Science and Technology UPDATE

July–Sep 2014

Science and Technology on a Mission

LLNL-MI-665261

LABORATORY CAPTURES FOUR R&D 100 AWARDS

LLNL received four awards in this year's R&D 100 competition, bringing to 152 the total number of awards LLNL has won in what is widely referred to as the "Oscars of invention." "These awards recognize the tremendous value of our national labs," said Secretary of Energy Ernest Moniz. "Research and development at the national labs continues to help our nation address its energy challenges and pursue the scientific and technological innovations necessary to remain globally competitive." The four winning technologies are as follows:

Portable kit for detecting explosives and drugs. A team of LLNL chemists developed a miniaturized, portable, thin-layer chromatography kit commercialized as **the product microTLC**, which can **detect and identify** explosives, illicit drugs, insecticides, pesticides, and other targets in samples. MicroTLC also won a 2014 award for technology transfer under the Federal Laboratory Consortium's Far West Regional Awards (see page 5).

High-precision spectrometer for identifying trace elements. The superconducting tunnel junction x-ray spectrometer can measure x-ray energies 10 times more precisely than current spectrometers based on silicon or germanium semiconductors. Built in conjunction with **STAR Cryoelectronics**, this **powerful tool can identify unknown substances** such as traces of evidence from crime-scene samples, impurities in computer-chip materials, and toxic metals in biomedical components. This advanced science and technology was developed over a long period, with early support from the Laboratory Directed Research and Development Program.

Faster, cheaper system for polishing laser optics. Optics for imaging systems, lithography, and fusion research at the National Ignition Facility can now be polished and finished more quickly and economically thanks to the **convergent polishing system**, which can finish flat and spherical glass optics in a single iteration, without operator intervention. This reduced-step technique achieves the precision optics industry's "Holy Grail" of convergence, comments an executive at a California precision optics company. This work was supported by the LDRD Program under **project 11-ERD-036**. The photo shows an LLNL optics polisher that incorporates the breakthrough method.

Beam-combining optical element. An optical technology named EXUDE (for "extreme-power, ultralow-loss dispersive element") enables the beams from many small lasers to be **combined into a single high-power beam**. Developed in partnership with Lockheed Martin Laser and Sensor Systems and Advanced Thin Films, EXUDE superimposes component beams into an electrically efficient, single-output system. A recent demonstration combined multiple fiber lasers into a single 30-kilowatt beam while maintaining excellent efficiency and beam quality, paving the way for advanced defense applications and material processing, such as cutting and welding.

About the Cover

A new material with a nanotubular structure achieves a high strength-to-weight ratio, overcoming a longstanding limitation of such materials. See "Ultralight, strong material on *Advanced Materials* cover," on page 11.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-7NA27344.

$7.8 MILLION GRANT FROM NIH FOR BIOMEDICAL RESEARCH

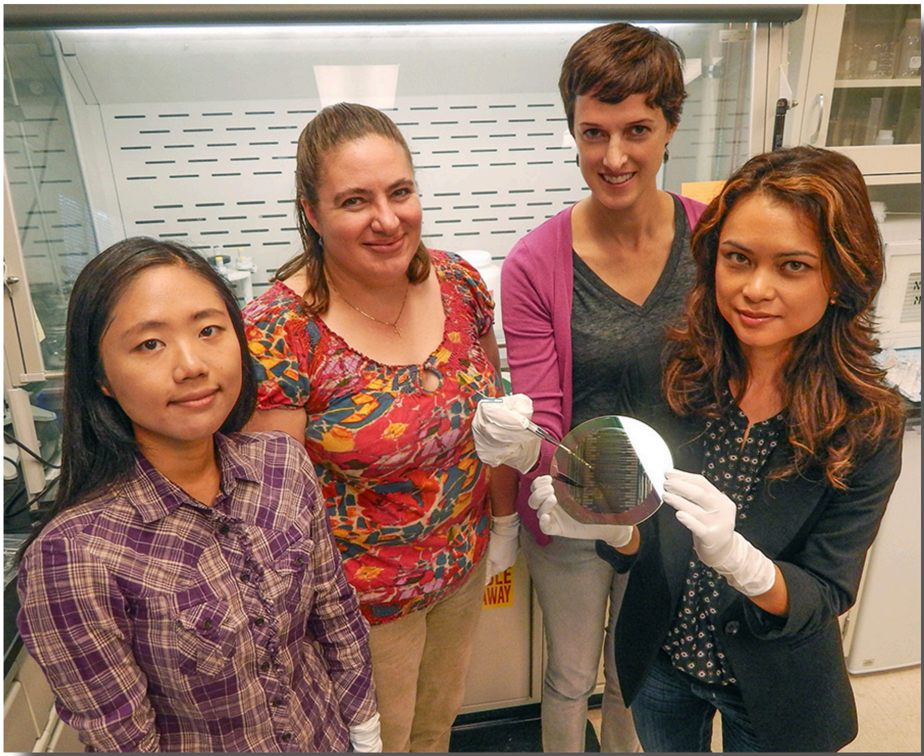
The National Institutes of Health (NIH) awarded a 5-year, $7.8 million grant for Lawrence Livermore to conduct biomedical research using the LLNL-pioneered technique of biological accelerator mass spectrometry (AMS). The work will be conducted by the Laboratory's **National Resource for Biomedical Accelerator Mass Spectrometry**, which currently collaborates with more than 60 medical centers, universities, and other entities around the world. The grant marks the fourth 5-year grant awarded over the past 15 years (the three others were in 1999, 2004, and 2009). This latest grant represents national recognition of Lawrence Livermore's leadership in biological AMS, including the recent development of a new system that is easier to operate and that can process liquid samples, bypassing the graphitization process. This new system now enables scientists to prepare and analyze samples in minutes instead of days. With the new grant, researchers will use the new system to **address important questions** in nutrition, toxicology, pharmacology, cancer research, drug development, and comparative medicine. They also hope to validate the new instrument for deployment to general clinical laboratories in about 5 years. In the photo, **Ted Ognibene** (center), a chemist who co-developed the technique enabling liquid samples, discusses operation of the instrument with biomedical scientist **Mike Malfatti**.

LABORATORY IN NEW PROJECT TO BUILD MOST COMPLETE EARTH SYSTEMS MODEL EVER

A new DOE-funded project will use high-performance computing to develop and apply the most complete climate and Earth system model to date to bolster research on climate change. Eight national laboratories, including Lawrence Livermore, are combining forces with the **National Center for Atmospheric Research** and others in the new effort. The project, Accelerated Climate Modeling for Energy (**ACME**), is being led by Livermore's own **Dave Bader** and is designed to accelerate the development and application of state-of-the-science Earth system models that can also support a broad range of scientific and energy applications. The initial focus will be on three climate change science drivers: water cycle (e.g., how the hydrological cycle and water resources interact with the climate system on local to global scales), biogeochemistry (such as how carbon, nitrogen, and phosphorus cycles regulate climate system feedback), and cryosphere systems (including whether a dynamical instability in the Antarctic Ice Sheet **could be triggered** within the next 40 years). Over a planned 10-year span, the project aims to conduct simulations and modeling on the most sophisticated supercomputers as they come online.

NIH Grant to Develop Electrode Array to Study Brain Activity

The National Institutes of Health (NIH) has awarded LLNL a grant to develop an electrode array system that will be used to help understand how the brain works. Lawrence Livermore's neural measurement and manipulation system—an advanced electronics system to monitor and modulate neurons—will be packed with more than 1,000 tiny electrodes embedded in different areas of the brain to record and stimulate neural circuitry. The goal is a system that will allow scientists to simultaneously study how thousands of neuronal cells in various brain regions work together during complex tasks such as decision making and learning. The project is a collaboration between Livermore's Neural Technology Group, the University of California–San Francisco, Intan Technology, and SpikeGadgets and is part of **NIH efforts to support** the White House's Brain Research through Advancing Innovative Neurotechnologies (**BRAIN**) Initiative, a new research effort to revolutionize our understanding of the human mind and uncover ways to treat, prevent, and cure brain disorders. (This grant follows an earlier award this year from the Defense Advanced Research Projects Agency to develop an implantable neural interface **to study post-traumatic stress disorder** and other ailments.) Early investments at LLNL to develop these electrode arrays were made by the Laboratory Directed Research and Development Program. In the photo, Lawrence Livermore's **Kye Lee**, **Angela Tooker**, **Sarah Felix**, and **Vanessa Tolosa** (left to right) hold a silicon wafer containing micromachined implantable neural devices.

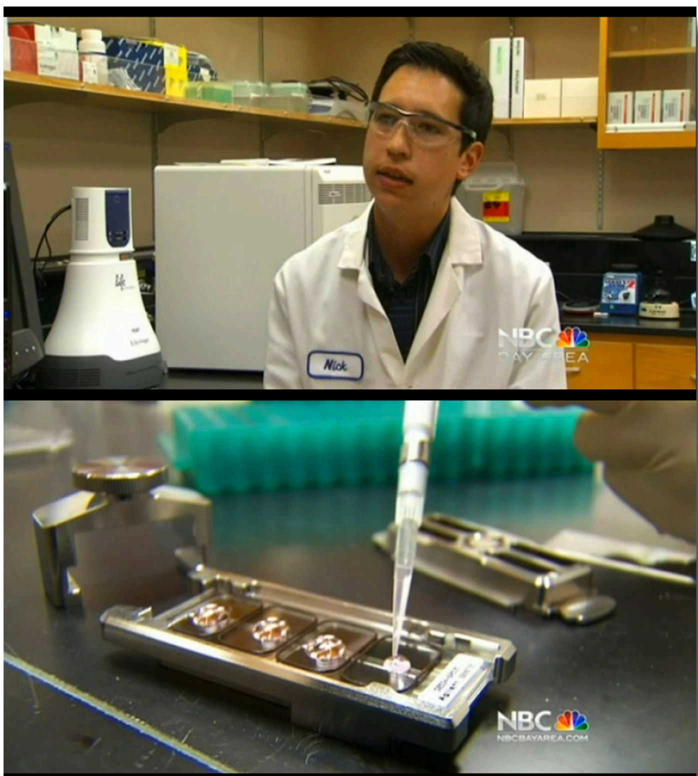


LLNL Researchers on List of "World's Most Influential Scientific Minds"

Lawrence Livermore scientists Charles Westbrook and William Pitz have been named to the Thomson Reuters list of "**The World's Most Influential Scientific Minds**." The list of 3,000 researchers was generated by analyzing citation data over the last 11 years to identify those ranking in the top 1 percent in citations in their subject area. Charles and William have published numerous research papers on combustion modeling, and their work has been incorporated into codes that simulate combustion in internal combustion engines—codes used by the auto industry and others to optimize engine design, increase efficiency, and reduce emissions. They also work on chemical kinetic code for biofuels and other next-generation fuels and simulations of advanced combustion engines for future vehicles. "This recognition is a great honor for Charlie Westbrook and Bill Pitz and extremely well deserved," said LLNL Director **Bill Goldstein**. "It also is indicative of the bright minds working together at Lawrence Livermore to solve some of the nation's most challenging problems."

MICROBIAL DETECTOR TOUTED AS POTENTIAL TOOL AGAINST EBOLA

The spate of media coverage of the recent Ebola outbreak included an NBC Bay Area **report on the potential use** of the Lawrence Livermore Microbial Detection Array (**LLMDA**) in the fight against the disease. "This is going to be faster and cheaper in most situations," says Livermore biomedical scientist **Nicholas Be** about the **already-licensed technology**. The story cites the LLMDA's 24-hour turnaround and the importance of doctors having such a tool, given the similarity of early Ebola symptoms to those of "the flu or a variety of other diseases" and because "the best chance at beating Ebola is by beginning treatment as soon as you've been exposed." The reporter concludes by commenting that the technology is currently "only being used for research, but if the FDA approves it, it could become a common test in hospitals all over the world." The screen captures show Nicholas Be being interviewed for the story and placing samples onto an LLMDA slide.



NUCLEAR ENGINEER ELECTED CHAIR OF ANS FUSION ENERGY DIVISION

LLNL nuclear engineer Susana Reyes has been elected chair of the American Nuclear Society's (ANS's) **Fusion Energy Division**. She has a long history of service with the ANS and won the society's **Mary Jane Oestmann Professional Women's Achievement Award** in 2012. Since joining the Laboratory in 2001 to work on the safety analysis of inertial fusion energy power plant designs, Susana has branched out into many other areas, with strong involvement in neutronics and materials damage simulations in support of high-energy accelerators and the National Ignition Facility (NIF). Her more than 12 years of experience in international fusion projects includes the U.S. ITER **Test Blanket Module**. From 2006 until early 2010, Susana took a leave of absence from LLNL to join the ITER Organization in Cadarache, France, to support the project by conducting and coordinating safety analyses and associated documentation in preparation for ITER licensing.

PROVIDING PROLIFERATION-PREVENTION AID IN TAJIKISTAN

Two Lawrence Livermore scientists—**Pejman Naraghi-Arani** and Jason Olivas—provided training and advanced technology for detecting foodborne pathogens to researchers in the Republic of Tajikistan, a mountainous, landlocked nation that borders Afghanistan to the south and China to the east. The effort was part of the National Nuclear Security Administration's Global Initiatives in Proliferation Prevention Program and **provided** molecular assays, instrumentation, and training on the use of the assays to detect pathogens from a variety of sources.

LLNL WINS THREE REGIONAL TECH-TRANSFER AWARDS

Lawrence Livermore scientists have been selected by the **Federal Laboratory Consortium** (FLC) for three awards for technology transfer in the FLC's Far West Regional Awards. The awards recognize the following technologies:

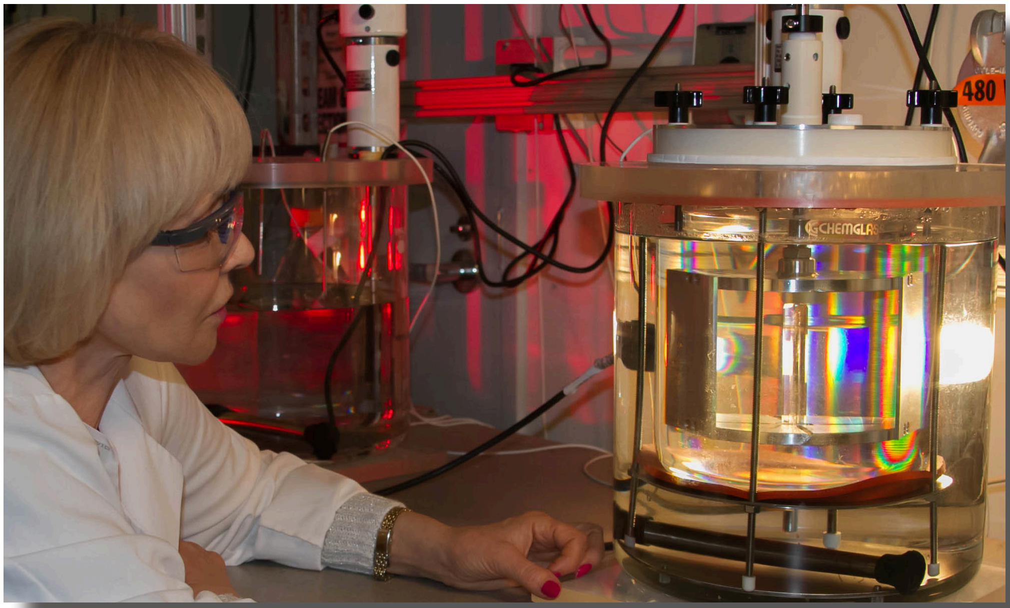
Portable kit for detecting explosives and drugs. A team of LLNL chemists developed a miniaturized, portable, thin-layer chromatography kit commercialized as the product **microTLC**, which can detect and identify explosives, illicit drugs, insecticides, pesticides, and other targets in samples. This technology also won an R&D 100 Award (see page 1).

Crystal for detecting nuclear materials. Working under a Department of Homeland Security (DHS) grant, a team of LLNL scientists developed technology to produce large-scale, **high-optical-quality stilbene crystals** for national-security applications. Their work, along with that of **licensee Inrad Optics**, was recognized as an "outstanding commercialization success." Inrad Optics also **won two awards** for its development of nuclear detection material licensed from LLNL, including an award from the DHS Domestic Nuclear Detection Office (see story on this page) for "exceptional contributions to advanced materials development for the neutron detection of nuclear materials." In the photo, LLNL **materials scientist Natalia Zaitseva**, a member of the winning team, examines a stilbene crystal.

Software tools for climate research. A partnership across government, academic, and private sectors has created a novel system that enables climate researchers to solve their most complex data analysis and visualization challenges. The Ultrascale Visualization Climate Data Analysis Tools (**UV-CDAT**) Project integrates more than 70 disparate scientific software packages and libraries for large-scale data analysis and visualization. This work was recognized by the FLC as an "outstanding partnership."

AWARD FROM DOMESTIC NUCLEAR DETECTION OFFICE

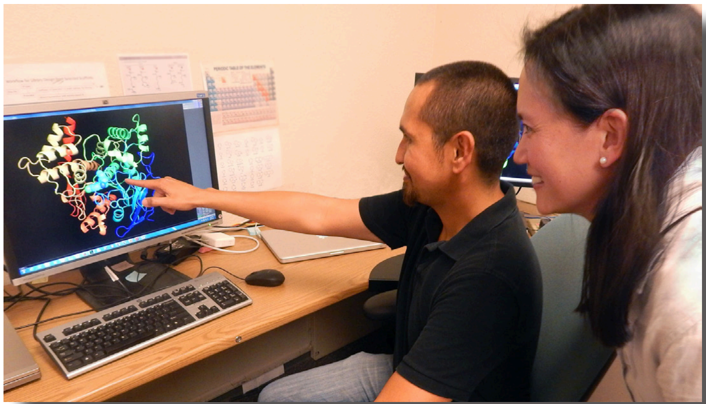
The Transformational and Applied Research Directorate of the Department of Homeland Security's Domestic Nuclear Detection Office (**DNDO**) has recognized **Natalia Zaitseva** and the Laboratory as a whole with the DNDO Award for Exceptional Performance. The award recognizes "exceptional support to the mission of DNDO" and was presented to Natalia at the plenary session of the **2014 Symposium on Radiation Measurements and Applications**, held in Detroit, Michigan, on June 10.

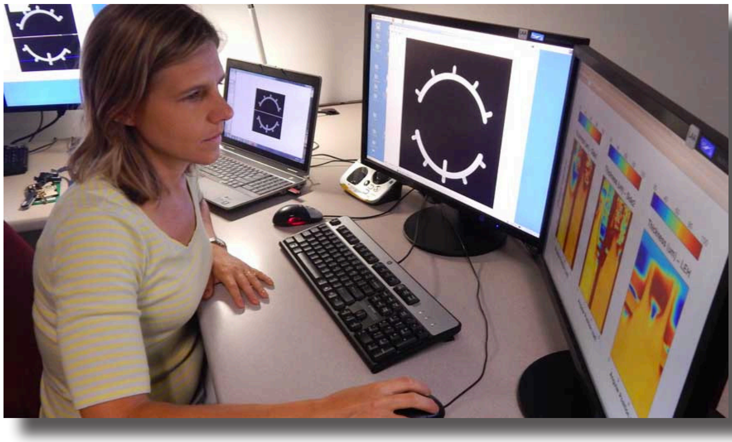


COMPUTATIONALLY PREDICTING ADVERSE REACTIONS TO DRUGS

Lawrence Livermore researchers have developed a computational technique that uses software running on **LLNL supercomputers** to determine whether a potential new drug could have adverse side effects in humans. Such side effects can be a significant public health issue and a source of major economic liability that inhibits future drug development. The LLNL team developed an algorithm that predicts whether a drug candidate could interact with important proteins in the human body. The team **published its findings in the journal *PLOS ONE***. "We need to do something to identify these side effects earlier in the drug development cycle to save lives and reduce costs," said Monte LaBute, the paper's lead author.

The paper describes how the team used the Livermore-developed program **VinaLC**, a parallelized version of **AutoDock Vina**, to dock 906 small-molecule drugs to a virtual panel of 409 protein targets. By comparing their results with those of FDA-approved drugs with known side effects, the team showed that in two categories of disorders their computational model delivers more-accurate predictions than are possible with current statistical methods. This achievement thus provides the drug industry with a cost-effective and reliable method to screen for side effects. Their goal is to expand their computational pharmaceutical research to include more off-target proteins for testing and eventually screen every protein in the body. "If we can do that, the drugs of tomorrow will have less side effects that can potentially lead to fatalities," says Monte. The photo shows Monte examining a docking simulation with team member **Felice Lightstone**.





CHEMICAL ENGINEER REPRESENTS LLNL AT NATIONAL SYMPOSIUM

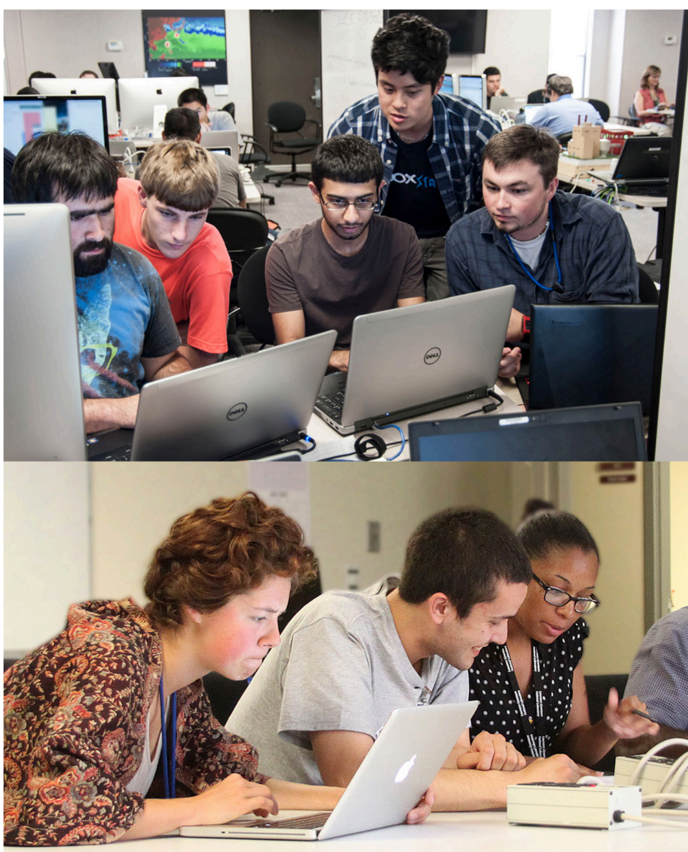
Chemical engineer Rebecca Dylla-Spears represented the Laboratory at the National Academy of Engineering's **2014 U.S. Frontiers of Engineering Symposium**. The event featured dozens of engineers from ages 30 to 45 who perform exceptional work in a variety of disciplines. Rebecca has been solving complex problems in support of the National Ignition Facility (**NIF**) for the past 4 years, including growing solid deuterium–tritium layers for ignition targets and an an R&D 100 Award-winning technology for polishing glass optics (see page 1). In the photo, Rebecca is inspecting a deuterium–tritium fuel layer for a NIF experiment.

IEEE YOUNG ACHIEVERS AWARD WON IN SCALABLE COMPUTING

Abhinav Bhatele received the 2014 Young Achievers Award from the Technical Committee on Scalable Computing of the Institute of Electrical and Electronics Engineers. Abhinav, whose work **has been supported by the LDRD Program**, was presented with his award at this year's Supercomputing Conference, held in New Orleans. The award recognizes up to three individuals each year who have made outstanding, influential, and potentially long-lasting contributions in the field of scalable computing within 5 years of receiving a Ph.D. degree.

STUDENTS GET DYNAMIC INTRODUCTION TO CYBER SECURITY

The Laboratory's **Cyber Defenders Student Program** was established in 2009 to provide hands-on training to potential future cyber security experts. This summer's 30 participants were selected from a pool of 580 applicants and include undergraduates, graduate students, and even professors representing science, engineering, and humanities programs at institutions across the nation. Working closely with LLNL mentors, participants develop skills in areas such as detecting and preventing intrusion and writing algorithms for network monitoring and analysis. One of the program's highlights is the Tracer Fire competition, **held this year** from July 22 to 24 at the **High-Performance Computing Innovation Center** on the Livermore Valley Open Campus. Teams race to complete computer security challenges that test skills such as code breaking and network engineering. "Our goals for the program," says Celeste Matarazzo, who founded and co-leads the program, "are to excite people about the range of activities available in cyber security, to ensure that they leave the program with really strong skills, and to build a pipeline of skilled candidates for jobs here, at other national laboratories and in government services."



TEACHING UC BERKELEY COURSE ON RARE-EVENT DETECTION

Livermore's Adam Bernstein has begun teaching a graduate course entitled "Rare Neutral Particle Detection in Fundamental and Applied Physics" in the UC Berkeley Nuclear Engineering Department. Twenty-five students have enrolled, including five physics graduate students and several undergraduates. Throughout the semester, guest lectures will be given by other members of LLNL's Rare Event Detection Group and other Livermore experts in radiation detection, introducing students to a range of ongoing LLNL research activities. The goals of the class, which will train students in experimental radiation detection methods common to both fundamental nuclear science and nuclear security, are well matched to the ongoing UC Berkeley–national laboratory partnership known as the **Nuclear Science and Security Consortium**, which seeks to prepare a new generation of experts in nuclear science and security for work in the national nuclear laboratory complex.

LIVERMORE ORGANIZES PLUTONIUM FUTURES CONFERENCE

Lawrence Livermore hosted the "Plutonium Futures: The Science 2014" conference, held September 7–12 in Las Vegas, NV. This was the eighth conference in the biennial series, which brings together people of diverse disciplines to provide an international forum for discussion of current research on the physical, chemical, and mechanical properties of plutonium and the technological implications of those properties. This year's conference drew approximately 250 attendees, who were welcomed by LLNL Director **Bill Goldstein** in his conference-opening address. The American Nuclear Society is the official conference sponsor, but the organizational committee, which is currently chaired by LLNL scientists **Kerri Blobaum** and **Scott McCall**, determines the agenda and selects speakers.

Partnership with Georgetown Greatly Expanded

LLNL Director **Bill Goldstein** and Georgetown University President John DeGioia signed a memorandum of understanding that renews and significantly expands a partnership entered into in 2009. The new memorandum represents a framework to broaden university-wide collaborations with Georgetown, including the Georgetown University Medical Center, and expands the fields of study to encompass data science and data analytics; biosecurity; emergency and disaster management; global climate, energy, and environment; food safety and security; and biotechnology—including infectious diseases, drug discovery, regenerative medicine, and urban resilience. The LLNL–Georgetown partnership has already achieved successes such as the launch in 2013 of a **master's program in emergency and disaster management**. Livermore has also worked with Georgetown to establish a biotechnology seminar series and host summer interns in the university's **biotechnology master's program**.

Co-Chairing International Detonation Symposium

The **15th International Detonation Symposium** was co-chaired by Lawrence Livermore's Jon Maienschein—director of the Energetic Materials Center—and the leader of the Naval Surface Warfare Center's Indian Head Division. Held in San Francisco, CA, on July 13–18, the conference was attended by over 300 scientists and engineers from 17 countries and featured presentations and discussions about the latest developments in detonation science and explosive hazards response. Of the over 180 oral and poster presentations, 39 were delivered by 44 scientists and engineers from LLNL. This presence represented the largest delegation from any organization, reflecting LLNL's international leadership in the field of detonation science. The symposium, which began in 1951 and is held roughly ever four years, is considered the preeminent international venue for detonation science.

Scientists Lead Gordon Conference and Seminar on High-Pressure Research

Lawrence Livermore staff organized and led both the 2014 **High-Pressure Gordon Conference** (chaired by **Gilbert "Rip" Collins**) and its associated 2014 High-Pressure Gordon Research Seminar (co-chaired by **Rick Kraus**). Both events were held at the end of June at the University of New England in Biddeford, Maine. One hundred and fifty of the leading researchers in high-pressure science from around the world attended the conference, while 60 postdocs and students attended the seminar. At both events, the presentations included announcements of several new discoveries related to the high-pressure behavior and properties of hydrogen, water, dense phases of silica, high-temperature superconductors, and other systems.

Laboratory's Role in Medical Technology Transfer Showcased at Forum

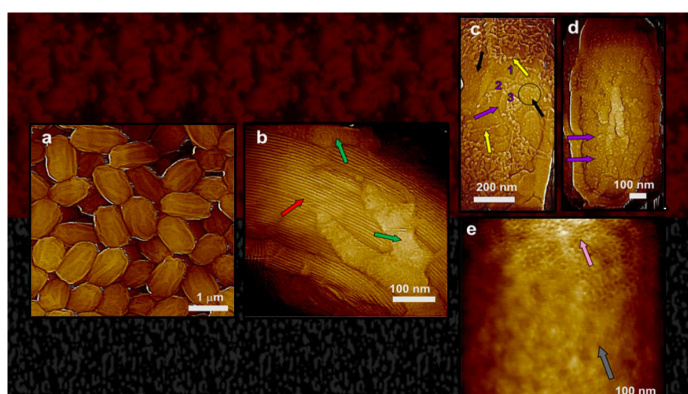
The Laboratory participated in the sixth annual **Innovation Tri-Valley Forum**, held July 23 in Pleasanton, California. This year's theme was the wealth of medical innovation in California's Tri-Valley area, with a spotlight on Livermore and Sandia National Laboratories "as a nexus for innovative medical devices and technology." Two panel discussions and a keynote speaker explored how partnerships with the two national laboratories can lead to innovation in medical technology and create a path to high-quality medical care. **Betsy Cantwell**, the Laboratory's director for economic development and one of the panelists, discussed LLNL's long history in biosciences, beginning with research on ionizing radiation that has since morphed into "a wealth of intellectual property." She stated that "economic value and technology transfer underwrite our national security. They are part of our mission, part of our DNA." She also stressed that "the Lab is always looking for partnerships," whether with Federal, academic, or industrial partners. Donald Bitting, program director for IBM Research Development, and Rich Stump, co-founder of **FATHOM**—the Bay Area's largest 3D printing production center—discussed their work with Lawrence Livermore. In addition, the Laboratory had a booth showcasing LLNL technologies such as **Cardioid**, the **Lawrence Livermore Microbial Detection Array**, and the **artificial retina**.

NIF COMPRESSES DIAMOND TO JUPITER-LIKE DENSITIES

The achievements by a team of LLNL researchers and colleagues from UC Berkeley and Princeton University who used the National Ignition Facility (NIF) to **compress diamond to the density of lead** are featured on the cover of the July 17 edition of *Nature*. As indicated by the accompanying headline—"Inside Jupiter: The Giant Planet's Interior Replicated at the U.S. National Ignition Facility"— the team's results will help validate not only first-principles density functional theory but also theories that have long been used—but not yet experimentally validated—to describe matter in the interiors of giant planets, stars, and inertial-confinement fusion experiments. At NIF, a sample of diamond was ramp compressed to a peak pressure 14 times greater than pressure at Earth's center. Such pressures have been reached before in diamond, but only in shock experiments, which are not relevant to planetary interiors because of the very high temperature to which the sample is heated. The unprecedented conditions attained in these NIF experiments provide new constraints on the equation of state of carbon at pressures more than 30 times that of previous static-compression measurements.

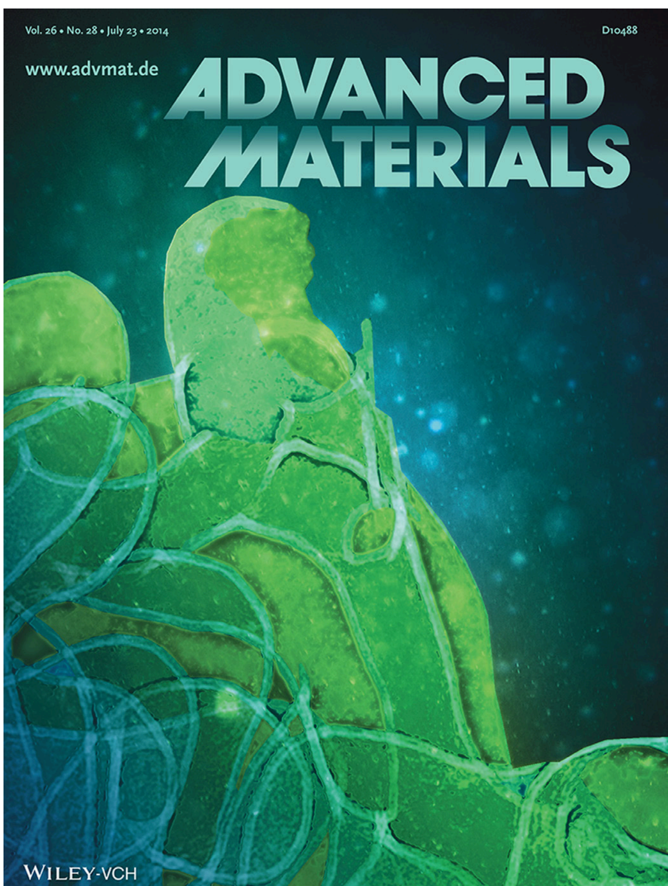
PAPER REVEALS NEW ASPECTS OF SPORE ARCHITECTURE

LLNL scientist **Alexander Malkin** and his team have discovered additional layers of a bacterial spore commonly found in soil and the human gut. This finding, **published in the journal *PLOS One***, may provide insight into how this organism develops, spreads, and survives in extreme conditions. Using high-resolution atomic force microscopy, the team studied the spore coats of *Bacillus subtilis* and found that in addition to the four known layers of the organism, the coats also contain a fibrous layer and a layer of "nanodot" particles. This finding allowed the team to formulate an improved model of the coat structure, which will improve our understanding of how this bacterium functions. This work, conducted with researchers at the University of Connecticut Health Center, was funded by the LLNL's Laboratory Directed Research and Development Program and with additional Federal funding. The figure shows high-resolution visualizations of the various spore coat structures, with yellow and black arrows marking the newly discovered dense fiber structural layer and nanodots, respectively.



ULTRALIGHT, STRONG MATERIAL ON *ADVANCED MATERIALS* COVER

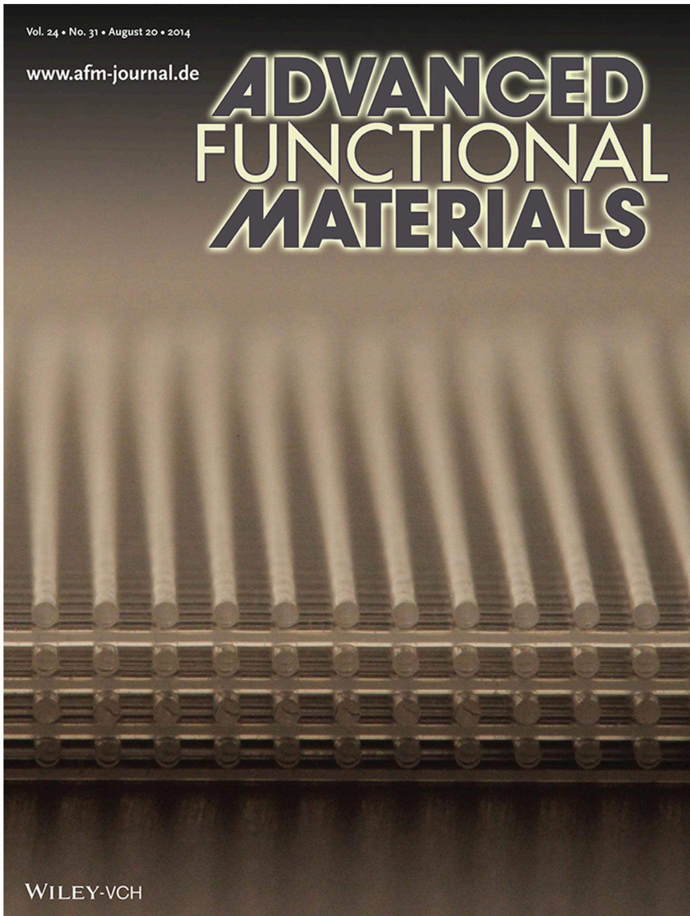
In **a paper featured on the cover of *Advanced Materials***, lead author **Monika Biener** and her Livermore colleagues report their success in synthesizing new ultralow-density, ultrahigh-surface-area bulk materials with an interconnected, nanotubular structure. This structure makes possible a high strength-to-weight ratio that overcomes a longstanding disadvantage of such ultralow-density materials, unlocking their potential for broad-ranging applications. The paper's authors developed an atomic layer deposition method using a tunable substrate of nanoporous gold. Their approach allows control over the material's density, pore size, and composition. With their narrow, tightly constrained pore-size distributions and thin-walled design, the resulting materials are 10 times stronger and stiffer than traditional aerogels of the same density, and are also thermally stable. The new technique can easily be extended to other atomic layer deposition processes and to other substrates. One possible use is enabling mass transport through two independent pore systems separated by a nanometer-thick three-dimensional membrane, which would have applications in fields such as energy harvesting, catalysis, sensing, and filtration. This work was supported by Livermore's Laboratory Directed Research and Development Program under **project 13-LW-031**, which was also led by Monika.



CALCULATIONS IN *PRL* FIRST TO PRESERVE QCD SYMMETRY IN BIRTH-OF-THE-UNIVERSE SCENARIO

In **a paper published in the August 18 edition of *Physical Review Letters***, Lawrence Livermore scientists present their calculations of the properties of a quantum chromodynamics (QCD) phase transition that occurred when the Universe was less than one microsecond old. (In the transition, a plasma of quarks and gluons formed into bound states of quarks—the protons and neutrons that make up most of the visible Universe.) The team is now the first to perform the calculation in a way that preserves a certain fundamental symmetry of QCD known as chirality. Livermore's Chris Schroeder, Ron Soltz, and Pavlos Vranas conducted the work as part of the Livermore-led **HotQCD Collaboration**, which also involves Los Alamos and Brookhaven National Laboratories, the Institute for Nuclear Theory, Columbia University, the Central China Normal University, and Germany's Universität Bielefed. The extremely computationally intensive calculation was performed on Livermore's 5-petaflop supercomputer, Vulcan, with **support from the Laboratory Directed Research and Development Program** and the **Grand Challenge Program**.

ADDITIVE MANUFACTURING YIELDS ENERGY-ABSORBING MATERIAL



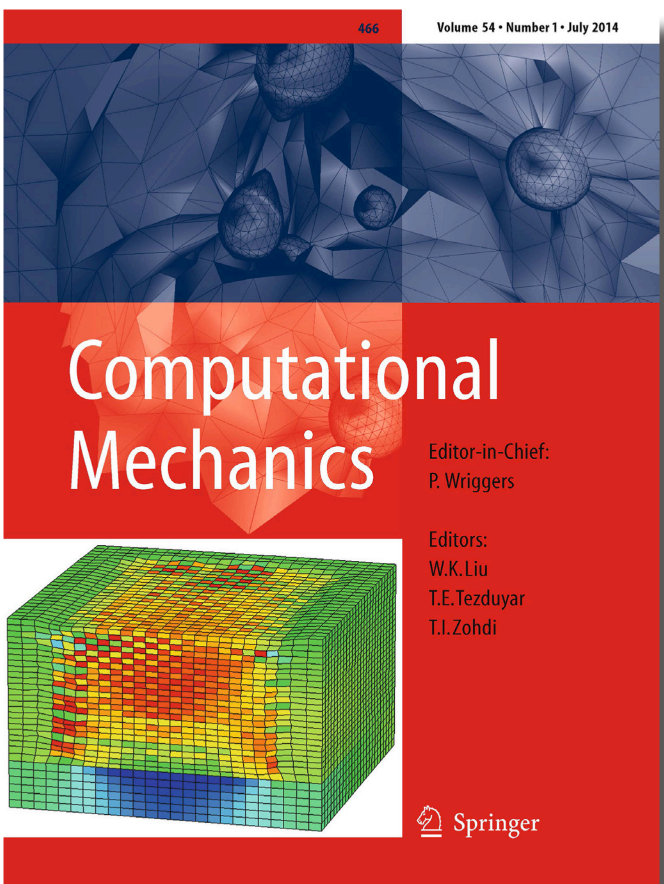
A team of engineers and scientists at Lawrence Livermore has developed an additive-manufacturing technique to design and fabricate, at the microscale, new cushioning materials with a broad range of programmable properties. The resulting material combines the advantages of gel and foam with an engineered architecture that actually overcomes the limitations of the component material—an example of the **power of additive manufacturing**. This research, led by Eric Duoss and Tom Wilson, is **described in a paper published in *Advanced Functional Materials***. Supported by the Laboratory Directed Research and Development Program as a strategic initiative (**project 11-SI-005**), the work focused on creating a micro-architected cushioning with a silicone-based ink that cures to form a rubberlike material. During printing, a first layer of ink is deposited as a series of horizontally aligned filaments, which can be as fine as a human hair. The second layer of filaments is then deposited vertically and so on, until the desired height and pore structure is reached. These novel energy-absorbing materials have many applications, including protective materials for sensitive instrumentation and in aerospace applications to combat the effects of temperature fluctuations and vibration.

PAPER ON LASER-BASED CHEMICAL VAPOR DEPOSITION FEATURED IN "SPOTLIGHT ON OPTICS"

A paper by LLNL researchers published in *Optics Express* has been selected as a "**Spotlight on Optics**" featured article by the Optical Society of America. The paper **describes the use of interferometry measurements as real-time feedback** to a laser-based chemical vapor deposition (LCVD) process using silica to obtain nanometer-scale sensitivity. A technique being explored to mitigate laser-induced damage to fused silica optics, LCVD deposits silica over the damaged area and shapes the final surface with nanometer-scale accuracy, resulting in a silica layer with a high damage threshold and a desired surface profile. High-energy laser systems typically require nanometer-scale flatness of mitigated optical surfaces to minimize perturbations to the laser light. To meet this requirement, LLNL researchers applied phase-shifting diffraction interferometry measurements of the surface profile to serve as feedback to control the LCVD parameters. In their article, LLNL authors Gabe Guss, Selim Elhadj, Arun Sridharan (now at General Electric), Michael Johnson, and Ibo Matthews show how utilizing diffraction interferometry and accounting for the kinetics of the modeled thermomechanical response resulted in increased control of the LCVD process. This work was supported by the Laboratory Directed Research and Development Program under **project 011-ERD-026**. The image shows the surface profile of laser-heated fused silica determined from the interferometry measurements.

COMPUTATIONAL TOOL FOR ADDITIVE MANUFACTURING

A paper describing a strategy for successfully implementing a thermomechanical model to simulate the additive manufacturing technique of selective laser melting was featured **on the cover of the journal *Computational Mechanics***. The special issue of the journal focused on modeling and simulation in support of advanced manufacturing processes. Lead author Neil Hodge and his colleagues in Livermore's Defense Technologies Engineering Division set forth problem formulation, numerical method, and constitutive parameters necessary to solve the problems associated with selective laser melting, a technique in which successive layers of metal powders are heated by laser to gradually build up an entire workpiece. This technique holds great potential in a new manufacturing paradigm that is already transforming the world's manufacturing sector—and that poses both opportunities and challenges in the arena of national security. The work in this article was funded by the Laboratory Directed Research and Development Program at LLNL under **project 13-SI-002**.



PAPER ON "SNOWFLAKE DIVERTOR" MAKES FUSION AWARD SHORTLIST

A paper by Livermore's **Vlad A. Soukhanovskii** and collaborators—"**Taming the plasma–material interface with the snowflake divertor in NSTX**"—was named to the 11-paper shortlist for the 2014 Nuclear Fusion Award, which is presented by the journal *Nuclear Fusion*. The winning paper will be determined by a secret ballot of the journal's board of editors and will be announced at the International Atomic Energy Agency's Fusion Energy Conference later this year. The research described in the paper was conducted by Livermore-led teams in the **National Spherical Torus Experiment** at Princeton Plasma Physics Laboratory in Princeton, NJ, and at the DIII-D National Fusion Facility at General Atomics in San Diego, CA. The snowflake divertor was first proposed by LLNL's Dimitri Ryutov in 2007 as a possible solution for the plasma–material interface problem in magnetically confined fusion plasma devices (that is, tokamaks), with foundational work on this groundbreaking concept **supported by Livermore's LDRD Program**. Dimitri and the team he led **won an R&D 100 Award** for this concept in 2012.

PAPERS DEMONSTRATE BREADTH OF LABORATORY'S ISOTOPIC SCIENCE

In three articles in two consecutive issues of the *Journal of Environmental Radioactivity*, LLNL's researchers working in environmental radiochemistry and isotopic signatures will publish results obtained with their deep expertise in using mass spectrometry and isotope ratios in a broad range of applications. The first paper, which originated as a summer intern project, **investigated contamination from an abandoned uranium mine** in the Sierra Nevada mountains of California. Measurements of the isotopic composition in water and sediment samples, combined with isotopic mixing models, show that the source of uranium contamination is weathering of uranium mine tailings.

The second article describes how a new high-sensitivity inductively coupled plasma mass spectrometry method can be used to **measure ultralow levels of neptunium-237**—a major contributor to radioactivity in spent nuclear fuel—in groundwater samples. The LLNL technique was shown to provide the best direct measurement of transport rates of neptunium-237 in groundwater and concludes that the isotope does not appear to pose significant environmental risks.

The third article demonstrates how fissiogenic xenon isotopes in radioactive fallout from a nuclear explosion **are uniquely able to constrain the timescale** of fallout formation, the chemical fractionation that occurs when fission products and nuclear fuel are incorporated into fallout, and the speciation of fission products in the fireball. In short, xenon isotopes provide a window into the chemical composition of the fireball in the seconds following a nuclear explosion, improving our understanding of the physical and thermo-chemical conditions under which fallout forms. The figures are optical microscope images of fallout particles analyzed in the study.

DISCOVERED: NEW PHASE TRANSITION IMPACTING DYNAMICAL STRUCTURES

In **a paper published in *Physical Review B*** as an Editors' Selection, a team including Livermore's **Jason Jeffries**, researchers from Oak Ridge National Laboratory (including former LLNL employee Michael Manley), National Institute of Standards and Technology (including former LLNL employee Nick Butch), and Santa Clara University report on their use of inelastic neutron scattering, x-ray diffraction, and heat capacity measurements to characterize the nature of intrinsic localized modes (ILMs) in sodium iodide (NaI) crystals. Spatially localized, anharmonic vibrations that break the translational symmetry of a crystal lattice, ILMs until recently were thought to occur as random pointlike features. Recent experiments, however, had indicated that ILMs can form dynamical patterns affecting physical properties. Now, these new results by Jason and colleagues show, for the first time, that when dynamical patterns of ILMs form, they trigger a series of phase transformations that couple to defects, creating new stacking faults in the system. These findings represent a new class of phase transitions defined by symmetry breaking in the lattice-dynamical structure rather than by the average crystal, electronic, or magnetic structure.

IN *NATURE*, A "MOLECULAR MOVIE" OF PHOTOSYNTHESIS

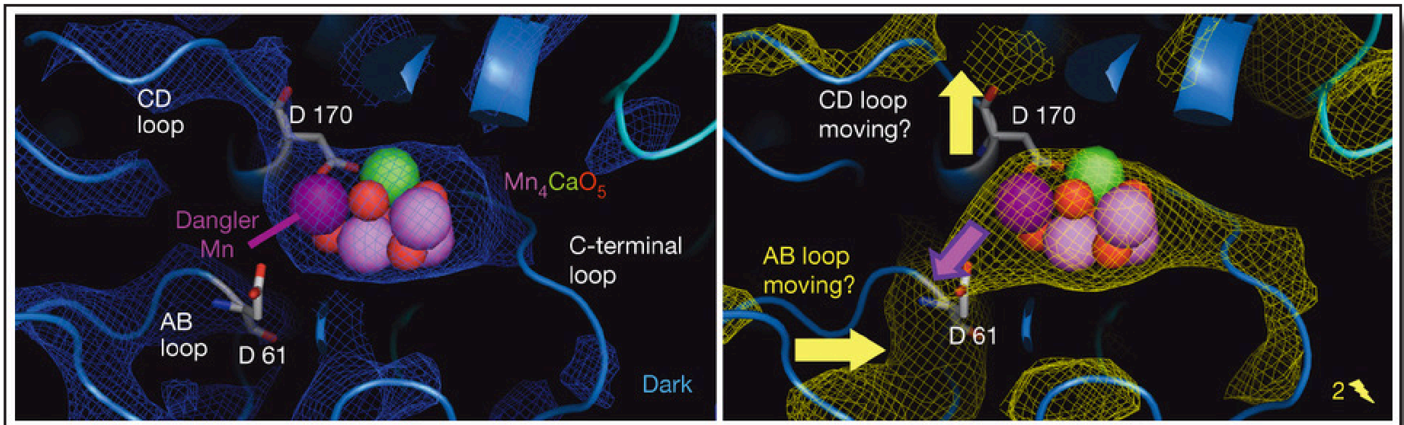
In a paper published in the July 9 online edition of *Nature*, an international team that includes Lawrence Livermore researchers **Mark Hunter**, Stefan Hau-Riege, and Matthias Frank reports the **light-induced structural changes they observed in photosystem II** (PSII), one of the two large protein complexes that catalyze photosynthetic reactions. The team used the x-ray free-electron laser at the Linac Coherent Light Source to perform femtosecond crystallography on nanocrystals of PSII, collecting time-resolved structural data. (This is in contrast to conventional x-ray diffraction, which provides merely a static picture of a molecule's structure.) From the data, they determined the molecular structures of the PSII complex in its dark and light-affected states, determining that specific molecular regions of the complex undergo significant conformational changes as photosynthesis proceeds. This work shows the great potential for time-resolved serial femtosecond crystallography for investigating catalytic processes in biomolecules. LLNL's participation in this work was funded through the UC Laboratory Fee Research Program and Livermore's Laboratory Directed Research and Development Program. The figure shows the simulated (left) dark and (right) flashed states of the highly radiation-sensitive Mn_4CaO_5 cluster of the PSII complex.

CONTRIBUTING CHAPTER TO MICROARRAY TECHNOLOGIES BOOK

LLNL scientists Kevin McLoughlin, Crystal Jaing, Shea Gardner, Nicholas Be, James Thissen, and Tom Slezak have contributed a chapter to the recently published book, ***Microarrays: Current Technology, Innovations and Applications***, edited by Zhili He and published by Caister Academic Press. The book focuses on current microarray technologies and their applications in environmental microbiology. The book begins by briefly introducing microarray technologies and applications, then offers detailed descriptions of microarray probe design, development, and evaluation and data analysis. Later chapters discuss phylogenetic arrays (e.g., **PhyloChip**) and functional gene arrays (e.g., GeoChip). The chapter by the LLNL authors listed above is titled "Broad Spectrum Viral and Bacterial Pathogen Detection by Microarrays."

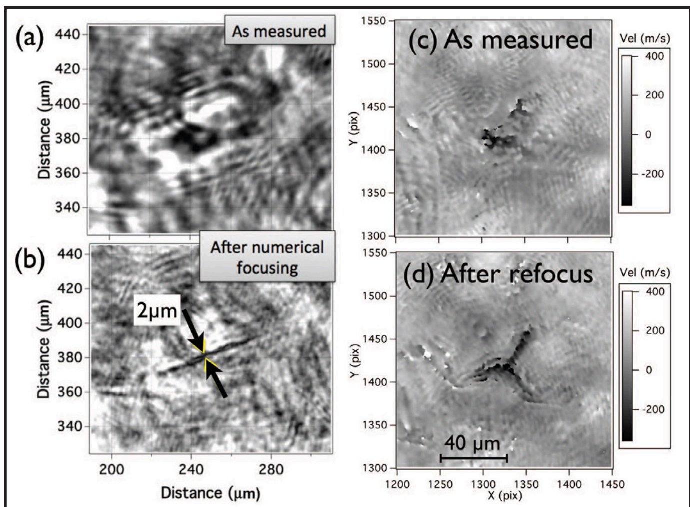
COMPUTATIONAL "FOCUSING" CAPTURES 3-D MATERIAL BEHAVIOR

In an article in *Review of Scientific Instruments*, a team led by LLNL scientists describe a technique for computationally processing high-speed velocity interferometry images of laser-shocked materials, bringing previously fuzzy features into focus. This achievement has potential applications in revealing a material's three-dimensional behavior. Velocity interferometer is conventionally used to measure a target along a line (that is, in one dimension), but the



team, led by David Erskine, used short laser pulses and the Velocity Interferometer System for Any Reflector (**VISAR**) system in two dimensions to capture snapshot-like images. Then, numerical postprocessing based on Fourier transform yielded 3-D, holographic images from the data. The team is planning to use this technique to explore how materials such as diamond fracture and disintegrate when decompressing from high pressure. Most of the experiments in this research were performed at LLNL's Jupiter Laser facility. The figure shows images of laser-shocked silicon before and after numerical focusing (top and bottom rows, respectively).

RECENT PUBLICATIONS BY LLNL



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