explains that the conventional HE in older weapon systems can be sensitive to extreme shocks, which can complicate safeguarding and transport. Livermore designers incorporated a widely used IHE, triaminotrinitrobenzene (TATB), in the design of the W87 ICBM warhead, which includes modern safety features. TATB. however, has not been produced in 20 years. Livermore chemists are evaluating current manufacturing techniques that would be more environmentally friendly, should it be decided to use TATB in the refurbished W78 warhead. Advanced safety and security options for the warhead depend on the use of IHE, as well.

Physicist Juliana Hsu leads the effort to understand how the modified W78 could effectively accommodate IHE and other modified components. She notes that LEPs provide the opportunity to add safety and security features without degrading overall effectiveness or introducing new military capabilities. "We will probably have the W78 for the foreseeable future," she says. As a result, "We will be proposing safety and use-control features that were not implemented in the original warhead design. It makes sense to have the warhead safer and with more effective safeguards." Hsu adds that physicists and engineers are also considering options to modify the

warhead so it can be adapted to multiple delivery platforms, which would provide a cost-effective hedge against future problems in the stockpile.

Many safety and security options ready for deployment on the W78 are based on results from past nuclear tests. Some features would provide enhanced protection from fire, while others would guard against unauthorized use and attack. One safety option being evaluated is a method to better ensure that the firing system commences only when an elaborate sequence of events takes place. To that end, Livermore engineers are working on an advanced mechanical safe arming detonator (MSAD). This intricate nuclear safety component prevents accidental or unintended detonation of a warhead. MSADs protect nuclear weapons by preventing an outside source from using the weapon detonators to successfully ignite the IHE main charge. The miniature notches on an MSAD pattern wheel encode a signal set that must be received for the weapon to be operable. This unique signal set ensures that naturally occurring signals or an improper input cannot cause the weapon to function.

Current Weapon Systems in the U.S. Nuclear Stockpile

Weapon	Type*	Delivery system	Primary use	Service	Date added	LEP status
W78	ICBM	Minuteman III	Surface to surface	Air Force	1979	Phase 6.1
W87	ICBM	Minuteman III	Surface to surface	Air Force	1986	Completed
W76	SLBM	Trident II (D5)	Underwater to surface	Navy	1978	Phase 6.6
W88	SLBM	Trident II (D5)	Underwater to surface	Navy	1989	Future LEP
B61-3/4/10	Bomb	F-15, F-16	Air to surface	Air Force	1979/1990	Phase 6.3
B61-7/11	Bomb	B-52H, B-2A	Air to surface	Air Force	1985/1996	Phase 6.3
B83	Bomb	B-52H, B-2A	Air to surface	Air Force	1983	Not needed
W80-1	Missile	B-52H	Air to surface	Air Force	1982	Delayed

*ICBM = intercontinental ballistic missile; SLBM = submarine-launched ballistic missile.

	Refurbish	Reuse	Replace
Performance margins	Limited improvements	Large improvements	Largest improvements
Primary high explosive (HE)	Retains conventional HE	Enables insensitive HE	Enables insensitive HE
Added surety for nuclear explosive package	No	Yes	Yes
Multiple delivery platforms	No	Yes	Yes
Production rate	Limited by new production	Not limited by new production	Limited by new production

Green = meets requirement, yellow = partially meets requirement, red = does not meet requirement.

U.S. government policy requires the W78 LEP to consider three options: refurbishing the existing design, reusing components from other stockpiled designs, and using nuclear-test-based designs that are not in the current stockpile. Of the three options, only reuse meets all LEP requirements.

S&TR March 2012

MSADs are an example of a so-called strong link—rugged mechanical safety devices that interrupt the firing chain until certain sensing systems indicate a normal launch sequence. These devices help safeguard the HE that detonates to begin the nuclear detonation.

A Better Look at the Fundamentals

"Stockpile stewardship is becoming scientifically and technically more challenging as weapons continue to age beyond their original design lifetimes," observes O'Brien. However, the physicsbased understanding of nuclear detonations has improved significantly over the past decade thanks to theoretical advances, experiments, and simulations, together with the existing nuclear-test database. (See the box on p. 11.) This improved capability allows weapon scientists and engineers to assess with confidence a wide range of options in the W78 LEP.

Because underground nuclear experiments ceased in 1992, simulations have become a major tool for assessing the stockpile and guiding LEP efforts. "Compared to the W87 LEP completed in 2001, we have a much greater technical basis for making decisions," says O'Brien. Full three-dimensional, high-fidelity simulations allow physicists to observe important nuclearrelated phenomena

nanosecond by nanosecond, with a level of spatial resolution and a degree of physics realism previously unobtainable.

"We're bringing substantially more computational power to bear on this LEP compared with the resources we had for the W87 LEP," says O'Brien. "Our codes have much more detail, allowing us to analyze options with even greater precision."

Advanced simulations require experimental validation, which, in the absence of nuclear testing, is provided by sophisticated nonnuclear experiments. For example, Laboratory physicists Aaron Puzder and Dana Goto designed experimental studies to investigate advanced safety technologies. Those experiments, which were fielded in 2010 and 2011 at the Dual-Axis Radiographic Hydrodynamic Test Facility at Los Alamos, provided valuable data for the W78 LEP.

In 2011, Livermore engineer Chad Noble received an NNSA award for a

Small-arms fire discharged into the triaminotrinitrobenzene surrounding a nuclear weapon component does not detonate this insensitive high explosive.





A mechanical safe arming detonator (MSAD) prevents accidental or unintended detonation of a nuclear warhead. Stockpile stewards at Livermore are working on an advanced MSAD for the W78.

hydrodynamic experiment at Livermore's Contained Firing Facility, which provided an improved understanding of use-control technology for consideration in the W78 LEP. Physicist Steve MacLaren also won an NNSA award for work as lead designer in high-energy-density experiments on the National Ignition Facility at Livermore and the Z-pinch machine at Sandia, New Mexico. Those experiments produced data that validated key stockpile stewardship simulations.

The National Boost Initiative (NBI) is also helping scientists better understand the thermonuclear burn process. "NBI is an effort to examine the primary's performance, or the boost process, in greater detail," says Hsu. "The W78 LEP will leverage the increased scientific knowledge from this initiative to quantify and potentially reduce our uncertainties during warhead certification." Hsu notes that Ray Tolar, a physicist working on the W78 LEP, is also supporting a major NBI milestone. As a result, he will be able to maximize the synergy between the two projects.

Livermore physicist Omar Hurricane, who specializes in secondary design, won

the Department of Energy's prestigious Ernest Orlando Lawrence Award for solving a mystery that had confounded weapon scientists for more than half a century. For decades, Hurricane says, scientists had to account for missing energy produced during nuclear tests. "There was consistent mysterious behavior of nuclear detonations from what we measured during underground tests. It was OK during the Cold War because we could do a test and make sure things were working properly. With the cessation of underground testing, we knew we had to resolve the discrepancy."

Over a decade, Hurricane led a team ranging from 20 to 40 physicists who worked on two vastly different areas of physics. "It was an intense, detailed effort," he says. The team identified the key physical processes involved and built computational tools to make predictions about the physics. They then conducted experiments to validate their theories. "We eventually resolved the problem and applied the solution to our codes," says Hurricane. That breakthrough has increased confidence in calculations that simulate performance for the modified W78 and other warheads.

Weapons scientists continue to benefit from a methodology known as quantification of margins and uncertainties (QMU). This methodology draws together the latest data from simulations, experiments, and theory to establish confidence factors for the key potential failure modes in weapon systems. QMU helps weapon scientists rank the design options identified for the W78 LEP. "QMU is a way to quantify our performance margins, to help us know we're in the regime where we're strongly confident," says O'Brien. "We want margins that are sufficiently robust."

Engineering's Major Role

The LEP effort requires input from engineers as much as from physicists. Engineers must ensure both the mechanical robustness of the overall system and the



Omar Hurricane received the Ernest Orlando Lawrence Award for helping to resolve a longterm mystery in weapons physics—accounting for the missing energy produced during nuclear tests.

complete integration of every component and system, explains Peter Raboin, project engineer for the W78 LEP. Raboin notes that the warhead's nuclear explosive

Understanding Plutonium

Among all the elements, plutonium is the most mysterious because it exhibits six different phases (orientations of its atoms) at ambient pressure, with a seventh phase under pressure. What's more, phases readily transform from one to the other and are accompanied by large volume changes. In addition, plutonium's radioactive decay causes self-irradiation damage that can change the metal's properties over time, a matter of concern to stockpile stewards evaluating whether a weapon system should undergo a life-extension program (LEP).

Livermore scientists have labored for decades to unravel plutonium's secrets, using a combination of experiments, theoretical advances, and simulations. Determining the long-term behavior of plutonium is important for stockpile stewardship and for the eventual dismantlement and disposition of warheads. The U.S. and Russia have withdrawn thousands of nuclear weapons from their arsenals, and the excess plutonium recovered from these warheads must be dealt with safely.

"We've only studied the basic fundamental properties of plutonium metallurgy and properties," says materials scientist Brandon Chung. "Many questions remain. It's very much an ongoing science." As part of the W78 LEP, special engineering test facilities will help researchers evaluate advanced safety and surety features that involve plutonium and uranium. Other facilities could help them explore the chemistry of new manufacturing methods for the warhead's plutonium pits. The National Nuclear Security Administration is changing the manufacturing process for plutonium pits because the production facilities of the Rocky Flats Plant no longer exist. "We need more efficient, cost-effective pit manufacturing," says Chung. "We will have no underground tests to prove that new manufacturing processes do not degrade pit performance, so a firmer understanding of plutonium is required."

Engineering efforts for the W78 LEP will simulate environmental stresses that components could experience from the time a warhead is produced until it arrives at a target. These stresses include being placed and driven on a truck, vibrations experienced at launch and during the flight sequence to a target, and high temperatures during reentry through the atmosphere. The planned tests include spinning components at high speed and subjecting objects to extreme heat and high gravitational forces. package resides in a deployment vehicle located in the nose cone of an ICBM. The package and its support structures must be "fit to fly."

"The Department of Defense expects the W78 to arrive on target intact and functioning," says Raboin. "We pay very close attention to making sure components will survive the flight from launch to target. Parts could potentially be damaged or break during reentry into the atmosphere, when the Mark 12A experiences decelerations as high as 100 times the force of gravity."

To approximate the vibrations during flight, Laboratory engineers use centrifuges and so-called jerk and shaker tables. By combining such physical experiments with simulations, they mimic what happens to the warhead from the moment it leaves a production facility to the point at which it hits a target.

Engineers also turn design concepts prepared by physicists into computer drawings, models, and eventually detailed engineering specifications to

be implemented by NNSA production facilities. In this activity, the Livermore team works closely with Sandia, which is responsible for the nonnuclear hardware that supports operation of the nuclear explosive package. Livermore and Sandia engineers then integrate the nuclear and nonnuclear hardware into fully functional warheads.

Chemists also contribute to this effort by searching for potential problems that stem from chemical incompatibilities in the widely different materials used in a warhead. Such problems could develop over time because components are in chemical contact with each other and are situated close to a field of high radiation. Engineers are also mindful of possible changes in the size of gaps separating components should a material shrink or expand. "Changes within the warhead

Storage

may occur at a very slow rate," says Raboin. "But over 30 years, they can add up to a considerable amount."

O'Brien adds that LEPs in general help NNSA maintain the expertise required for stockpile stewardship into the future. (See the box on p. 13.) The special skills required for nuclear weapons work are developed over time through experience and mentoring. The W78 LEP provides the Laboratory with an opportunity to develop the next generation of scientists, engineers, and technicians to help sustain the nation's nuclear deterrent.

Best Analysis of Options

"The W78 LEP is a significant development program," says O'Brien. "It's the biggest effort of this decade for the Livermore weapons program. We're getting ready to present to the U.S. government our best analysis of options, including the advantages and risks of each." Those options will address aging issues observed

Transport

As part of the W78 LEP. Livermore engineers will evaluate the benefits of adding safety and security features to the warhead over its complete lifecycle, from fabrication to deployment.





Assembly



Deployment



platforms

Training the Next Generation of Stockpile Stewards

The W78 life-extension program (LEP) presents an excellent opportunity to develop and train stockpile stewards. The program will help the Laboratory maintain a knowledge pipeline by allowing the next generation of LEP scientists and engineers to work with mentors who have LEP experience.

W78 LEP manager Hank O'Brien notes that neither Livermore nor Los Alamos can execute all the LEPs needed to sustain the nation's nuclear deterrent. Of equal importance, stockpile stewardship in the absence of nuclear testing vitally depends on the two laboratories providing expert technical review of each other's work. To sustain expert judgment, both laboratories must be involved in all elements of stockpile stewardship, and each laboratory must attract, develop, and retain talented scientists, engineers, and technicians needed to maintain the nation's nuclear arsenal. The specialized skills and expertise required for nuclear weapons work take a long time to develop through hands-on experience and mentoring. In 2011, Laboratory Director George Miller (now retired) told Congress, "Confidence in the stockpile ultimately depends on confidence in the stockpile stewards at the [National Nuclear Security Administration] labs and production facilities."

"The W78 LEP will proceed as the last of the nuclear testexperienced designers will reach the end of their careers, while the first generation of stockpile stewards is in their professional prime, and will develop the next generation," said Miller. "This program is a vital element in maintaining the competency and capability of the Laboratory's weapons specialists through a project involving design, engineering, and manufacturing."

For the past three years, the Enterprise Modeling Group led by physicist Cliff Shang has been tracking the skill sets of current stockpile stewards at Livermore and projecting needs for the future. Shang notes that the W78 LEP effort is valuable because it "exercises" many key capabilities in the U.S. nuclear security enterprise: production plants, design laboratories, and most of all, the people. "The nation has made an enormous investment in developing a cadre of weapons scientists and engineers," says Shang. "In the past, one way to mastery was achieved by leading and testing nuclear devices. Very few of these people remain in our current workforce. In today's era of science-based stockpile stewardship, mastery is achieved by integrating large-scale simulations with the design work required to field nonnuclear experiments. The scientists and engineers we hired for the W80 and W87 LEPs are the technical leaders for the W78 effort. The challenge for us now is to grow a new generation of scientists and engineers so they will have the skills, knowledge, and abilities needed to maintain the nation's strategic deterrent."



Livermore physicists with nuclear test experience are reaching the end of their careers, and the first generation of stockpile stewards is in its professional prime. The W78 life-extension program is thus critical to the Laboratory's efforts to maintain the skills, knowledge, and abilities required for effective stewardship of the nation's nuclear deterrent.

in surveillance of W78 units and will feature warhead designs that increase confidence in performance and meet requirements for enhanced safety and security.

Over the next decade, Livermore stockpile stewards will produce detailed engineering documents, supervise advanced experiments, and simulate every proposed modification and new part in three dimensions. And they will coordinate closely with NNSA production centers as the modifications slowly take shape.

The result will be a new lease on life for a warhead that was not designed to remain in service for 40 years. Thanks to the LEP, the W78 will have another three decades of service life, potentially with advanced safety and security features in place and changes that will give stockpile stewards greater confidence in its performance.

—Arnie Heller

Key Words: B61, intercontinental ballistic missile (ICBM), life-extension program (LEP), mechanical safe arming detonator (MSAD), quantification of margins and uncertainties (QMU), stockpile stewardship, triaminotrinitrobenzene (TATB), W78, W87.

For further information contact Hank O'Brien (925) 423-5017 (obrien6@llnl.gov).

Materials by Design

Additive manufacturing techniques deliver three-dimensional microstructures with previously unobtainable material properties.

VER wonder why on hot days a door sticks in its jamb or a car's fuel gauge registers more gas than is actually in the tank? The answer is thermal expansion. Rises in temperature cause materials, including solids, liquids, and gases, to swell and grow in volume as the heat increases but pressure stays relatively constant. Thermal expansion is one of many properties scientists look for when adapting materials for new applications. Others include fracture toughness, strength, and thermal conductivity.

A material's properties and overall performance are determined by its chemical composition, crystalline state, and underlying microstructure-how the constituent elements within the material are arranged relative to one another. These characteristics force scientists to accept certain trade-offs when choosing a material for a specific application. British materials engineer M. F. Ashby developed charts that provide selection guidance by categorizing materials such as metals, ceramics, polymers, and foams based on their properties in bulk form. An example chart comparing a material's stiffness (Young's modulus) with its density illustrates how the two properties are coupled, or linked,

so that typically the denser a material is, the stiffer it is. (See the figure on p. 16.)

Livermore materials scientists and engineers Chris Spadaccini, Joshua Kuntz, and Eric Duoss are designing a class of materials that will open up new spaces on many Ashby material selection charts, such as those for stiffness and density as well as thermal expansion and stiffness. In collaboration with partners at the University of Illinois Urbana-Champaign, the Massachusetts Institute of Technology (MIT), and the University of Wisconsin-Madison, the Livermore team is advancing three additive manufacturing techniques to fabricate three-dimensional (3D) microstructures with micrometer resolutions. Spadaccini, who leads the effort, says, "By controlling the architecture of a microstructure, we can create materials with previously unobtainable properties in the bulk form."

In projects funded by the Laboratory Directed Research and Development Program and the Defense Advanced Research Projects Agency, the collaborators are combining sophisticated computer modeling with projection microstereolithography, direct ink writing, and electrophoretic deposition to design, build, and test designer materials. "Our goal is to use these techniques to effectively alter the chemical composition and crystalline state of materials at their microstructural level so we can control their properties and performance," says Kuntz, who leads the team's work on electrophoretic deposition.

In particular, the researchers will focus on creating materials that exhibit high strength but low density or ultralow thermal expansion or improved energetics. Such materials are important for a wide range of national security applications and in the areas of energy, photonics, microfluidics, and semiconductor manufacturing.

From the Bottom Up

Additive manufacturing is the process of building 3D structures by sequentially layering one material on top of another in a desired pattern. It is a dramatic departure from more conventional fabrication techniques in which material is removed from a bulk piece through processes such as etching or machining. Contrary to what the name might imply, additive

Livermore engineers Chris Spadaccini (left) and Eric Duoss experiment with the direct ink-writing process. 6.5

B camund Optics' 66382



Livermore scientist Joshua Kuntz (left) is working with Spadaccini and Duoss to develop additive manufacturing techniques for designing materials with improved properties.



Materials designed with new additive manufacturing techniques exhibit high stiffness and low density, occupying a previously unsettled area of the Ashby material selection chart for Young's modulus (stiffness) versus density. The octet truss structure recently fabricated by Livermore researchers is a stretch-dominated lattice.

manufacturing actually requires less material than "subtractive" fabrication methods. It also results in less waste and can reduce manufacturing costs.

Over the last decade, additive manufacturing has become a burgeoning industry, enabling rapid prototyping of components for automotive, medical, and electronic applications. News headlines in recent years have showcased the oftenremarkable capabilities of 3D printers that produce macroscale objects, such as a prototype musical instrument. Although specialized technologies are available for developing 3D structures with small, mesoscale (millimeter-length) features hearing aids, for example—they are limited to a small number of materials as well as component size and shape specifications.

According to Duoss, who leads the team's direct ink-writing effort, commercial additive manufacturing systems can at best fabricate single-material structures at resolutions of about 100 micrometers. "In contrast," he says, "our techniques can incorporate several materials into structures with feature sizes in the micrometer and even submicrometer range."

To date, no single technology that fabricates 3D mesoscale objects with micrometer-size architectures and submicrometer precision is compatible with the wide range of materials available. The Livermore-led project is integrating projection microstereolithography, direct ink writing, and electrophoretic deposition into a process that can manufacture materials with these characteristics in high volumes at low cost. In doing so, the team will significantly improve additive manufacturing capabilities and advance material design. "The broad diversity of potentially relevant materials, length scales, and architectures underscores the need for these flexible additive micromanufacturing techniques," says Duoss. "We believe our new patterning methods and design approaches will drive scientific and technological advances in

materials science, chemistry, physics, and biology."

Building Complex Structures

Projection microstereolithography, direct ink writing, and electrophoretic deposition offer a unique combination of advantages for fabricating microscale structures from multiple materials. "These three technologies complement each other," says Kuntz. "Where one is weaker in a certain capability, the others are strong."

Projection microstereolithography, for example, can reliably create structures in three dimensions, but for now, it is compatible with only a few materials. Direct ink writing and electrophoretic deposition, on the other hand, work well with more materials but do not offer the same 3D capability as projection microstereolithography. Electrophoretic deposition would have to burn out excess, or fugitive, material within a fabricated component to create void space, but direct ink writing and projection microstereolithography can build these spaces where needed during component fabrication. Says Kuntz, "By combining the techniques, we can create more complex structures than we can produce using one method alone."

With each fabrication approach, the team first applies a computer-aided design program to section an image of the desired structure into 2D slices in the horizontal plane. In a project with MIT professor Nicholas Fang and his colleague Howon Lee, the team used projection microstereolithography to display 2D images on a digital photomask made from a micromirror or liquid crystal on a silicon chip. An ultraviolet light-emitting diode illuminates the miniature display, which reflects light and an image of the component to be fabricated through a series of reduction optics onto a photopolymer liquid resin. As the resin cures, it hardens into the shape of the image. The substrate holding the resin is then lowered using a motion-controlled stage, and the next 2D slice is processed.





The Livermore team fabricated this heterogeneous polymer structure (left) using projection microstereolithography and integrated microfluidics. The schematic (right) delineates the two materials incorporated into the final structure: (red) polyethylene glycol with rhodamine B dye and (black) hexanediol diacrylate. (Courtesy of Nicholas Fang, Massachusetts Institute of Technology.)

Projection microstereolithography is a high-speed parallel process that can fabricate structures at both micro- and macroscales within minutes. "Using projection microstereolithography, we can rapidly generate materials with complex 3D microscale geometries," says Spadaccini, the principal investigator for the technique.

However, the method does have its limitations. "The quality of a component depends on the uniformity of light at the image or polymerization plane and both the lateral and depth resolution of the system," he says. "Resolution is restricted both by the optical resolution and the physical-chemical characteristics of the exposed monomer solution."

Expanding the technique's capabilities requires a thorough understanding of the physics involved in the fabrication process. The team is developing process models based on differential equations to assess physics parameters, such as lightscattering effects, chemical composition, and fluid dynamics. Through these computational methods, parameters can be altered to determine the best ones for achieving a desired resolution and geometry.

Microfluidic systems can also be incorporated with projection microstereolithography to create heterogeneous structures that integrate multiple materials into one component. "After we fabricate structures from one material, we can flow the remaining uncured resin out of the fabrication zone and flow a new resin in," says Spadaccini. "By simply shining light in a new pattern, we can fabricate a second structure with the new material on the same device layer." With the combined process, researchers can develop a two-material composite with void space, the same structures that form the building blocks for designer bulk materials.

Inking a Material

The direct ink-writing process can also create micro- to macroscale structures with

extreme precision. With this technique, a print head mounted to a computercontrolled translation stage deposits inks into programmed designs on various substrates. The process works layer by layer, adding a continuous filament to a substrate. The patterns it generates range from simple, one-dimensional wires to complex, 3D structures.

Inks are administered through one or more nozzles, and filament diameter is determined by nozzle size, print speed, and rates of ink flow and solidification. The time required to build a final part is determined by the distance from the nozzle to the substrate and by print speed. The finest feature size obtained with this technology is approximately 200 nanometers-smaller than the features produced with projection microstereolithography. Recently, the team constructed two direct ink-writing platforms that can travel 30 centimeters at up to 10 centimeters per second while maintaining micrometer and submicrometer resolution.

Direct ink writing can rapidly pattern different materials into multiscale, multidimensional structures for an array of applications. However, process improvements, including more sophisticated inks, are needed to achieve the arbitrary, complex 3D structures required for designer materials. To date, the researchers have designed particleand nonparticle-based inks derived from metals, ceramics, and polymers.

"We carefully tailor the fluid properties and solidification behavior to obtain inks that readily flow through micronozzles without clogging," says Duoss. "We also want the inks to set rapidly so they will maintain their shape with minimal shrinkage."

In addition, the team is working on a direct ink-writing process specifically designed for building 3D geometries. Adds Duoss, "Through improved ink chemistries, better material characterization, modeling of ink dynamics during deposition, and improved robotic and ink delivery systems, we can create a 3D printing process with ever greater spatial and compositional control."

Electrifying Attraction

Although typically used for creating protective or performance-enhancing coatings, electrophoretic deposition has great potential for building 3D designer materials. Among its advantages are the ability to incorporate multiple materials into one structure, extreme precision, and potential for large-scale production. In the electrophoretic deposition process, an electric field is applied to a liquid medium that contains suspended colloidal nanoparticles. "Within these suspensions, the particles exhibit an induced surface charge," says Kuntz. "By altering that charge, we can use electric fields to control the particles."



Scanning electron micrographs of titanium dioxide structures show the fine-scale features and precision that can be achieved with direct ink writing. (Courtesy of Jennifer Lewis, University of Illinois Urbana-Champaign.) Typically, the suspension is flowed into a deposition cell that has opposing electrodes. Once an electric field is applied to the deposition cell, the induced surface charge causes the particles within the liquid to travel parallel to the electric field, attracting the suspended particles to the substrate electrode. With this process, the team has built 2D structures with resolutions smaller than 7 micrometers and horizontal gradients of about 1 micrometer.

Achieving 3D geometries with electrophoretic deposition is a novel concept, one the team is validating through an innovative electrode scheme. As with projection microstereolithography, an optical system projects a pattern onto a transparent photoconductive layer attached to a dynamic electrode. The electric field emanates only from the illuminated area of the electrode and can be varied throughout the deposition process. Because the image is also adjustable, the team can alter the 2D pattern on the deposition plane during an experiment to build complex 3D structures.

The team is again turning to process models to speed experimental redesign of the electrophoretic deposition technique. "These models save us time," says Kuntz. "They allow us to effectively sculpt the electric field for producing a specific deposited geometry. In this way, we can narrow deposition parameters and the electric field profile to those that are the most successful prior to actually conducting experiments." Armed with a better understanding of processes such as particle motion, electrophoresis, and hydrodynamic interactions, the team has already identified ways to change the electrode design for improving its fidelity and subsequently the surface topography of the fabricated components.

Things that Go Boom

The Livermore researchers are applying the three techniques to improve the performance of thermites—pyrotechnic compositions that combine a metal oxide, such as copper oxide, with a metal powder, such as aluminum. Thermites are designed to produce an exothermic reaction through a process of oxidation and reduction. Such materials typically have a slow burn rate, limited by the irregular placement of the fuels and oxidizers. "Improved performance in energetic materials is contingent upon achieving microstructural control that is not currently available," says Spadaccini. "If we can adjust the thermite microstructure, we can control its burn rate."

Using electrophoretic deposition, the team strategically arranged an oxidizing agent and a fuel to produce a highly ordered, optimized thermite. "With this placement, we can potentially alter the directionality of the thermite reaction as



Electrophoretic deposition can be used to fabricate (a) highly ordered and (b) disordered structures. The computational models shown in the bottom row match the experimental results in the top row, where μm = micrometers.

it propagates through the material," says Kuntz. The team's first heterogeneous thermite structure had a power density approximately two times greater than that achieved with more conventional thermite compositions, with half the burn time and twice the burn velocity.

Thermite performance could be improved further by combining the fabrication techniques. A recent experiment showed that direct ink writing and electrophoretic deposition could create a novel 3D microstructure made from multiple materials. In this experiment, the scientists used direct ink writing to build an initial lattice structure complete with void space. They then applied a new material to the void with electrophoretic deposition.

"Working with Jennifer Lewis and her team at the University of Illinois, we've developed copper oxide and aluminum inks and are trying to better understand the fundamental reaction mechanisms of the materials," says Duoss. "We will print both inks in 2D and 3D configurations to study the effects of stoichiometry and structure on properties such as propagation velocity and energy density."

"Uncharted" Territory

Using projection microstereolithography, the team fabricated a 3D microstructure with high stiffness and low weight in the form of a very small octet truss. This geometric configuration is the stiffest and



In a recent experiment, Livermore researchers fabricated a highly ordered thermite structure by combining two additive manufacturing techniques. They applied direct ink writing to build an aluminum lattice structure complete with void space. They then filled the void with copper oxide using electrophoretic deposition.

Scanning electron micrographs compare (left and middle) a single unit-cell octet truss and (right) a 3 × 3 × 3 array fabricated with projection microstereolithography.



lowest weight architectural arrangement for a mechanical structure. The singlematerial truss can be bound with other identical unit cells to create a bulk material with a precisely arranged lattice structure. Such materials occupy a new realm on Ashby material selection charts for stiffness and density.

In another project, the team developed lattice structures from two materials, arranging the void space such that the composite offered zero or graded thermal expansion but remained structurally sound. "By designing a structure with both high and low expansion materials, we can strategically place void spaces or small amounts of bending or twisting in a local structural member to accommodate growth or shrinkage from temperature changes," says Spadaccini.

Materials that maintain their relative shape under extreme temperatures offer a variety of potential applications, for example, in weapons systems, thermalimaging diagnostics, energy technologies, and medical devices. Three-dimensional mesoscale structures with microscale features and restricted thermal behavior may also be beneficial in fusion energy experiments, such as those conducted at Livermore's National Ignition Facility, and in developing lightweight, high-strength materials for aerospace components.

A Boon for Manufacturing

Although the researchers are working on the three techniques in parallel, their goal is to integrate the strengths of each process into one technology that does it all. A streamlined fabrication method for producing 3D microstructured materials would benefit academia, scientific research, and the manufacturing industry. "With the ideal technology, users could upload a computer model of a component with an arbitrary shape and size and merely press a button," says Kuntz. "The machine would then build the part to precise specifications with no additional assembly required."

According to Spadaccini, a lower cost, highly efficient fabrication process could also improve the status of the U.S. manufacturing industry in the global market. As opposed to the standard assembly-line process in which several workers build components piece by piece, this tool would require only one skilled technician and one or two designers to develop the computer models. Spadaccini adds, "One way we can help make U.S. manufacturing competitive again is through more advanced fabrication methods."

By pushing the limits of additive manufacturing and material design, the team is demonstrating Livermore's scientific prowess. Says Spadaccini, "As a result of this effort, the Laboratory and our collaborators are becoming scientific and technological leaders in 3D fabrication and micromanufacturing of engineered materials." In providing a boon for the manufacturing industry and enabling previously unobtainable material properties, it is no wonder that these tiny 3D microstructures have such big possibilities.

-Caryn Meissner

Key Words: additive manufacturing, designer material, direct ink writing, electrophoretic deposition, microstructure, projection microstereolithography.

For further information contact Chris Spadaccini (925) 423-3185 (spadaccini2@llnl.gov).

Research Highlights

Friendly Microbes Power Energy-Producing Devices

Livermore researchers Fang Qian (left) and Michael Thelen display a canister of wastewater sludge, which contains plenty of organic nutrients and microorganisms. The team's solar-microbial energy device is designed to use this sludge to purify water.

THE tiniest living organisms on Earth could become key to addressing some of the world's biggest energy challenges. For decades, researchers have pursued energy generation by bacterial processes, most recently through the development and wider application of microbial fuel cells (MFCs), devices that convert biomass directly into electricity. These bioreactors are powered by select strains of bacteria capable of oxidizing organic matter and transferring electrons from their outer cell surface to an external electrode, thereby producing electrical current. But for all the ingenuity behind this technology, practical applications for MFCs have been limited because of the low efficiency of the bacterial energy conversion.

Livermore scientists are currently seeking ways to maximize microbial-based energy generation and develop novel applications for MFC technologies and the special bacteria that power them. Fang Qian, a scientist in the Physical and Life Sciences Directorate, is leading a study to demonstrate enhanced MFC performance using the *Shewanella oneidensis* MR-1 bacteria and a unique bioreactor design that incorporates carbon cloth electrodes with micro-size chambers. In experiments, the device yielded a power output of 250 nanowatts (billionths of a watt)—an order of magnitude increase in performance compared to most previously reported MFCs of similar dimensions.

MPT

Qian views this accomplishment as a first step toward developing new MFC technologies that integrate improved microbial metabolism with advances in materials science and fuel cells. Qian's goal is to design and build novel bioelectrical systems that combine a variety of renewable energy sources, including solar power. Ultimately, she aims to couple MFCs and solar cells to produce hydrogen, creating a hybrid system that supports more efficient and environmentally friendly energy production.



Electrogenic Bacteria Fuel Bioreactors

MFC technologies use a relatively rare type of bacteria known as electrogenic bacteria, which transfer excess electrons produced by their central metabolism to the cell surface. "Most bacteria use organic compounds as nutrients, oxidizing the carbon source and generating electrons," Qian says. "But most of these bacteria are insulators—they generate electrons but do not release them. They are needed in biosynthetic processes to produce biomass. Electrogenic bacteria have developed unique types of transmembrane proteins that deliver unused electrons to the outside, one by one."

This characteristic makes electrogenic bacteria excellent candidates for use in electricity-generating devices. MFCs use a pair of battery-like terminals (anode and cathode electrodes) connected to an external circuit and an electrolyte solution to conduct electricity. When bacteria physically attach to the anode, electrons generated in the interior of the cell are transferred to an external electrode, producing electrical current.

"Because bacteria are some of the oldest living systems on the planet, they have invented ways to interact with the environment very efficiently," explains microbiologist Michael Thelen, Qian's mentor at the Laboratory. "As an example, they are able to gain energy from minerals. We can exploit this process by isolating the bacteria and then examining their genes and the encoded proteins that are actively involved in the electron transfer."

Most of Qian's research into electron transfer pathways has focused on *Shewanella*, a dissimilatory metal-reducing bacteria considered a model microbe for fundamental research. The bacterium, which she used in the optimized micro-MFC study, is well understood and easy to identify, culture, and manipulate. But for all its great qualities, *Shewanella* is inefficient at generating power because it cannot completely oxidize organic compounds to maximize the energy extraction process. Moreover, a pure culture such as *Shewanella* always generates less power than do mixed cultures that contain a rich variety of microorganisms, including perhaps yet-unidentified electrogenic bacteria. Such microbial assemblies, or communities, can be found in natural environments or in municipal wastewater—a potential gold mine for bacterial prospectors like Qian and Thelen, who seek to improve MFCs.

Turning Wastewater into Drinking Water

Electrogenic bacteria exist in sludge, the by-product of wastewater treatment, which contains rich organic nutrients and diverse microbes that feed on them. While studying wastewater as a potential energy generator, the scientists realized that these clever microbes could do even more: They can purify water. To this end, Qian devised a method to inoculate MFCs with bacteria-filled sludge collected from a local water reclamation plant. The bacteria attached to the MFC anode, coating it with a biofilm that converts organic waste into carbon dioxide, producing electrical current while also reducing organic matter in the water. "We can consider this microbial fuel cell a multifunctional device," Qian says. "It produces energy and also treats wastewater. We hope to develop this technology and scale it up for broader use."

The research, funded by the Laboratory Directed Research and Development Program, is a collaboration with the University of California at Santa Cruz and the Livermore Water Reclamation Plant. During the first year of the project, Qian and her colleagues have designed different devices that can generate electricity from wastewater. Once they achieve a self-sustaining, continuous-flow system in a laboratory setting, they plan to scale up the device to operate continuously in the water plant. By the end of this year, the team wants to produce hydrogen from wastewater as well, which would add value to the water reclamation process.

More importantly, Qian's research with bacterial communities could lead to the discovery of new, more efficient strains of electrogenic bacteria. Scientists are constantly searching for microbes with performance characteristics that will improve the bacterial-colonizing anode. As microbes are found, their genomes can be sequenced for optimizing future microbial technologies. "Our research could open up a whole new world for bioenergy applications," says Thelen.

Adding a Solar Device

While working on the wastewater purification project, Qian devised another ingenious application for MFCs. The system uses bacteria, wastewater, and sunlight to produce clean, renewable energy. The hybrid device integrates an optimized MFC with a photon-absorbing semiconductor to convert light to electrical current. The result is a solar-driven microbial photoelectrochemical cell that Qian anticipates will harvest solar light and recycle biomass, generating hydrogen in a self-sustained way while simultaneously purifying water. "No one has developed a way to couple a semiconductor photocathode and a microbial anode and have them work together synergistically," Qian says. "This innovation is really exciting in terms of fundamental science."

The hybrid system takes advantage of the best features of both technologies. Semiconductors transfer electrons at a much faster rate than microbial systems do, but most semiconductors need additional external electrical input to work as photoelectrodes. "Fang's idea was to couple the two systems so that the bacteria will provide that extra energy," says Thelen.

For now, the solar-driven microbial reactor is not envisioned as a competitor to solar cells because microbial systems are intrinsically slower than semiconductors. Instead, the team would like to use this device to enhance the capabilities of water



Livermore's hybrid solar-microbial energy device is designed to recover energy from the Sun and wastewater. The microbial fuel cell chamber (left) contains a bioanode, where electrogenic bacteria thrive and extract electrons from organic nutrients in wastewater. A cuprous oxide photocathode in the photoelectrochemical chamber (right) works with the anode to produce hydrogen. In this laboratory setup, the device is mounted to a solar simulator to mimic energy from the Sun.

reclamation plants and to sow the seeds of future research. "Microbes are easy to work with and they reproduce," says Thelen. "Just give them a little food, which we can get from sludge, and we have an infinite supply."

While applications for MFC technologies are still in their infancy, Qian's creative uses of electrogenic bacteria for energy harvest and environmental applications are providing a glimpse into their future potential. One day, solar-driven devices that incorporate microbial photoelectrochemical cells may be useful on military bases or in other operations that necessitate the transport of water to remote facilities. Having the capability to treat and purify water locally in such environments could prove extremely valuable. In the meantime, the research conducted at Livermore is improving our fundamental understanding of key processes at the interface of biology, environmental science, nanotechnology, genetics, and other disciplines that will define science in this century.

-Monica Friedlander

Key Words: bioanode, electrogenic bacteria, microbial fuel cell (MFC), *Shewanella oneidensis* MR-1, solar-driven microbial photoelectrochemical cell, transmembrane protein.

For further information contact Fang Qian (925) 424-5634 (qian3@llnl.gov).

Chemical Sensor Is All Wires, No Batteries

Sensor technology keeps advancing with the development of smaller and smaller sensors that have higher and higher sensitivities. However, when it comes to conventional chemical detectors, most (if not all) still require a power source, that is, a battery, and therein lies a challenge. Battery-powered sensors require regular maintenance and replacement, making them problematic for field use. And, with sensors shrinking in size, the power source is often larger than the sensor itself, which defeats the purpose of miniaturization.

Fortunately, Livermore materials scientist Morris Wang and colleagues have found a way to bypass the power source requirement. Their "batteryless" nanosensor can identify different chemical species in less than a second, giving it potential for homeland security and medical applications.

Scientific Serendipity at Work

Wang and former colleague Xianying Wang (a visiting scientist from the University of Shanghai for Science and Technology) stumbled across the batteryless nature of nanowires while conducting tests for energy conversion applications. The scientists had embedded zinc-oxide (ZnO) nanowires in a polymer responsive to environmental conditions such as humidity and temperature. Changing conditions cause the polymer to swell or shrink, which in turn puts a force on the nanowires. Because the ZnO nanowires are piezoelectric, applying a force induces a voltage in the wires. On this particular day, the scientists were dripping solvents on the polymer to make it swell and stretch the nanowires. After applying ethanol, they saw an unexpected voltage spike—a far greater blip than the swelling mechanism would cause. The batteryless nanowire sensor is sensitive, fast, and small—about 2 millimeters long—and could be the basis of a small-scale handheld chemical detector.

On seeing the strong signal, Livermore's Wang thought something odd might be going on. He explains, "I always tell my postdocs that getting unusual, unexpected, or abnormal experimental results can often be a very good thing. It may mean they have discovered something new. The weirder the results, the more exciting they may be. In this particular case, we had a very weird result." Upon further examination, they discovered that the nanowires—which poke out of the polymer base like teeny fingers—were interacting directly with the alcohol molecule.

From Alcohol to TNT

Using specialized Livermore facilities—including the Engineering Directorate's Center for Micro- and Nanotechnology and the Physical and Life Sciences Directorate's Nanoscale Synthesis and Characterization Laboratory—the team fabricated and tested two different platforms to verify their initial discovery. The first platform was fabricated from single-crystalline, vertically aligned ZnO nanowires. The second platform used silicon (Si) nanowires in a random tangle. "Zinc-oxide and silicon have proved to be good sensor materials," says Wang.

In the first platform, the 6- to 7-micrometer-long ZnO nanowires were infiltrated with a polyvinyl chloride polymer and etched with oxygen plasma, leaving exposed "fingers" about 0.1 to 0.5 micrometers tall. For the sensing experiments,

a gold–titanium film and silver paste were used to make the top and bottom electrical contacts. The scientists then monitored the change in electric potential on the two ends of the nanowire.

The second platform used randomly aligned Si nanowires up to tens of micrometers long. About 80 percent of the nanowire tangle was sealed with polymer, leaving the remaining 20 percent exposed. Gold-titanium film was evaporated on two opposite sides of the substrate as electrical contacts. In this system, scientists monitored the change in electrical potential between the exposed and unexposed nanowires.

The team experimented with more than 15 different organic solvents, including acetone, chloroform, toluene, and ethanol, by dripping each chemical onto a sensor at room temperature. With ethanol, for example, the electric voltage rose sharply, peaking at approximately 170 millivolts. The signal rise was almost instantaneous and decayed slowly to zero as the ethanol evaporated. Other solvents produced different characteristic signals, yielding voltage "fingerprints" for each substance.

Wang then worked with engineer Chris Spadaccini in the Center for Micro- and Nanotechnology to test the nanowire device on explosives such as TNT (trinitrotoluene) and RDX (1,3,5-trinitro-1,3,5-triazacyclohexane). The results were very encouraging. The sensor was able to distinguish between different types of chemical explosives, which offers many new possibilities. "The device is potentially very sensitive and fast," says Spadaccini. "In addition, because it is so small, it could be easily integrated into a handheld system." Alex Hamza, director of the Nanoscale Synthesis and Characterization Laboratory, also sees the future benefits of batteryless technology, adding, "Developing techniques to power sensors and other nanostructured devices is vitally important to furthering their widespread use."

How It Happens

The nanosensors take advantage of a unique interaction between a chemical species and the surface of a semiconductor nanowire. The interaction stimulates an electric charge between the two ends of the exposed, vertically aligned ZnO nanowires or between the exposed surfaces of a Si tangle. When chemical molecules attach to surface molecules of the nanowire, they induce a change in the charge distribution (density of the electrical charge) on the nanowire surface. This change produces a voltage between the ends of the nanowires, generating a measurable electric signal.

To better understand what was happening at the atomic level, Wang turned to physicists Daniel Aberg and Paul Erhart in the Physical and Life Sciences Directorate. Aberg and Erhart focused on the chemisorption effects of the ethanol molecule to look for an



Chemical sensor designs use (a) zinc-oxide (ZnO) nanowires aligned vertically in a polymer sealant and (b) silicon nanowires in a tangled, randomly aligned formation, partially in sealant. Scanning electron micrographs show (c) ZnO nanowires and (d) a silicon nanowire tangle. In each system, chemical molecules cause changes in the charge distribution of the nanowire surface, producing a detectable electrical signal. explanation. In chemisorption, a chemical coats an exposed surface of a material, and the chemical and surface molecules create new electronic bonds. This process results in a new chemical species that forms a thin surface film, sometimes only one molecule thick. Corrosion and oxidation are two common products of the chemisorption process.

Aberg and Erhart used HERA, a large-capacity Linux cluster in Livermore's Open Computing Facility, to run quantum mechanical calculations on detailed interactions at the atomic level. Results from the calculations indicated that the ethanol molecule had a negative adsorption energy when interacting with the top or side surfaces of the ZnO molecule. Aberg and Erhart experimented with a dozen or so different positions before determining the lowest energy level for the system. In this state, the oxygen atom in ethanol bonds with a zinc atom in the nanowire. Another bond (a hydrogen-bridge bond) forms between a hydrogen atom in ethanol and an oxygen atom in the nanowire.

The researchers also found that the degree of detection sensitivity is linked to the polarity of the molecules involved. "Signal strength is directly tied to the dipole moment of the



In the lowest energy configuration of ethanol on ZnO nanowires, a chemical bond forms between the oxygen (red) atom in ethanol and a zinc (blue) atom, and a hydrogen-bridge bond forms between a hydrogen atom (white) of ethanol and an oxygen atom of the ZnO molecule. Yellow halos indicate the electron density, which is a measure of the probability of an electron occupying an infinitesimal element of space surrounding any given point. (Violet dots indicate carbon atoms in the ethanol molecule.)

molecule," says Wang. Many molecules have a dipole moment, which is a function of the molecule's asymmetric electrical nature. Water, for example, has a negatively charged oxygen atom at one end and two positively charged hydrogen atoms at the other. As a result, water molecules have a different charge at each end, and thus a polarity, much like the negative and positive poles of a battery. When molecules with a given dipole moment attach to a surface created of molecules that also have a dipole moment, the attaching molecules bind in a preferred direction. "The strength of the signal is determined by the dipole moment of the attaching chemical species and the surface area of the nanowire," says Wang.

Charging Forward with Batteryless Nanowires

Work will continue on refining the structure's detection of chemicals in liquids and on other aspects of the device as well. Jianchao Ye from the University of Shanghai for Science and Technology is on a one-year assignment at Livermore to help further develop the nanowire sensor. Ye, whose Ph.D. studies focused on the microscale mechanical characterization of metallic glasses, will investigate the device's sensitivity to very small amounts of chemical species, probably down to the parts-permillion scale, and look for ways to improve sensitivity. "One possible approach is to increase the surface area exposed to the chemical," says Ye. He also will explore the selective detection of certain biomolecules, a process which may be possible with some surface modifications to the ZnO nanowires. Ultimately, this work may lead to miniaturized sensor devices that are energy efficient and ecofriendly. "The beauty of this research lies in discarding an external power source," Ye notes. "Also, because zinc-oxide nanowires possess both semiconducting and piezoelectric properties, we hope to develop a nanosystem that has both sensing and actuation functions."

Batteryless, small, fast, inexpensive, and simple, these nanosensors are on their way to "electrifying" the chemical sensor field. The sensors made the inside cover of *Advanced Materials* last year, and commercialization of the technology is a possibility. Born out of researchers' willingness to explore an out-of-place result from a different experiment, the batteryless chemical nanosensor is proof that it pays to heed scientific serendipity and see where the unexpected may lead.

-Ann Parker

Key Words: battery, batteryless, Center for Micro- and Nanotechnology, chemical detector, chemical sensor, homeland security, medicine, nanoscience, nanowire, power source, semiconductor.

For further information contact Yinmin (Morris) Wang (925) 422-6083 (wang35@llnl.gov).

In this section, we list recent patents issued to and 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.

Patents

Laser Diode Package with Enhanced Cooling Robert J. Deri, Jack Kotovsky, Christopher M. Spadaccini

U.S. Patent 8,018,980 B2

September 13, 2011

This package includes a reservoir filled with a fusible metal in close proximity to a laser diode. The metal absorbs heat from the laser diode and undergoes a phase change from solid to liquid. Once the laser diode is turned off, the liquid metal cools and resolidifies. The reservoir is designed such that the metal does not leave the reservoir even when in a liquid state. The laser diode assembly also includes a lid with one or more fin structures that extend into the reservoir and contact the metal.

Local–Global Alignment for Finding 3D Similarities in Protein

Structures

Adam T. Zemla U.S. Patent 8.024.127 B2

September 20, 2011

This method can be used to locate three-dimensional (3D) similarities in the protein structures of two molecules. Selected information about the two molecules is compared using three approaches: longest continuous segments analysis, global distance test analysis, and local global alignment scoring function analysis. The constructed alignment is then verified, and the steps are repeated to find the regions of 3D similarities in protein structures.

Colorimetric Chemical Analysis Sampler for the Presence of Explosives

Peter J. Nunes, Joel Del Eckels, John G. Reynolds, Philip F. Pagoria, Randall L. Simpson

U.S. Patent 8,025,856 B2 September 27, 2011

A device that detects explosives has a container filled with an explosivesdetecting reagent. A dispenser delivers the reagent to a lateral flow swab unit connected to the container.

Particle Measurement Systems and Methods

Paul T. Steele

U.S. Patent 8,031,339 B2 October 4, 2011

In this system, a sampling mechanism directs a particle through the light fringes generated by a light source. At least one detector then measures the light scattered as the particle passes through the fringes. A method for generating the fringes, directing the particles, and detecting the scattered light is also described.

Dual Resolution, Vacuum Compatible Optical Mount

John Michael Halpin U.S. Patent 8,031,417 B1

October 4, 2011

This mount for an optical element includes a mounting plate, a lever arm pivot, and an adjustment plate. A flexure pivot mechanically couples the adjustment plate to the mounting plate and a lever arm. An adjustment device extending from the adjustment plate contacts the lever arm. A projection of a line from the first contact point to a pivot point, measured along the lever arm, is a first predetermined distance. A second adjustment device extends from the adjustment plate to a second contact point on the lever arm. A line projected from the second contact point to the pivot point, measured along the lever arm, provides a second distance, which is greater than the first distance.

Transparent Ceramics and Methods of Preparation Thereof Joel P. Hollingsworth, Joshua D. Kuntz, Zachary M. Seeley, Thomas F. Soules

U.S. Patent 8,039,413 B2

October 18, 2011

Oxide particles suspended in a solvent are added to a mold and uniformly cured to form a transparent ceramic preform. The suspension includes a dispersant but no gelling agent. A mixture that includes inorganic particles, a solvent, and a dispersant can also be created without a gelling agent. The inorganic particles have a mean diameter of less than about 2,000 nanometers. The mixture is agitated, added to a mold, and cured at a temperature of less than about 80°C to form a preform. Other methods for forming transparent ceramic preforms are also described.

Catalyst for Microelectromechanical Systems Microreactors

Jeffrey D. Morse, David A. Sopchak, Ravindra S. Upadhye, John G. Reynolds, Joseph H. Satcher, Alex E. Gash U.S. Patent 8,057,988 B2

November 15, 2011

In this system, a microreactor has a silicon wafer with multiple microchannels that are coated with a catalyst. In one arrangement, the catalyst is made of a nanostructured material. In other setups, it is made of an aerogel, a solgel, or carbon nanotubes.

Multiplexed Photonic Membranes and Related Detection Methods for Chemical and/or Biological Sensing Applications Sonia E. Letant, Tiziana C. Bond

U.S. Patent 8,059,924 B1

November 15, 2011

A photonic detection system has a flow-through photonic membrane with pores distributed along multiple regions. One type of target-specific anchor is attached to the pore walls in the first region, and another type is attached to the pore walls in the second region. The system can also include a pore region without anchors, so that optical detection occurs differentially. In a stack of photonic membranes, the pore diameter of one membrane is larger than that of the membrane in the next layer. Thus, the size of a target organism can be determined as it flows through the membrane stack.

Ultrafast Chirped Optical Waveform Recorder Using Referenced Heterodyning and a Time Microscope Corey Vincent Bennett

U.S. Patent 8,064,065 B2

November 22, 2011

A new technique can capture both the amplitude and phase of an optical waveform. Signals with many terahertz of bandwidths can be captured in a single shot (for example, at a temporal resolution of about 44 femtoseconds), or the process can be operated repetitively at a high rate. That is, each temporal window (or frame) is captured as a single shot in real time, but the process may be run repeatedly or only once. This invention expands on previous work in temporal imaging by adding heterodyning, which can be self-referenced for improved precision and stability, to convert frequency chirp (the second derivative of phase with respect to time) into a time-varying intensity modulation. Various demultiplexing techniques can be included to scale the process for recording continuous signals.

Computerized Method and System for Designing an Aerodynamic Focusing Lens Stack

Eric Gard, Vincent Riot, Keith Coffee, Bruce Woods, Herbert Tobias, Jim Birch, Todd Weisgraber

U.S. Patent 8,065,119 B2 November 22, 2011

A computerized system for designing an aerodynamic focusing lens stack uses input factors such as the particle size range to be considered, characteristics of the gas that will flow through the system, the upstream temperature and pressure at the top of a first focusing lens, the flow rate through the aerodynamic focusing lens stack equivalent at atmosphere pressure, and a Stokes number range. Based on the design parameters, the system determines the total number of focusing lenses and the respective orifice diameters required to focus the particle size range to be considered. The system calculates the orifice diameter of the first focusing lens in the Stokes formula. It then uses that value to determine, in iterative fashion, the intermediate flow rates required to calculate the orifice diameters of each succeeding focusing lens in the stack design. The results are output to a designer. The Reynolds numbers associated with each focusing lens and exit nozzle size may be calculated to enhance the stack design.

Hyper Dispersion Pulse Compressor for Chirped Pulse Amplification Systems Christopher P. J. Barty U.S. Patent 8,068,522 B2

November 29, 2011 A grating pulse compressor configuration is introduced to increase the optical dispersion for a given footprint and to make practical the application for chirped-pulse amplification to quasi-narrow bandwidth materials, such as neodymium-doped yttrium-aluminum-garnet. The configurations often use cascaded pairs of gratings to increase angular dispersion by an order of magnitude or more. Increased angular dispersion allows for decreased grating separation and a smaller compressor footprint.

Methods of Using Ionic Liquids Having a Fluoride Anion as Solvents Philip Pagoria, Amitesh Maiti, Alexander Gash, Thomas Yong Han, Christine Orme, Laurence Fried

U.S. Patent 8,071,813 B2

December 6, 2011

In this method, a strongly hydrogen bonded organic material contacts an ionic liquid that has a fluoride anion for solubilizing the organic material. The ionic liquid is maintained at a temperature of about 90°C or less during the contacting. The method can also use an ionic liquid with an acetate or formate anion for solubilizing the strongly hydrogen bonded organic material. In this setup, the ionic liquid is maintained at a temperature of less than about 90°C.

Amorphous Metal Formulations and Structured Coatings for Corrosion and Wear Resistance

Joseph C. Farmer U.S. Patent 8,075,712 B2

December 13, 2011

This system uses an amorphous metal made of more than 11 elements to produce a corrosion-resistant coating on a structure. The apparatus includes a deposition chamber with a source that produces the composite spray and a system that directs the spray onto the surface to be coated.

Awards

David Fittinghoff of Livermore's Physical and Life Sciences Directorate and **Edward Moses**, principal associate director for the National Ignition Facility (NIF) and Photon Science, have been elected fellows of the **Optical Society of America** (OSA). The OSA fellow designation is awarded to members of distinction who have made significant contributions to the advancement of optics.

Fittinghoff was recognized for his "foundational work in optical field ionization using ultrashort pulses and innovative engineering in ultrafast optics and [for] outstanding contributions to OSA." He was one of the key developers of the frequencyresolved optical gating technique, which was designed to measure ultrashort laser pulses. Since 2000, he has served on numerous OSA committees.

Moses was cited for his "outstanding technical leadership of the construction, completion and use of the world's largest and most energetic laser system, the National Ignition Facility." He has 30 years of experience developing and managing complex laser systems and high-technology projects. Since his time as NIF project manager and now as principal associate director, Moses has been responsible for bringing NIF into full operation. He also serves as program director for the National Ignition Campaign.

Mike Dunne, director for the Laser Fusion Energy Program at Livermore, received the **2011 Excellence in Fusion Engineering Award** from **Fusion Power Associates** (FPA). FPA honored Dunne for his technical contributions to high-energy-density physics and laser facility design and operations and for his leadership on the Laser Inertial Fusion Energy project. A Laboratory employee since 2010, Dunne previously led the European laser fusion program, HiPER, a consortium of 26 institutions across 10 countries. He also served as director of the Central Laser Facility in the United Kingdom and spent 10 years at the Atomic Weapons Establishment in Aldermaston, England. FPA established the annual Excellence in Fusion Engineering Award in 1987 to honor individuals who have demonstrated technical accomplishment in fusion engineering and have the potential to become exceptionally influential leaders in this field of research.

Extending the Life of an Aging Weapon

A team of about 30 Livermore physicists, engineers, and chemists are working on the first phase of a projected 10-year effort to extend the service life of the W78 warhead, which is deployed on many U.S. Air Force Minuteman III intercontinental ballistic missiles. During the LEP's first phase, scientists and engineers explore a wide range of options and review the performance characteristics, manufacturing issues, and technical challenges associated with each one. They are also determining expected improvements in performance margins, identifying safety and security improvements, and predicting long-term maintenance and surveillance requirements. Throughout the W78 LEP, advanced simulations and nonnuclear experiments will play important roles. Engineers will ensure the mechanical robustness of the overall system and the complete integration of every component and system. The biggest Livermore Weapons Program effort of this decade, the W78 LEP is helping to maintain a knowledge pipeline by having the next generation of stockpile stewards work with mentors-the scientists and engineers who have conducted previous LEPs. Laboratory weapon scientists also bring their expertise to the W78 effort, building on their long-standing work to better understand the physics of plutonium by combining experiments with theoretical research and computer simulations. Contact: Hank O'Brien (925) 423-5017 (obrien6@llnl.gov).

Materials by Design

A material's properties and overall performance are determined by its chemical composition, crystalline state, and underlying microstructure. These characteristics force scientists to accept certain trade-offs when choosing a material for a specific application. With funding from the Laboratory Directed Research and Development Program and the Defense Advanced Research Projects Agency, a Livermore team is collaborating with academic partners to advance three additive manufacturing techniques to fabricate threedimensional (3D) microstructures. The three techniques-projection microstereolithography, electrophoretic deposition, and direct ink writing-create composite materials with properties that were previously unobtainable. The team recently demonstrated how the techniques could be used to improve the performance of thermite compositions and to create ultralightweight, high-strength materials and materials that exhibit zero or negative thermal expansion. These "materials by design" have many potential applications, including in weapons systems, thermal-imaging diagnostics, energy technologies, and medical devices. Ultimately, a streamlined, scalable process for producing bulk materials made from 3D heterogeneous, microscale structures would dramatically advance the additive manufacturing industry in the U.S.

Contact: Chris Spadaccini (925) 423-3185 (spadaccini2@IInI.gov).

Space-Based Traffic Cameras



In the STARE project, Livermore researchers are designing nanosatellites to more accurately determine the trajectory of space objects orbiting Earth.

Also in April/May

• Resonance ionization mass spectrometry improves the response time for nuclear forensics by eliminating much of the sample preparation required for isotope analysis.

• Livermore researchers find that a modest increase in the foam padding for Army helmets could better protect soldiers against head trauma.

• Laser experiments with thin films of aluminum provide an unprecedented look into the physics of shock waves traveling through a metal.

www.llnl.gov

Science & Technology Review Lawrence Livermore National Laboratory P.O. Box 808, L-664 Livermore, California 94551

PRSRT STD U.S. POSTAGE PAID San Bernardino, CA PERMIT NO. 3330

