Lawrence Livermore National Laboratory

Science & Technology Review

January/February 2015

Additive Manufacturing Innovations

Also in this issue:

- Accelerated Certification of Components
- Detecting Optical Damage Precursors
- Basic Science Exploration

About the Cover

As the article beginning on p. 4 describes, additive manufacturing (AM), often called three-dimensional (3D) printing, offers the National Nuclear Security Administration (NNSA) a new avenue for creating replacement nuclear weapons parts and related stockpile materials. Lawrence Livermore is collaborating with other NNSA laboratories and production plants to expand the range of materials and components compatible with AM, develop a better fundamental understanding of the materials involved, and exploit the flexibility of AM manufacturing processes. The cover image shows a 3D printer that uses a laser to produce complex metal parts (the glowing green object). (Rendering by Ryan Chen.)

Cover design: Amy E. Henke. Rendering by Ryan Chen.

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.

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Prepared by LLNL under contract
DE-AC52-07NA27344

Science & Technology REVIEW

January/February 2015

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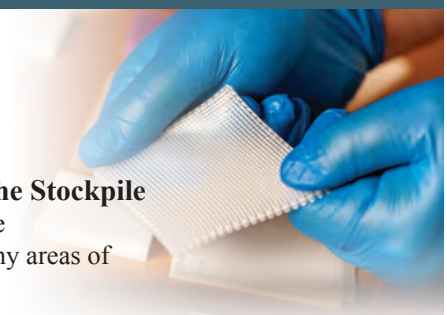

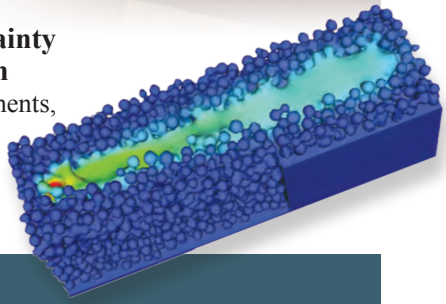

Research Highlights

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S&TR Staff

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-52000-15-1/2
Distribution Category UC-99
January/February 2015

Ocean Warming in Southern Hemisphere Underestimated

Using satellite observations and a suite of climate models, Livermore scientists have found that long-term warming in the upper 700 meters of the Southern Hemisphere oceans has been likely underestimated. "This underestimation is a result of poor sampling prior to the last decade and limitations of the analysis methods that estimate temperature changes in data-sparse regions," says Livermore oceanographer Paul Durack, lead author of a report in the October 5, 2014, issue of *Nature Climate Change*. "Our results suggest global ocean warming has been underestimated by 24 to 58 percent. The conclusion agrees with previous studies, but it's the first time scientists have estimated how much heat we've missed."

The team found that climate models simulating the relative increase in sea surface height—a leading indicator of climate change—between Northern and Southern hemispheres are consistent with highly accurate altimeter observations. However, separating the simulated upper-ocean warming in the Northern and Southern hemispheres is inconsistent with observed estimates of ocean-heat-content change. These sea-level and ocean-heat-content changes should be consistent, suggesting that Southern Hemisphere ocean-heat-content changes were likely underestimated. Since 2004, automated profiling floats (named Argo) have been used to measure global ocean temperatures up to depths of 2,000 meters. The 3,600 Argo floats observing the ocean provide systematic coverage of the Southern Hemisphere and, with earlier data, show gradual warming. (Background image is an iceberg sighted off the Amery Ice Shelf in the Southern Ocean.)

Ocean heat storage is important because it accounts for more than 90 percent of Earth's excess heat associated with global warming. The Southern Hemisphere oceans make up 60 percent of the world's oceans. Given that most of the excess heat associated with global warming is in the oceans, this study has significant implications for how scientists view Earth's overall energy budget.

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Tiny Carbon Nanotube Pores Make Big Impact

Livermore scientists along with collaborators have created a new type of ion channel consisting of carbon nanotubes (CNTs) inserted into synthetic bilayers and cell membranes to form tiny pores (called porins) that transport water, protons, small ions, and DNA. Collaborators include colleagues from the Molecular Foundry at Lawrence Berkeley National Laboratory, University of California at Merced and Berkeley, and University of the Basque Country in Spain.

Research showed that CNT porins display many behaviors of natural ion channels. The CNT porins spontaneously insert into membranes, switch between metastable conductance states, and display macromolecule-induced blockades. The team also found that local channel and membrane charges could control the ionic conductance and selectivity of the CNT porins. Livermore's Kyunghoon Kim, a postdoctoral research team member, says, "We expect that CNT porins could be modified with synthetic gates to alter their selectivity."

"Nanopores are a promising biomimetic platform for developing cell interfaces, studying transport in biological channels, and creating biosensors," says Aleksandr Noy, a Livermore biophysicist who led the study and is senior author of a paper in the October 30, 2014, issue of *Nature*. "Many efficient drugs that treat diseases of one organ are quite toxic to another," says Noy. Unlike taking a pill that is delivered to the entire body, CNTs can help deliver the drug to an area without affecting surrounding organs. These CNT porins have significant implications for the future of health care and bioengineering through drug delivery, novel biosensors, DNA sequencing applications, and as components of synthetic cells.

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Holography Reveals Hidden Cracks in Shocked Targets

A research team led by Livermore scientists developed a technique for three-dimensional (3D) image processing of a high-speed photograph of a target. "We are interested in how fast-moving surfaces crack, crumble, and disintegrate after they are shocked by a laser pulse, because these details provide us with important information about a material's properties," says David Erskine, lead author of a paper in the June 2014 online issue of *Review of Scientific Instruments*.

Most of the relevant experiments were performed at Livermore's Jupiter Laser Facility. This technique is particularly applicable in targets that are shocked with lasers, suddenly undergoing intense energy waves. The process described uses an apparatus called VISAR (velocity interferometer system for any reflector) to measure velocities of targets. VISAR is traditionally used to measure a target along a line or at a single point. The team instead used VISAR two-dimensionally to take snapshot images using high-resolution detectors with a short laser flash to freeze target motion. Holographic properties became apparent, making it possible to recover 3D information from 2D images. "We didn't set out to do holography, but when our target moved, blurring cracks, we were able to refocus the data by numerical processing and bring blurred features into focus," says Erskine.

"We plan to explore how materials, such as diamond and silicon, fracture and disintegrate when they decompress from high pressure. These fundamental materials can be obtained in high purity and are used in many shock experiments," says Erskine. "The decompression process provides information about the strength of a material under the conditions encountered in all momentary shock experiments."

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Commentary by Charles Verdon

Partnerships Help Power Additive Manufacturing Research

AS a leading center for materials science research and high-performance computing (HPC), Lawrence Livermore is an ideal institution at which to perform innovative manufacturing research to advance technologies in support of national security. Additive manufacturing (AM), also known as three-dimensional (3D) printing, is a particularly exciting area that we think could revolutionize how the National Nuclear Security Administration (NNSA) produces the parts needed to maintain the safety, security, reliability, and effectiveness of the nuclear stockpile and to bring about a more cost-effective and responsive stockpile. To this end, we are pioneering new approaches and customizing existing AM technologies to meet our unique manufacturing needs. This effort is described in the article beginning on p. 4.

Successfully carrying out a mission of such magnitude requires partnerships with industry, academia, and other federal laboratories. Lawrence Livermore has been working closely with Sandia and Los Alamos national laboratories and the NNSA production plants on a range of stockpile-related AM projects, from fundamental research of the materials and processes involved in AM to the application and refinement of methods for additively manufacturing tools and weapons components. Livermore has helped form the California Network for Manufacturing Innovation, an organization that brings together manufacturers, national laboratories, government agencies, universities, and workforce and economic development organizations to accelerate manufacturing innovation. We are also part of America Makes, a network of companies, nonprofit organizations, academic institutions, and government agencies working to foster collaboration and encourage growth in 3D printing technology and applications. External engagements and collaborations not only help the Laboratory fulfill its national security research and development mandate but also support the nation's economic competitiveness.

Livermore's computing and simulation capabilities, originally developed to understand and predict nuclear weapons performance, have proven to be a powerful tool for analyzing and optimizing manufacturing processes and efficiencies. The Accelerated Certification Initiative, discussed in the article beginning on p. 12, unites HPC, uncertainty quantification (UQ), materials science, and manufacturing research in an effort to better understand the connection between manufacturing processes, material structure, material properties, and component performance. UQ tools such as data mining help winnow the number of parameters involved in process and part optimization to a reasonable quantity for further study and experimentation, while HPC-based modeling and simulation support more efficient virtual design, prototyping, and testing of parts.

Livermore is developing these robust HPC-based AM process modeling capabilities in partnership with other NNSA laboratories and production plants. As our process understanding and predictive modeling capability improve, we should be able to significantly reduce the amount of trial and error involved in manufacturing and more quickly arrive at qualified materials and components with fewer required tests. These tools are also attracting interest from potential industry and university collaborators. Their wider application could in turn help drive AM process improvements. A related area of AM research at the Laboratory involves implementing process inspection and control features into 3D printers. Real-time process analysis—an area in which we excel—could enable us to precisely control part quality and perhaps even to produce parts that are "born certified."

Livermore's core national security mission remains focused on the maintenance of a safe, secure, reliable, and effective nuclear stockpile, but the science discoveries and technology developments made in support of this mission benefit a broad portfolio of national security work performed at the Laboratory. For example, the accelerated design and prototyping of parts that AM enables could also help us rapidly evolve battlefield capabilities and strengthen our nonnuclear defense. On the intelligence front, AM research gives us unique insights into potential proliferation paths that might be taken elsewhere in the world. Although rooted in our stockpile mission, AM research under way at Lawrence Livermore is likely to bear diverse fruit.

■ Charles Verdon is principal associate director for Weapons and Complex Integration.

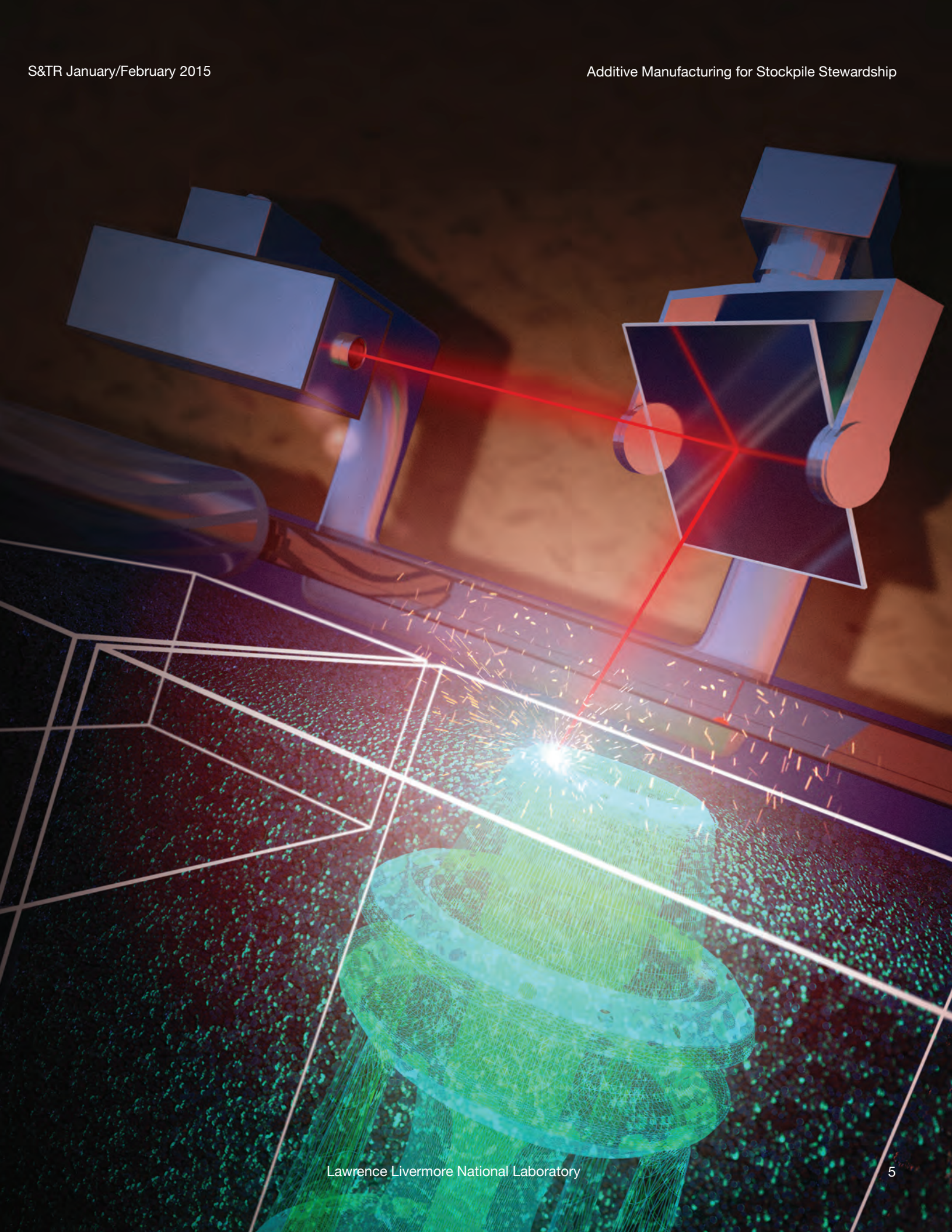
NEXT-GENERATION MANUFACTURING FOR THE STOCKPILE

Additive manufacturing may help transform the nuclear weapons enterprise.

WEAPONS refurbishment efforts called life-extension programs (LEPs) enable the National Nuclear Security Administration (NNSA) to maintain the nation's nuclear deterrent without resuming the production of new weapons or underground nuclear tests, both of which ceased roughly a quarter century ago. (See *S&TR*, March 2012, pp. 6–13; July/August 2010, pp. 4–11.) Sustaining the legacy manufacturing processes used for LEP component production is growing increasingly challenging for the NNSA laboratories and production facilities, which are tasked with keeping the aging weapons safe and operational. Many of the procedures are five decades old and geared toward mass production of weapons components. They entail lengthy multistep methods, expensive facilities, large lot sizes, and undesirable levels of hazardous waste generation. Some processes are no longer operationally feasible because of environmental issues, while others call for materials difficult to obtain.

Advanced manufacturing technologies such as additive manufacturing (AM), together with high-performance computing (HPC), could be used to develop next-generation manufacturing processes and materials for the NNSA complex. AM methods, in which layers of material are built up as prescribed in a digital file, can be used to quickly, easily, and precisely create objects with complex shapes. The superior material design and manufacturing process control available through AM can facilitate the creation of objects with more desirable material properties and performance than conventional subtractive manufacturing technologies. AM is already being exploited by a wide range of industries to drastically reduce product development and production time lines, particularly for low-volume specialty parts and tooling.

Recognizing that AM could greatly benefit national security missions, NNSA has launched a multiyear, multipronged initiative to explore, mature, and adapt the most promising commercial AM technologies and to develop new techniques. NNSA's success will rely on the manufacturing expertise of its production plants and the unique science-based stockpile stewardship capabilities of its laboratories. "For NNSA to realize additive manufacturing's important benefits in a reasonable time frame, it needs multidisciplinary labs such as Lawrence Livermore working closely with its production plants," says Melissa Marggraff, deputy principal associate director for Livermore's Weapons and Complex Integration Principal Directorate and coordinator for NNSA's many AM activities. "We have materials science, engineering, high-performance computing, and certification expertise that can help make this effort a success." Lawrence Livermore has five AM labs and more than 80 material scientists, chemists, physicists, engineers, and computational scientists developing advanced materials and manufacturing processes.



In collaboration with other NNSA laboratories and production plants, the Laboratory is studying and expanding the range of materials and component types amenable to AM. The collaboration is also exploiting the flexibility of AM processes to enhance the properties and performance of components. In addition, Livermore scientists are using HPC-based modeling and simulation to accelerate AM process qualification. NNSA's AM experts envision widespread use of the technology across the weapons complex, from manufacturing tooling and simple weapon replacement parts, such as cushions, to developing advanced materials, such as high explosives and nuclear components.

Tailoring Industry Processes

NNSA researchers have begun to strategically adopt existing AM capabilities and methods for stockpile-relevant applications and have already achieved some early successes. For instance, the Y-12 National Security Complex, with support from Livermore AM experts, has been exploring the feasibility of using industry-developed metal AM machines and processes to manufacture tools.

As part of this effort, Y-12's Derek Morin spent a year at Livermore, during which he worked with the Laboratory's AM experts and Y-12 end users to manufacture select metal tools. For several of these tools, the Livermore–Y-12 team fabricated both an AM replica of the wrought part and an enhanced version of the part. "We wanted to show how AM expands the design possibilities," says Livermore mechanical coordinator Steve Burke. "We no longer need to make a round hole when a square or oval hole will work better."

The ongoing collaboration has also demonstrated how AM can shrink production costs for intricate components such as gears by largely eliminating assembly and machining. A match drill fixture, the first piece of production-qualified tooling made by AM, has already entered use at Y-12. The new approach for producing this tool consolidates 5 parts into 1, thereby eliminating 12 welds and reducing waste.

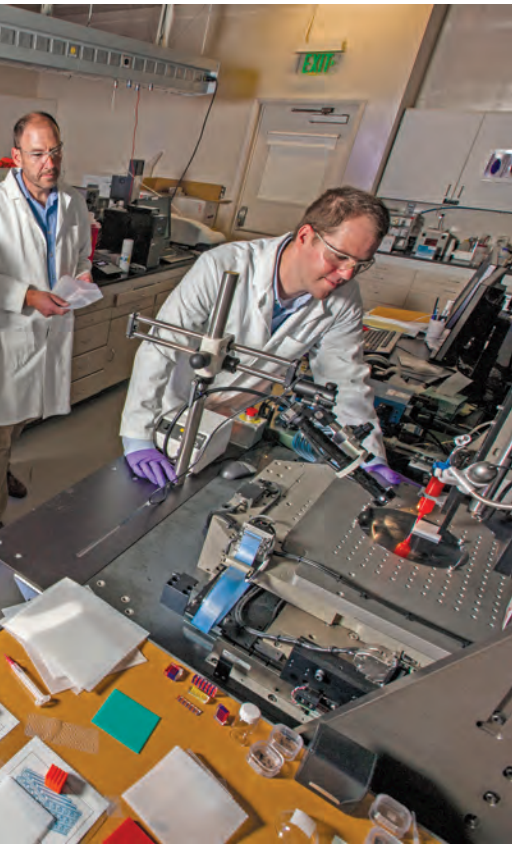
Livermore AM technician Manuel Iniguez holds a metal part produced in partnership with the Y-12 National Security Complex. This match drill fixture is the first additively manufactured part to be qualified for NNSA production and takes one-fifth the labor hours to produce as compared with previous manufacturing methods. (Photo by George Kitrinos.)

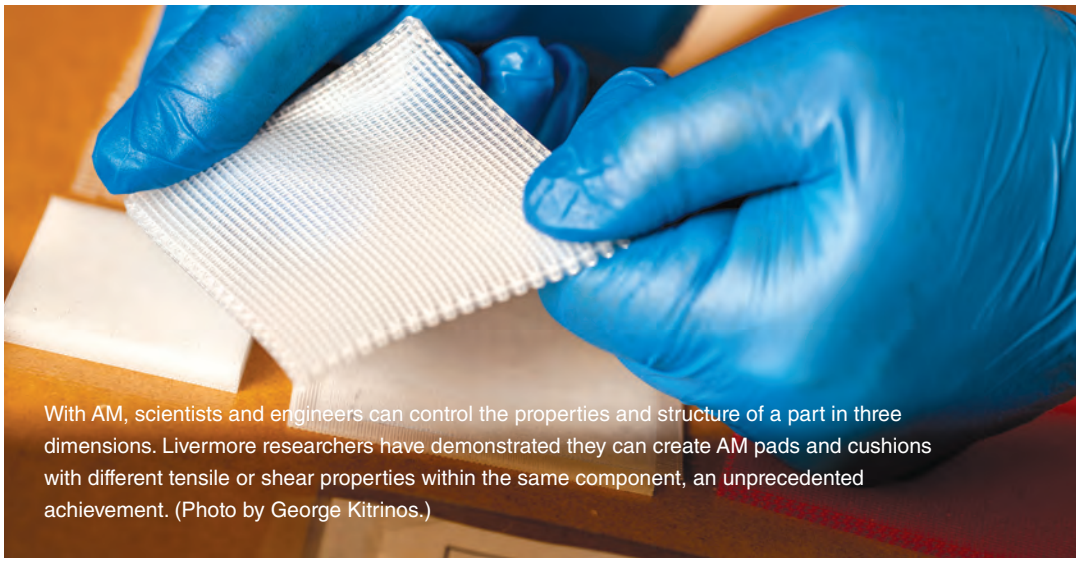
Additive manufacturing (AM) researchers produce polymer parts using Livermore's direct-ink-writing machine. Shown here (left to right) are Chris Spadaccini, Tom Wilson, Robert Maxwell, and Eric Duoss. (Photo by George Kitrinos.)

NNSA sites estimate that 50 percent of its tools could be made using AM in five years. In which case, tooling production costs would be reduced 75 percent, development time 80 percent, and production time 60 percent, while potentially improving tool performance. Further, the items could be printed on demand, reducing inventory and freeing space.

Designing Special Properties

Livermore is engaged in challenging materials research in an effort to control and customize a weapon





With AM, scientists and engineers can control the properties and structure of a part in three dimensions. Livermore researchers have demonstrated they can create AM pads and cushions with different tensile or shear properties within the same component, an unprecedented achievement. (Photo by George Kitrinos.)

component's properties with AM. For one project, a team of engineers and materials scientists has developed a method for additively manufacturing cushions and pads that protect and position components within a nuclear weapon. (See *S&TR*, September 2014, pp. 20–23.) Traditionally, cushions and pads have been made of foam through a manufacturing process that does not allow for complete control of the shape, size, and distribution of air pockets. Consequently, the performance of the material cannot be precisely predicted.

Using a silicon-based "ink" that cures into a rubbery material, the team has designed and fabricated pads and cushions with direct ink writing (DIW). (See *S&TR,* March 2012, pp. 14–20.) DIW machines deposit ink on a substrate one layer at a time, in a predetermined pattern. The resulting structure is then cured with heat or ultraviolet light. With this technique, the team can better control the material's mechanical and directional properties than when working with foam. Engineer Chris Spadaccini says, "By controlling the architecture of a microstructure, we can create materials with previously unobtainable properties in the bulk form."

The team can also create novel combinations of properties, such as a pad that is easily compressible at one end and stiff at the other. The new method increases production uniformity and allows researchers to better model the materials and their performance. Moreover, DIW-produced polymer cushions are 85 percent cheaper than foams manufactured with legacy approaches and can be made in a tenth of the time. DIW pads will likely be among the first additively manufactured components incorporated in an LEP. Livermore researchers are working with manufacturing experts at the Kansas City National Security Campus to establish the AM production infrastructure, refine processes, and produce qualified parts.

Livermore researchers are also optimizing the structure of metal components using AM. Mechanical engineer Howard Rathbun develops strong yet lightweight lattice structures on a scale too fine for conventional metal manufacturing techniques. "We want to take advantage of the strength and stiffness of lattice structures to help resolve some stockpile stewardship technical challenges," says Rathbun."

To achieve a stronger, stiffer structure, each lattice is configured so that none of its struts can bend. Standard design tools could not create lattice structures of the desired complexity, with thousands or millions of individual millimeter-high struts, so Rathbun's team developed computational design tools that run on Livermore's supercomputers. Using these tools, the researchers can create lattices that conform to a curved surface while retaining superior lattice performance. "HPC is a significant aspect of developing metal lattice structures and ensuring we have confidence that they will meet performance requirements," says Rathbun.

These standards can be demanding. For instance, one stretch-dominated lattice structure can absorb very high loads and spring back without exhibiting permanent deformation. Metal lattices can be designed to serve multiple simultaneous roles, too. For example, the open spaces

within a lattice can be used to pass fluid, allowing the lattice to function as both a heat exchanger and a load-bearing structure. The Laboratory is also exploring other paths for maximizing the mechanical properties of lattice and multimaterial components while minimizing weight, with the aid of sophisticated tools. For instance, Daniel Tortorelli of the University of Illinois at Urbana–Champaign has been working with Spadaccini's team to use computational modeling methods known as topology optimization to create designs for AM fabrication.

Printing Exotic Materials

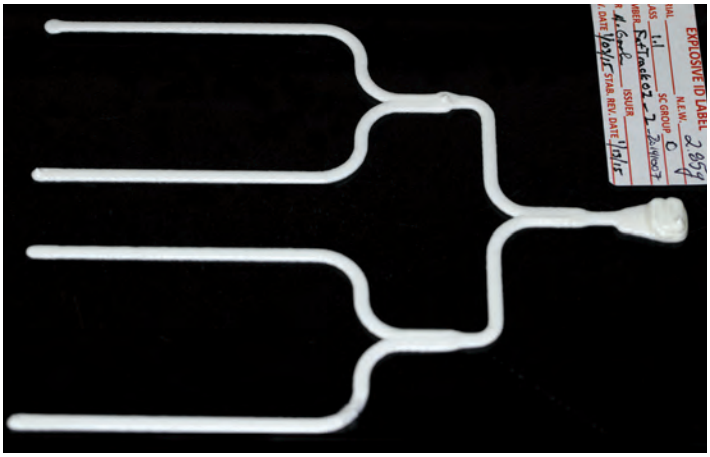
An effort to print exotic materials, such as explosives, has necessitated the development of new AM methods as well as the adaptation of some commercial technologies. Using AM methods, Laboratory scientists aim to improve a manufacturing process and product that have remained essentially the same for the past 65 years. Materials chemist Alex Gash observes, "AM provides an opportunity to gain more control over the sensitivity, safety, and performance of the explosive."

A high explosive's crystal structure is pocked with defects, or pores. When the explosive is shocked, these pores both collapse and heat, initiating the explosion. "We know that explosive performance and safety are affected by defects in the material," Gash adds. "These defects exist at the mesoscale, from about 1 to 100 micrometers. AM gives us the potential to manipulate structures on that scale, unlike conventional manufacturing." Controlling the distribution of the pores should yield a safer and more predictable explosion. For instance, the team could design parts with a density gradient, which might enable reliable initiation.

For its feasibility experiments, the team targets small components, such as the boosters that set off the main high-explosive charge of a nuclear device. Detonators and boosters are more practical to print than larger components at this stage. Thus far, Livermore researchers have demonstrated, using mock energetic materials, that they can manipulate material microstructures at critical length scales for controlling the response and performance of explosives. Printing of actual high explosives began in September 2014 in a specially constructed laboratory for remotely operating AM techniques at Livermore's High Explosives Applications Facility. Preliminary printing and test results are encouraging.

Livermore researchers are also developing new techniques for manufacturing other components, including materials associated with dispersion-type nuclear fuels. Initial efforts focus on using selective laser-melting (SLM) technology to produce parts from a uranium–niobium alloy that are high strength as well as oxidation resistant. The SLM powder-bed AM technique uses intense laser energy to fuse fine metal particles and produce a three-dimensional (3D) part. To enable this and other AM research, a multidisciplinary team set up a laboratory and SLM machine specifically for working with reactive and radioactive powders, a significant effort. "It was challenging to determine the potential hazards and to develop creative ways for implementing the required controls," observes Paul Alexander, lead SLM machine operator. "However, with a diverse team of experts, we were able to establish a research and development facility that is well prepared for these unique challenges."

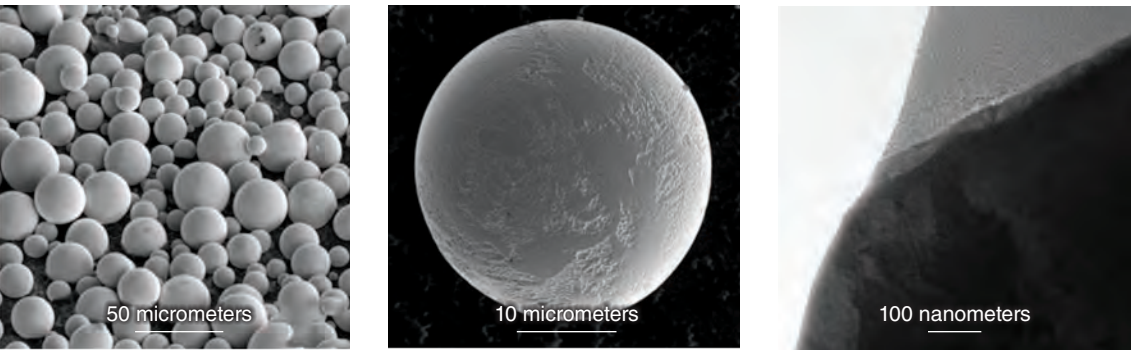
In May 2014, the facility became operational, and the uranium–niobium alloy was printed for the first time using a commercial SLM machine. The team is now proceeding to characterize the SLM-produced test objects. Compositional studies using various microscopy techniques have helped the research team understand how uranium and niobium atoms are distributed during printing, how particle size affects printing results, how laser settings determine the material's porosity, and how impurities affect the material's properties.



An object made using an extrudable explosive demonstrates Livermore's ability to additively manufacture conventional high explosives.

Intensive Characterization

The success of ongoing AM research relies on the ability of researchers to understand and control the properties and performance of additively manufactured materials in order to ensure qualification of AM components. AM entails not only a new production process but also potentially different component materials. Chemist Larry Fried explains, "Even if we begin



Material scientists Geoffrey Campbell, Luke Hsiung, and Joseph McKeown have characterized the surface oxide layer and microstructure of uranium–niobium powder using (left and center) scanning electron microscopy and (right) transmission electron microscopy. This information contributes to understanding how factors such as size distribution and quality of the particles affect the AM process.

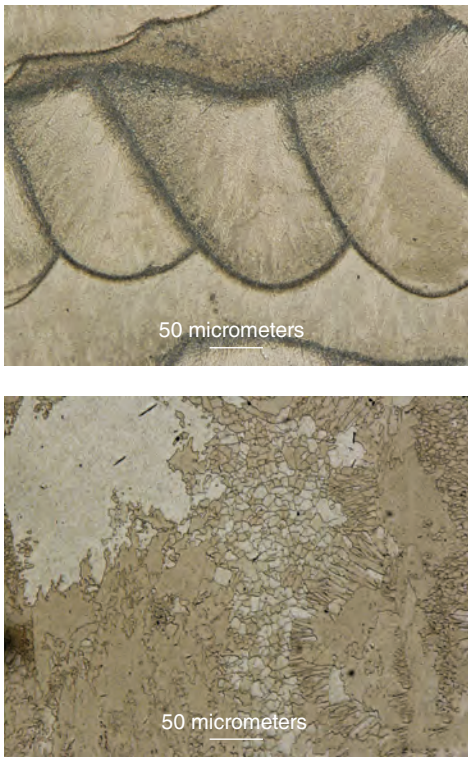
with the same metal, the AM process changes the metal's microstructure."

AM-produced metals can exhibit structures, properties, and performance that differ from their cast and wrought counterparts. This issue continues to dominate concerns with exploiting AM for commercial applications. For example, any pores and pockets of unmelted powder that form during the SLM powder-bed process will affect the metal's density. Furthermore, the rapid melting and solidification that SLM and other metal AM techniques impose on the material can change the distribution of crystal orientations within the resulting product. A significant amount of industrial and academic research and development is directed at determining the effects of these differences on a wide range of material properties.

"AM methods generally produce metal structures with more impurities and finer grain sizes, both of which make them stronger," says materials scientist Geoffrey Campbell. "Trade-offs exist, of course. More strength usually means less ductility, and ductility is what allows many metals to bend and deform without catastrophic failure." Significant future research and development will be directed toward understanding and exploiting these trade-offs.

Livermore researchers subject AM-produced metals to the full range of characterization methods in a materials scientist's toolkit, such as computed tomography, electron microscopy, x-ray diffraction, and ultrasonic sensing, as well as some less common tools. At the nanosecond and nanometer scale, they use the dynamic transmission electron microscope (see *S&TR*, September 2013, pp. 4–11) to study how metals solidify under laser-melting conditions. To characterize residual stresses within AM parts, they have collaborated with colleagues at Los Alamos National Laboratory to perform neutron diffraction studies. Optical metallography provides them with information on impurities in the microstructure. Other experiments performed include simple comparisons of weight and density, chemical analyses, and tests for characteristics such as strength and elasticity.

Experiments at other Department of Energy facilities complement Lawrence Livermore's examination techniques. Materials scientist Amanda Wu is collaborating with scientists from Los Alamos, Argonne, and Brookhaven national laboratories to examine the effects of AM on the fine-scale crystallographic structure of uranium–niobium, using Argonne's Advanced Photon Source. Materials scientist Holly Barth is conducting in situ mechanical testing of AM materials using synchrotron radiation microtomography at the Advanced Light Source at Lawrence Berkeley National Laboratory.



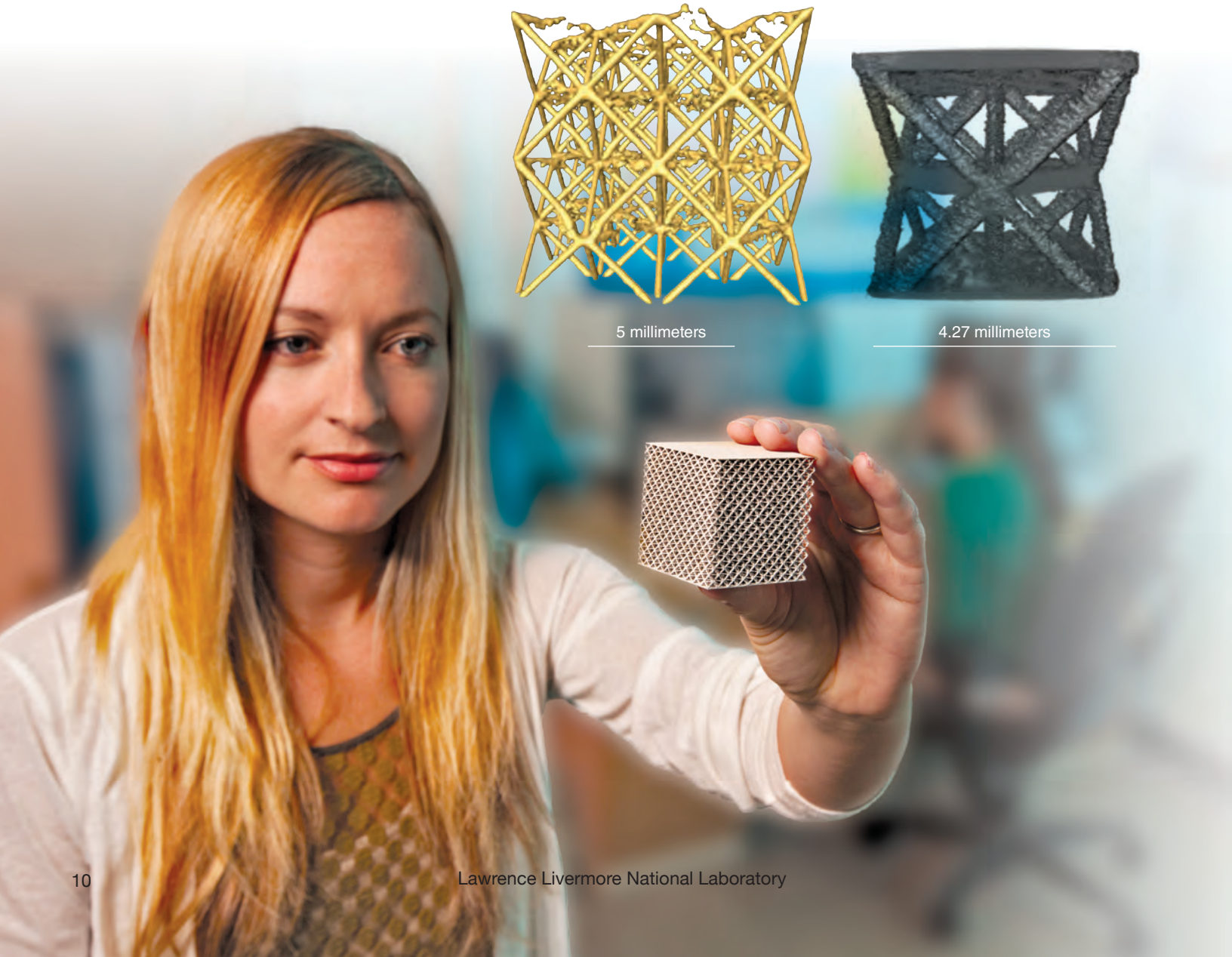
Characterization has revealed that with common postprocessing methods such as heat treatment, AM metal samples can achieve similar microstructures to those of conventionally manufactured metals. Optical micrographs created by Amanda Wu depict (top) an additively manufactured uranium–niobium sample without postprocessing and (bottom) a sample that has been radically transformed through solution annealing. The transformed microstructure resembles that of samples produced by other methods.

(below left) Materials scientist Holly Barth holds an additively manufactured metal lattice structure. A combination of modeling and synchrotron radiation microtomography experiments helped identify and correct some initial printing problems compromising structural integrity. (below center) This tomographic three-dimensional (3D) rendering of a stainless-steel lattice structure shows higher-than-desired porosity and disconnected struts, while (below right) the other tomographic 3D rendering shows a titanium alloy lattice structure with acceptable density and strut connectivity. (Photo by George Kitrinos.)

Barth's goal is to relate mechanical properties to microstructural observations in SLM-produced titanium alloys and stainless-steel samples. Her experiments generate micrometer-scale 3D images of samples as they are compressed or stretched. These images are used to track the damage evolution of potentially performance-limiting features such as misprinted lattice struts, large pores, or uneven pore distributions. For one study, Barth compared wrought stainless steel with AM stainless steel of two densities and found the AM metals that had been heat-treated to achieve the desired microstructure displayed similar properties to wrought metals, up to a certain threshold of porosity. At times, the build "errors" accumulate beyond acceptable ranges. Livermore computational efforts are attempting to quantify these ranges.

More Testing Ahead

Livermore researchers will soon begin more extensive laboratory testing of AM parts to assess their dynamic behavior. Experimentalists will use a combination of techniques, including laser-driven shocks, dynamic compression, conventional gas-gun tests, and explosives compression. Using laser-driven ultrafast shock experiments, Fried's group will study the material response of AM plastics on



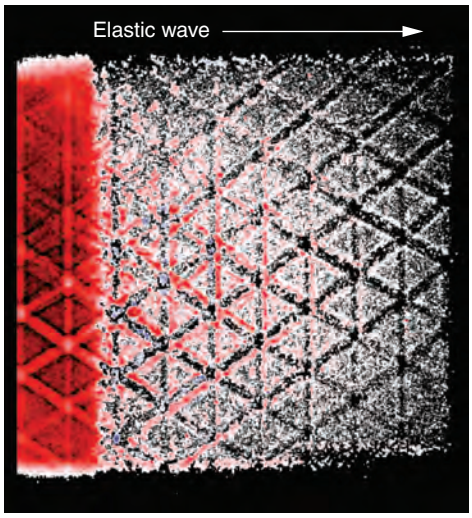
scales of hundreds of picoseconds and micrometers. This technique complements standard gas-gun tests, which interrogate material behavior on scales of centimeters and microseconds.

Materials scientist Mukul Kumar's team has begun conducting gas-gun experiments on plastic and metal AM samples at the dynamic compression sector of the Advanced Photon Source. This facility enables time-resolved x-ray diffraction and imaging measurements during compression experiments with spatial resolutions of about 10 micrometers. The technique will help researchers understand how metal lattices respond to shock waves similar to what would occur during weapon operation. Ultimately, the deeper understanding of AM materials gained through ongoing characterization and testing activities will inform the development both of AM stockpile components and of accelerated approaches for certifying AM parts. (See the article beginning on p. 12.)

National Security Applications

Livermore researchers and their NNSA partners are demonstrating how strategic use of AM can speed the development and enhance the quality of metal and polymer replacement weapon parts, prototypes, test objects, and related materials for stockpile stewardship activities. In time, AM could fundamentally change the way the nuclear weapons complex produces parts by shrinking the manufacturing production footprint, revitalizing the stockpile infrastructure, and helping bring about a leaner, more sustainable, and more agile nuclear enterprise. As a side benefit, AM's challenging multidisciplinary science and compelling mission may also help attract and retain the next generation of stockpile stewards at laboratories such as Lawrence Livermore.

"As we develop the core capabilities with NNSA, we will also support the development of national security capabilities more broadly," says Marggraff. For example, AM can be used to enhance capabilities to disarm nuclear weapons, train nuclear emergency responders, and gain insights regarding high-explosives performance and new conventional weapons concepts. Further, it can help intelligence experts understand how new manufacturing technologies could be exploited by other nations or entities to produce weapons that are otherwise difficult to make or that do not currently exist.



Dynamic compression experiments at Argonne National Laboratory's Advanced Photon Source performed by Livermore materials scientist Mukul Kumar and his team are providing insights into the physics associated with the deformation of AM metal and polymer lattices, including the propagation of traveling waves and their interaction with the material's microstructure.

Because the payoffs for the AM initiative won't be realized for at least a few years, maintaining the necessary momentum for the project demands dedication and passion from the researchers. "Our 'secret weapon' at Livermore is our enthusiastic and engaged management and staff," observes Rathbun. "We are excited about additive manufacturing's possibilities, and together we have the experience and abilities to make it happen."

—Rose Hansen

Key Words: additive manufacturing (AM), direct ink writing (DIW), foam, high-density part, high explosives, High Explosives Applications Facility, high-performance computing (HPC), life-extension program (LEP), National Nuclear Security Administration (NNSA), nuclear stockpile, nuclear weapon, pore, selective laser melting (SLM), uranium.

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BUILDING THE FUTURE

MODELING AND UNCERTAINTY QUANTIFICATION FOR ACCELERATED CERTIFICATION

Livermore technician Manuel Iniguez removes a finished component from the build chamber of a selective laser-melting (SLM) additive manufacturing (AM) machine. (Photo by George Kitrinos.)

Advanced manufacturing methods have motivated Livermore researchers to rethink how to better qualify components.

IN industries such as aerospace, defense, and medicine, the manufacturing processes and materials used to produce critical components must be formally qualified to ensure they perform to specification, as failure could prove disastrous. The extensive empirical testing and evaluation required to develop a material and qualify a component often encompass many thousands of individual tests, at a cost of millions of dollars and 5 to 15 years of effort. Later, even a minor manufacturing process change could necessitate complete requalification. This traditional qualification approach makes it difficult for producers to leverage the speed, flexibility, and cost savings that advanced techniques such as additive manufacturing (AM) offer. (See *S&TR*, September 2014, pp. 20–23.) AM refers to a category of manufacturing processes in which a polymer- or metal-based material is added layer by layer in concordance with a virtual blueprint. (See *S&TR*, March 2012, pp. 14–20.) AM methods can be used to create objects with shapes or properties that are difficult or impossible to achieve through traditional

subtractive manufacturing methods such as machining.

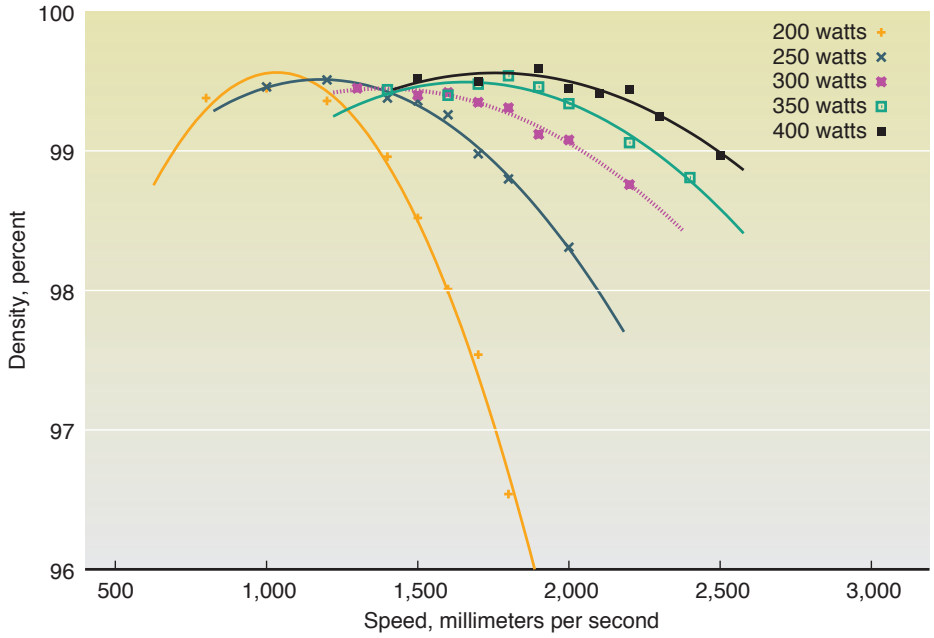
AM can also speed the development of complex designs, accelerating the development cycle and enabling customization. However, to realize AM's full potential, Livermore scientists posit that the processes to qualify components and certify systems must also be accelerated. "One of the most serious hurdles to the broad adoption of additive manufacturing of metals is the qualification of additively manufactured parts," says materials scientist Wayne King. "At this time, concern is focused on the quality of the final product." King leads Livermore's Accelerated Certification of Additively Manufactured Metals (ACAMM) Initiative, which began in late 2012. ACAMM is supported by Laboratory Directed Research and Development (LDRD) funding and builds on Livermore's foundational capabilities and previous successes in areas such as materials synthesis, predictive simulation, advanced manufacturing, and materials characterization.

Rather than undertaking exhaustive experimentation, King's team borrows a formula that has proven highly effective for stockpile stewardship work: modeling and simulation paired with targeted experiments and guided by data mining and uncertainty quantification (UQ). "With deep scientific knowledge, we develop more confidence in the process, and this confidence leads to qualification," says King. "High-performance computing plays a key role. We have used it to support certification of the stockpile by simulating systems and building confidence, and we believe high-performance computing can help us in a similar way in the metal AM arena." In turn, the results of this LDRD project may, with additional development effort, be applied to Livermore's nuclear stockpile mission. Nuclear engineers and AM experts are presently exploring how AM methods could benefit weapons refurbishment endeavors. (See the article beginning on p. 4.)

In the first two years of the project, King's team of computational experts has built and begun testing platforms for its multiscale modeling and data-mining efforts. With these platforms, the researchers are progressing toward understanding and optimizing the rapid heating, melting, cooling, and solidification processes at the heart of metal AM.

Less Trial and Error

For selective laser-melting (SLM) AM, Livermore researchers are using data-mining techniques to efficiently hone the optimal process parameters that result in parts with desired properties. With SLM, a high-energy laser beam fuses metal powder particles, layer by layer, to produce a three-dimensional (3D) part. Some SLM applications require parts with greater than 99 percent density, because voids, or pores, weaken

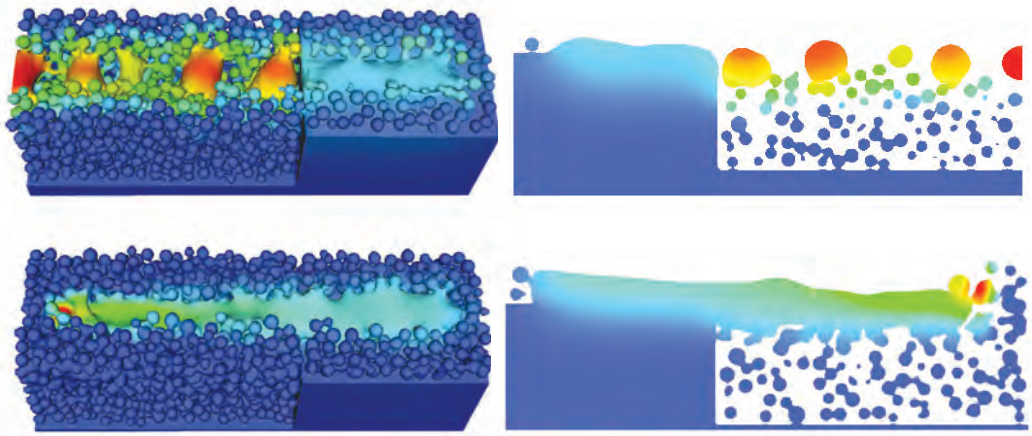


Livermore researchers have shown that modeling combined with a set of experiments is an efficient and reliable method for determining AM process parameters. This approach has helped them understand how various laser power and laser-scanning speeds during SLM influences the density of the part produced. For certain applications, parts with greater than 99 percent density are needed because of their superior strength.

the material and cause parts to fail. Unfortunately, the sheer number of process parameters that influence the quality of the material produced—more than 130—can make it difficult to determine the best settings without many rounds of experimentation. Some of these parameters include laser power, laser-scanning speed, distance between the laser scan lines, scanning pattern, and powder-layer thickness.

A team of researchers, led by computer scientist Chandrika Kamath, has used a combination of simulations and experiments to streamline the optimization process and identify variables likely to influence the density of stainless-steel parts. The team began by performing more than 500 simple, computationally efficient laser-melting simulations to pinpoint the parameters that played the largest role in determining the dimensions of the melt pool, which is the pool of liquid formed when the laser melts the metal powder particles. Using data-mining techniques to uncover patterns in the simulation results, the researchers found that laser power and scanning speed were the most crucial parameters. They also identified ranges of power and speed that would result in melt pools of the right depth. "We mined the simulation output to identify important SLM parameters and their values such that the resulting melt pools are just deep enough to melt through the powder into the substrate below," says Kamath.

Focusing on just these two parameters in the physical experiments enabled the team to reduce the number of experiments necessary to achieve high-density parts. The researchers first used a subset of speed and power values to perform basic single-track experiments, in which a laser creates a series of tracks in a metal plate. They found that when the speed was too low, the laser drilled into the material and produced pores, reducing the metal's density. Too high a speed generated insufficient melting. Once equipped with a subset of values deemed most likely to produce the right melting conditions, the team printed a series of small steel pillars with more than 99 percent density on the first attempt. The experiments also yielded significant data on the role of laser power in particular. For the stainless-steel powder under study, the density remained high over a wider range of scanning speeds at higher powers than at lower powers, which suggests that higher powers offer greater flexibility when choosing process parameters.



Powder-scale modeling with the code ALE3D provides an efficient avenue for understanding how to adapt process parameters to build a part with an overhang geometry. In the top scenario, both the laser power and scan speed are high, a combination that produces an undesirable balling effect. By lowering the scan speed and power (bottom scenario), a better build can be achieved.

This effort helped demonstrate that computer simulations, data mining, and a select set of experiments can be used to quickly and reliably determine process parameters. The team expects that a similar approach could be used to optimize other properties of a manufactured part or other materials. Furthermore, data mining is just one tool that helps the researchers make efficient use of the vast quantities of data that experiment and simulation are producing. In the future, a growing role will be played by UQ techniques as they are used to understand how uncertainties in inputs, such as powder quality and laser power and scanning speed, will affect the properties of parts manufactured using AM.

Micrometer-Scale Insights

Since the cessation of nuclear testing in the early 1990s, the Laboratory has focused particular attention on developing predictive models for regimes where experimental data are not always available. These tools are aiding the ACAMM team in developing a multiscale predictive modeling capability based on physics first principles and validated through physical experiments. Modeling AM processes and predicting AM part performance can be challenging, because the materials science involved is complex and covers a broad range of time and length scales. Such modeling may be computationally intensive but is possible with Livermore's exceptional high-performance computing (HPC) resources. Researchers use information provided by these models

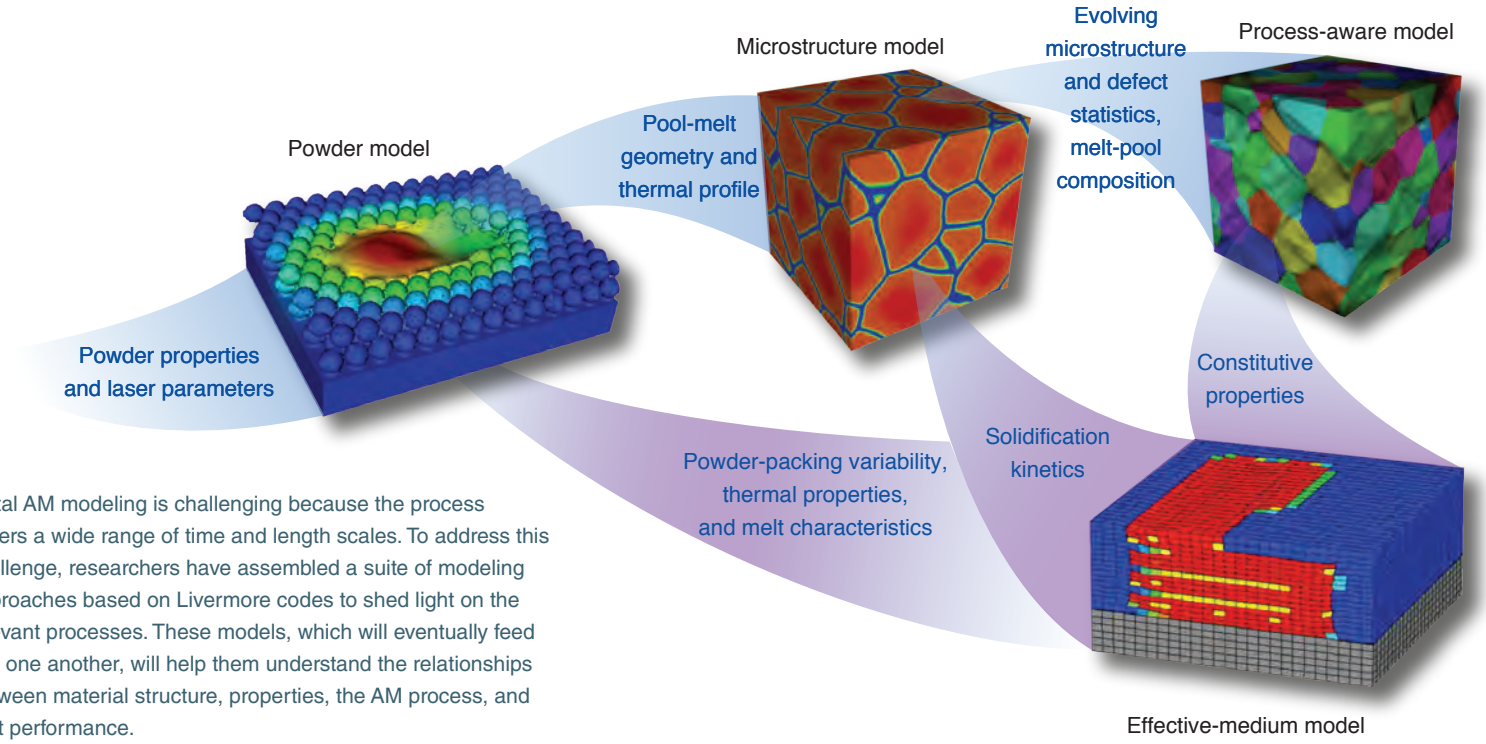
to improve AM processes, obtain desired microstructures, and reduce manufacturing errors. Two models, based on Livermore-developed codes, have already shown significant promise.

As the range of AM applications grows, so do the variety of metals Livermore researchers desire to additively manufacture. Some of these materials may never have been tested in AM machines, while others may not meet the machine manufacturer's specifications. For instance, a powder with a more varied particle size than recommended may be much cheaper, but it could also have performance implications. Engineer Andy Anderson and physicist Saad Khairallah have developed a model to help researchers understand whether a given powder can be processed by AM and, if so, what are its optimal processing conditions. Powered by Livermore's massively parallel multiphysics code ALE3D and HPC resources, the tool is the first high-fidelity, 3D powder-scale model of an SLM process.

This model resolves the melting and solidification of individual powder particles on submicrosecond timescales. "The simulations reveal that the surface-tension effects on topology and heat transfer drive the SLM process," says Anderson. The researchers observed behaviors in the melted region that resembled Plateau–Rayleigh instabilities, such as those that occur when a thin water stream breaks into droplets. These instabilities can occur at high laser speeds and create undesirable effects such as surface roughness and disconnected balls of material, both of which were observed in some experiments.

Khairallah and Anderson used the powder model to better understand the main physical processes occurring and to optimize process parameters. They found that for a fixed laser power and at high laser-scan speeds, less heat is deposited, and therefore the particles do not fully melt. This scenario can cause surface roughness and porosity to increase. Lower laser-scan speeds enable the particles to melt completely and produce conditions favorable for achieving the low porosity, smooth surface, and high density that the researchers desire. However, if too much heat is deposited, the material can enter a keyhole regime, where the laser drills into the sample, causing extensive material evaporation and creating plasma.

These simulations complement Kamath's efforts to efficiently optimize process parameters. She is analyzing the data from the simulations to understand how to create parts with smoother surfaces. Notes Khairallah, "We were surprised and pleased the first iteration of our model captured the essential characteristics of the melt track. Now that we understand the magnitude of our



Metal AM modeling is challenging because the process covers a wide range of time and length scales. To address this challenge, researchers have assembled a suite of modeling approaches based on Livermore codes to shed light on the relevant processes. These models, which will eventually feed into one another, will help them understand the relationships between material structure, properties, the AM process, and part performance.

approximations, we can add more physics effects to the model."

Building a Virtual Part

While the powder model looks at a single layer of metal powder and its interactions with the laser, the Livermore-developed effective-medium model is intended to computationally build a complete part and predict material properties such as residual stress and part characteristics such as unwanted distortions. The development team based this model on the Livermore engineering code Diablo, which is used to look at slowly evolving processes. Simulations cover a time period as long as several hours and a length scale of centimeters.

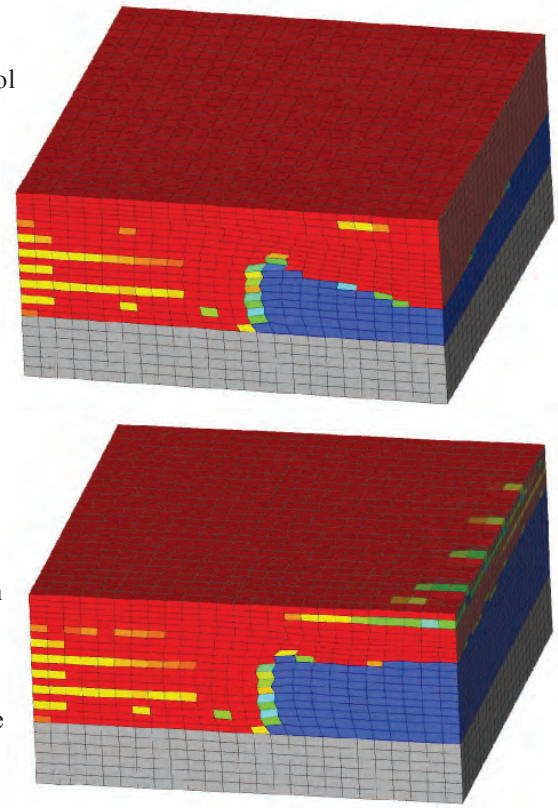
The effective-medium model has been successfully used to simulate several phenomena. Computational engineer Bob Ferencz explains, "We're interested in studying effects such as the cyclical shrinking a material undergoes as its layers are heated to thousands of degrees and then cooled. We have found the material near the melt layer, including the fused layers beneath, undergoes significant thermal processing over time. We need to know how that reworks the material." By sharing their temperature data with material scientists, Ferencz and his team hope to gain insight into how these temperature fluctuations influence the metal's microstructure, which could in turn enhance the model.

Early studies focused on modeling just a cubic millimeter domain of powder, which equals about 20 layers of particles. Even this small scale has shed light on problems such as rough surfaces in overhang regions. An overhang is a downward-facing surface of a part that is supported only by underlying unconsolidated powder as opposed to melted and solidified metal. Creating overhang features with SLM often results in an undesirable finish on the underside that necessitates further machining. Using overhang construction simulations, computational engineer Neil Hodge found that an uneven surface forms when the laser melt pool penetrates the previously unmelted layers. He demonstrated through further simulations that adjusting the laser power several times over the course of part production could mitigate excessive melting. With the acquisition of a sophisticated SLM machine from Germany's Fraunhofer Institute for Laser Technology, Livermore researchers soon will be able to verify simulation results and experiment with laser power modulation during the printing process.

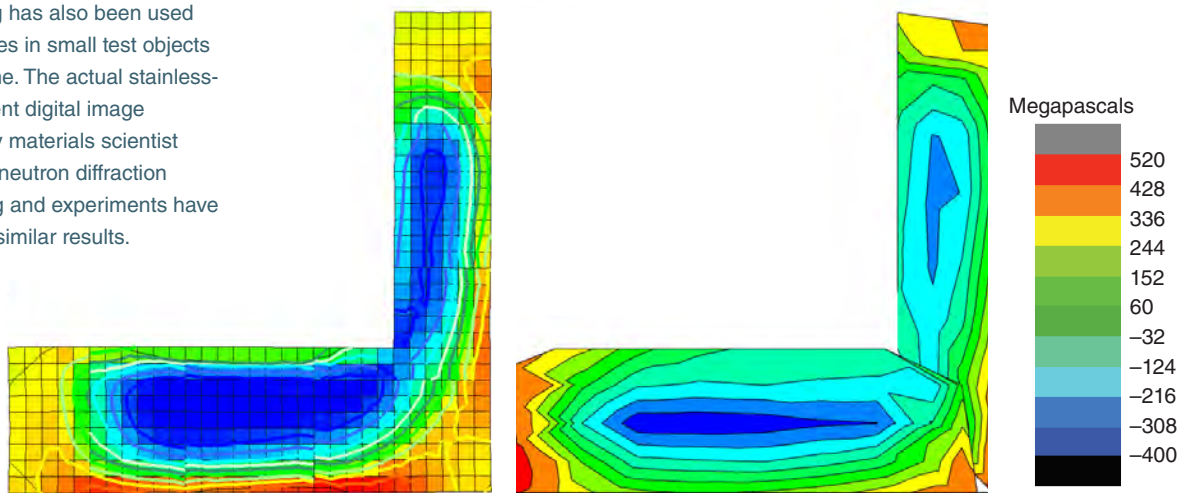
Ferencz's team also had some initial success in modeling residual stresses in centimeter-scale parts. These stresses are induced by the laser-melting process and change with the part's subsequent removal from the base plate on which it was built. Understanding these stresses is important for predicting part performance and improving the SLM process. The researchers modeled stresses in prism- and L-shaped stainless-steel test objects both before and after the objects were removed from their base plates.

For comparison, the actual parts were evaluated experimentally using nondestructive neutron diffraction at Los Alamos National Laboratory. The experimental results provided information on residual stress. Livermore materials scientist Amanda Wu also used digital image correlation to study the parts. This technique involves first painting a speckled pattern on the surface of a part and then photographing the part with a pair of cameras as the part separates from its base plate. Wu analyzed the image series to determine how much the material had distorted from the residual stresses.

The team found that predicted and actual stresses were quite similar. Given



Livermore researchers have used Diablo part-scale modeling to understand and correct the formation of uneven surfaces in overhang regions. (top) When the laser sweep proceeds at a uniform speed and power, it tends to produce excessive melting and consolidation (red) beneath the intended overhang, causing previously unprocessed powder (blue) to fuse and form a rough downward-facing surface. (bottom) By modulating the power, the simulations suggest this problem can be mitigated and a more even surface produced.



(left) Part-scale modeling has also been used to predict residual stresses in small test objects such as this L-shaped one. The actual stainless-steel test object underwent digital image correlation, performed by materials scientist Amanda Wu, and (right) neutron diffraction measurements. Modeling and experiments have achieved encouragingly similar results.

that modeling at this larger scale required simulations of "metalayers" rather than individual layers to speed up the simulation, the researchers were pleased to find that they were still able to reasonably capture stresses in the parts. They have now begun modeling residual stress in parts where a larger percentage of the surface area touches the base plate, which poses a greater challenge.

Diagnostics Complement Modeling

Future efforts will tie in the powder and effective-medium models with two others—a microstructure model designed to predict the microstructures that develop during the AM process and a process-aware model that predicts temperature and behavior for the effective-medium model. Ultimately, these models will be used to connect the AM process with the resulting material microstructure and properties and accurately predict the performance of the material.

While the deep understanding of the AM process that simulation affords is essential, it is not enough for qualification. The ACAMM team will also be integrating sensors and diagnostics into the Fraunhofer SLM machine to ensure that the process developed through modeling and simulation proceeds as planned during part production. Once process-monitoring capabilities are fully established and coupled with a mature multiscale model, it may become possible to qualify each part as it is built.

—Rose Hansen

Key Words: Accelerated Certification of Additively Manufactured Metals (ACAMM) Initiative, additive manufacturing (AM), data mining, digital image correlation, effective-medium model, high-performance computing (HPC), Laboratory Directed Research and Development (LDRD) Program, neutron diffraction, powder model, predictive modeling, process monitoring, selective laser melting (SLM), uncertainty quantification (UQ).

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Sleuthing an Optical Mystery

IN the pursuit of science, the recipe for understanding complex phenomena can often require several parts perseverance and one part good old-fashioned detective work. Lawrence Livermore scientists have shown that this formula holds true for advancing our knowledge of laser optics and how to preserve their functional lifetimes for laser-based applications, including those at the National Ignition Facility (NIF).

Large-area optical components such as lenses, mirrors, and frequency-conversion crystals are essential for effectively directing and focusing laser energy onto a target. Many of NIF's optics are made of fused silica because the material exhibits excellent properties, but they are also susceptible to damage when routinely subjected to the high energies produced by the laser. During manufacturing and processing, microscopic defects, called damage precursors, can form on an optic's surface. These precursors absorb and transfer energy to the optic, initiating damage sites that grow with additional laser shots. Eventually the impaired components must be refurbished or replaced. Livermore scientists have been involved in a decades-long effort to understand the sources of damage with the goal of developing techniques for mitigating their negative effects.

In 2011, Livermore scientists completed a project funded by the Laboratory Directed Research and Development (LDRD) Program that resulted in the advanced mitigation process (AMP). AMP is a chemical-etching method that uses optimized hydrofluoric acid to remove damage precursors, such as the defect layers found on fractured surfaces associated with fine scratches or impurities. Scratches are introduced to an optic's surface predominantly during the final polishing and handling phases of fabrication. "With AMP, we can effectively mitigate sources of damage and increase an optic's lifetime," says Jeff Bude, a physicist in the NIF and Photon Science Principal Directorate, who along with materials scientist Tayyab Suratwala helped lead the study. This process significantly reduces damage sites caused by precursors, primarily at lower energies—less than about 10 joules per square centimeter. (See *S&TR*, September 2011, pp. 17–19.)

In a more recent three-year LDRD study completed in 2014, Bude and colleagues set out to uncover the source of optics damage at higher fluences. "Despite our continued improvements, such as AMP, the surface damage threshold of most optical materials was still far below the intrinsic bulk limit of the material, which told us that other extrinsic factors were affecting optic performance," says Bude. Through detailed detective work, they discovered that precipitates of trace impurities found in processing chemicals are the most significant damage precursors in the high-fluence range. The work demonstrated that by minimizing the presence of precipitates during chemical processing and drying, the silica damage produced from high-fluence events can be reduced by

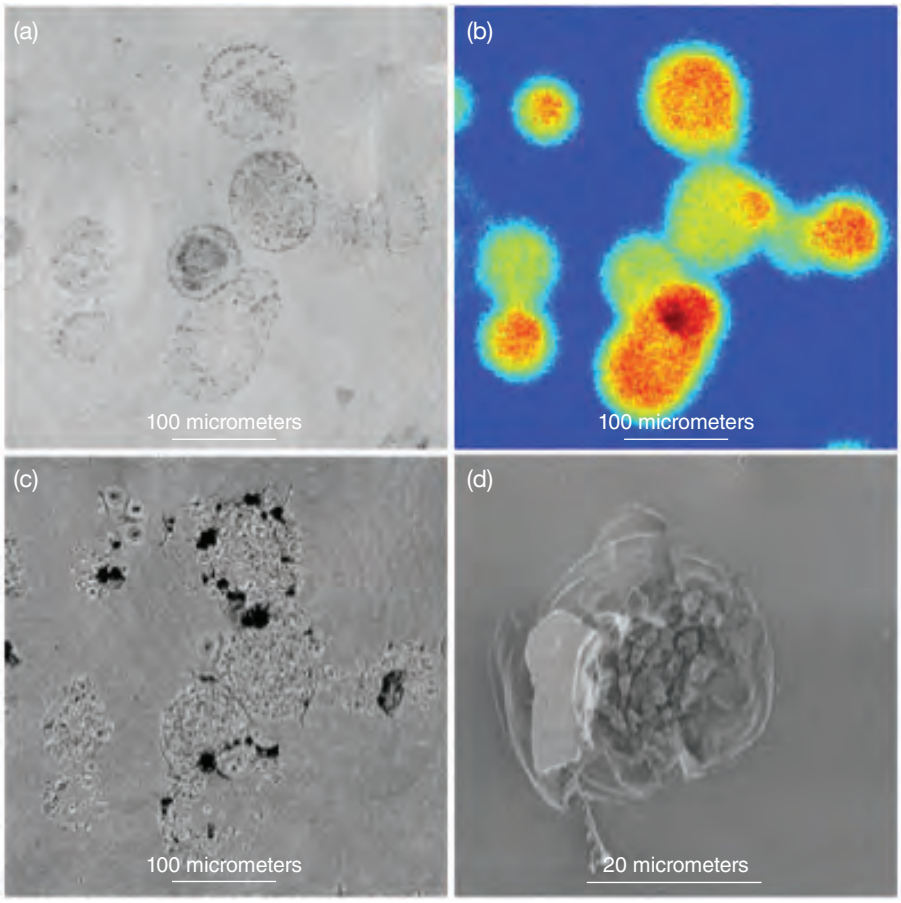
more than two orders of magnitude. The new process, called AMP3, has potential to significantly extend the functional lifetime of NIF optics, helping to further reduce overall operational costs and improve performance.

An Invisible Adversary

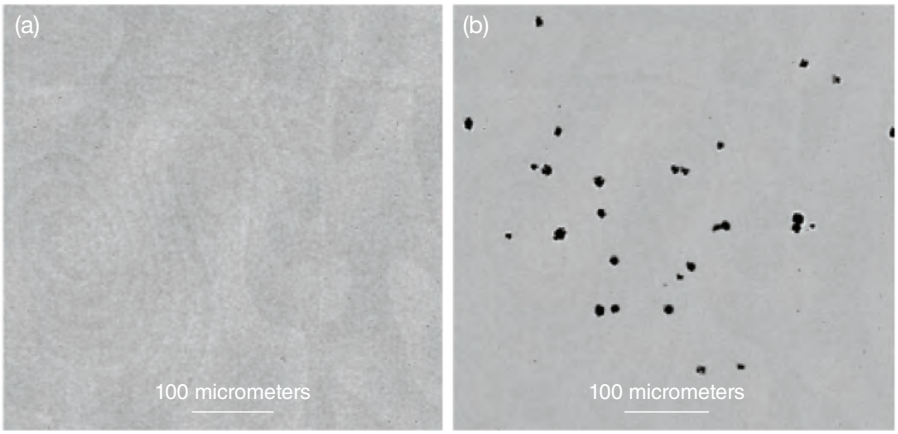
High-fluence damage precursors are characteristically different from their low-fluence counterparts in that they exist at much higher density and are spread more uniformly over an optic's surface. In addition, low-fluence precursors are large enough to be seen with scanning electron microscopes or optical microscopes, while high-fluence precursors are much smaller—submicrometer in scale—and are not readily observable until the damage sites have been initiated, earning them the name "invisible" precursors. "Surface damage requires that an absorbing defect couples laser energy into the bulk material," says Bude. "If one of these submicrometer precursors absorbs enough laser energy to reach temperatures at which the glass begins to absorb light, it can launch a damage-causing absorption front into the glass. Absorption by nanoscale precursors leads to macroscale damage."

Identifying these precursors was challenging. In addition to being invisible, they seemed immune to initial AMP improvements. "Our first process changes did not improve the damage, which exceeded 10^5 sites per square centimeter at high fluence," says Bude. "However, we knew from previous silica damage mitigation studies, that heating a small spot on an optic's surface to about 2,000 kelvins for a few seconds could remove some of these precursors." Bude and his team used this technique to locally increase the surface damage threshold for arrays of sites on AMP-treated silica substrates. They then passed these samples back through the steps of AMP to determine whether any of them reintroduced damage precursors to the heated regions. Surprisingly, the team found that each of the wet chemical steps produced damage precursors, even the deionized (DI) water rinse at the end of the process. Thus, the researchers concluded that precipitates of contaminants carried in the water and other processing liquids were a likely source of damage precursors.

To prove this hypothesis, Bude and his team performed tests to determine whether precipitates of trace impurities in processing liquids could absorb laser light and damage the optic. The team prepared test samples of 50-millimeter-diameter fused silica optics using AMP. Each step of etching, rinsing, and drying was carefully controlled to ensure the optics were as clean as possible prior to laser experiments. The entire process was conducted in a Class 100 clean room to minimize airborne impurities. Subsequently, the team applied different salt-based solutions of common impurities to the samples using an aerosol



(a) Optical microscopy shows precursors formed by sodium chloride (NaCl) droplets applied to an optic via an aerosol solution. (b) Photoluminescence spectroscopy demonstrates that these precipitates absorb light and transfer energy to the optic's surface. (c) NaCl precipitates are damage precursors that initiate damage sites after exposure to high-fluence laser light. (d) Scanning electron microscopy shows a typical silica damage site.



(a) Optics sprayed with an aerosol of deionized water showed no visible submicrometer precipitates under optical microscopy prior to laser exposure. (b) After large-area damage tests with nanometer light pulses, precipitate sites could be clearly seen.

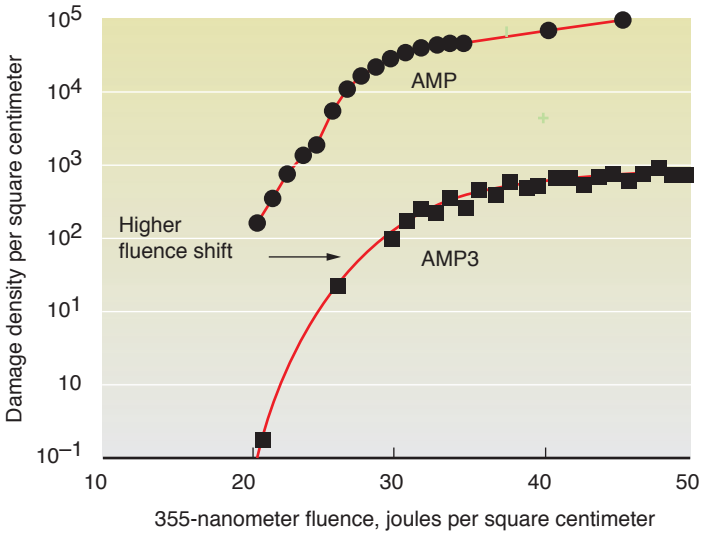
or direct aqueous deposition and then examined the impurities' photoluminescence and propensity to damage.

Crystals of these salts—such as sodium chloride—do not absorb ultraviolet light in their bulk state and as such are typically used to create high-transparency optics. Interestingly, the team found that precipitates of these salts are photoactive and, when exposed to laser light, easily damage the optic's surface. Bude explains, "What we found is that each of the salt crystals studied absorbed sufficient light to initiate a damage event, and the way a precipitate is formed governs its laser damage behavior more than its chemical composition and bulk optical properties."

Because the concentration of impurities in these experiments was high, the precipitates were micrometer in size, much larger than the nanometer-sized damage precursors expected to be on actual AMP-treated surfaces. To determine whether nanoscale precipitates could also cause damage, the team sprayed optic surfaces with an aerosol of DI water. The formed droplets contained impurities naturally found in the water and at a much lower concentration than in the salt experiments. "The precipitates in this case were submicrometer in size and invisible to optical microscopy, but when exposed to laser energy, they created damage sites many micrometers in size," says Bude. Such evidence led the team to deduce that precipitates of impurities derived from solutions during wet chemical processing could form high-fluence damage precursors on the surface, and that the DI water itself also may be to blame. The next step was to prove that these precipitates were the fluence-limiting precursors responsible for high-fluence damage.

Perseverance Pays Off

The team sought to improve the damage resistance of the optics by reducing the sources and probability of precipitation during all wet chemical-processing steps. Pinpointing the exact source of impurities was no simple feat. "Anything could have been causing the problem," says Bude. "Impurities could have been introduced



This graph compares damage density between the advanced mitigation process (AMP) and the newer AMP3, which is optimized to reduce the probability of precipitation from wet chemical processes. AMP3 achieves a 300 times reduction in overall damage density and a 7-joules-per-square-centimeter shift to higher fluences at 5-nanosecond pulses.

by the equipment used to process the optics or by the chemicals for etching and cleaning. They could have even come from the DI water system itself or from airborne contaminants during the final drying process." After working aggressively to isolate and analyze all of the steps, the team was able to significantly reduce the damage density on sample optics.

By surveying the parts produced in the experiments, the team finally found a direct link between precipitates and damage. Atomic force microscopy studies of the optics' surfaces indicated the presence of precipitates, hundreds of nanometers in diameter and tens of nanometers high, and the concentration of these precipitates was correlated to the damage density.

The team then introduced controlled quantities of impurities in each step of the process to determine how pure the DI water and other processing chemicals needed to be to achieve stable damage-resistant surfaces. The researchers found that impurities introduced to the etch bath at 10 to 100 parts per billion produced a noticeable increase in damage even when the parts were rinsed with high-purity water after the etch. Ultimately, the team discovered that in an optimal process, impurities at parts per billion introduced at the end of the final rinse were predominantly responsible for the increased damage. In fact, the most damage-resistant surfaces required semiconductor-grade water with an impurity content too low to detect by standard conductivity measurements.

Case Closed

The team's findings led to a comprehensive protocol for wet chemical processing (AMP3) that significantly reduces precipitation of impurities during critical steps. "In addition to processing all samples in a Class 100 clean room, we renewed all ion exchange beds used to prepare our DI water supply, introduced standardized high-purity Teflon fixtures, and instituted standardized pre- and postetch cleaning and rinsing protocols," says Bude. "We have optimized the etching and rinsing to achieve a stable, damage-resistant surface."

Not only can AMP3 reduce damage on optics by more than two orders of magnitude compared to AMP, but it also enables a 60 percent increase in the amount of energy that can pass through an optic without damage. Recent results show a continued progression toward zero damage through a reduction of 2,000 precursors in damage density, which doubles the damage threshold. AMP3 is now under development to be scaled to full-size NIF optics. Although Bude and his team suggest that further advances in understanding the complex chemistry involved in etching, cleaning, rinsing, and drying optical materials will lead to further NIF performance improvements and reductions in operational costs, its work has brought closure to a long-standing optics dilemma. "We met all our project milestones and deliverables to the point of eliminating high-fluence damage precursors for optics," says Bude. For these scientists turned detectives, the case is closed on the source of high-fluence damage precursors and how to eliminate them.

—Caryn Meissner

Key Words: advanced mitigation process (AMP), atomic force microscopy, damage precursor, deionized (DI) water, fused silica, Laboratory Directed Research and Development (LDRD) Program, National Ignition Facility (NIF), optics mitigation.

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Investing in Early Career Researchers

AMONG the forces driving innovation, scientific discovery, technical advancement, and career development at Lawrence Livermore, none have been as effective as the Laboratory Directed Research and Development (LDRD) Program. Established by Congress in 1991 to maintain the health and technical vitality of the Department of Energy's (DOE's) national laboratories, LDRD is the largest single source of internal investment in Lawrence Livermore's future. Currently funded at about $81 million annually, the program supports about 150 Livermore projects selected through an extensive peer-review process.

A high-priority goal of LDRD is to advance the frontier of basic science in support of the Laboratory's missions. LDRD-funded projects have made essential contributions to every facet of national security, including stockpile stewardship, high-energy-density matter, high-performance computing and simulation, materials science, chemistry, information systems, biosecurity, cybersecurity, and energy. Many Livermore programs trace their roots to research that began under LDRD sponsorship.

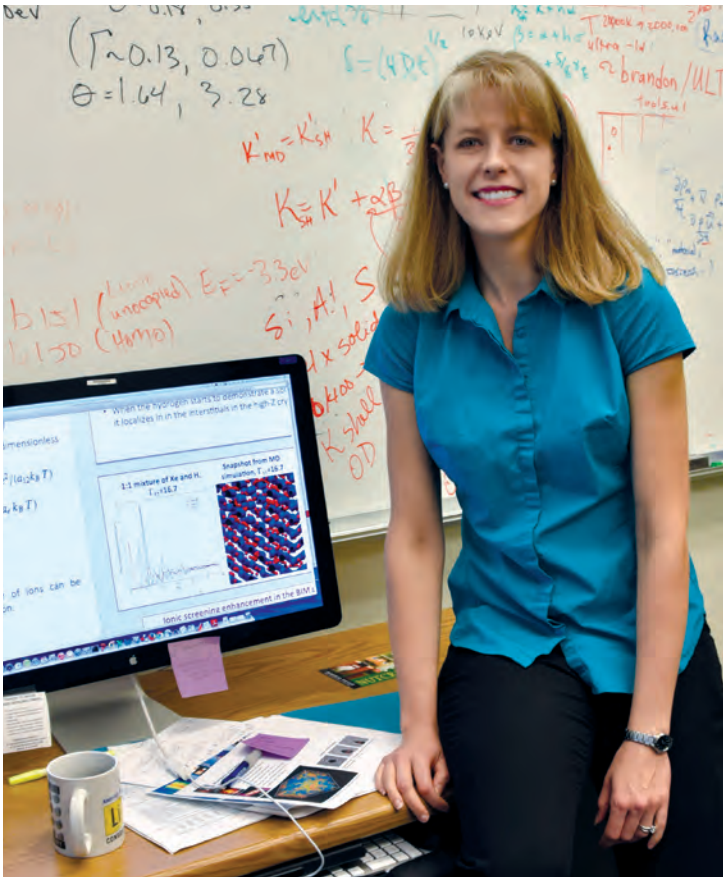
"LDRD is critical for anticipating future needs and avoiding technical surprises," says Rokaya Al-Ayat, who oversees the LDRD Program as special assistant to the Laboratory director. "Its focus is on high-risk, high-payoff research not yet ready for a program sponsor to fund." For example, the LDRD Program invested in research advancing biosecurity and biodetection long before they became indispensable tenets of national security.

By any measure, the LDRD Program has been a success. The projects funded by the program have frequently earned national recognition through awards, papers published in peer-reviewed journals, and patents. Roughly one-half of patents and one-half of Livermore's R&D 100 awards have stemmed from LDRD projects. The program has also been a major vehicle for attracting, training, and retaining new technical staff.

A comprehensive peer-reviewed proposal submission process results in about 10 percent of the entries being selected for LDRD funding annually. The competition is open to all Laboratory scientists and engineers. However, early career scientists and engineers (within 10 years of having received an advanced degree), including postdoctoral researchers, are particularly encouraged to apply. Three outstanding recent recipients—theoretical chemist Heather Whitley, physicist Miguel Morales-Silva, and particle physicist Gianpaolo Carosi—exemplify LDRD-funded early career scientists who are making a difference in their fields. In addition, all three have been honored with prestigious external awards: two earned a Presidential Early Career Award for Scientists and Engineers (PECASE), and one earned a DOE Early Career Research Program Award.

Microphysics of Dense Plasmas

Whitley came to the Laboratory in 2007 as a postdoctoral researcher from the University of California at Berkeley. She initially joined a quantum simulations group, where she used supercomputer simulations to study the properties of semiconductor nanomaterials that could eventually be applicable to solar cells and other clean-energy technologies.



Scientist Heather Whitley uses supercomputer simulations to expand understanding of dense plasma microphysics. (Photo by Alexandria Ballard.)

Taking advantage of her supercomputer simulation expertise, Whitley collaborated with physicist Frank Graziani on his LDRD effort focused on using simulations to enhance the fundamental understanding of complex plasmas. This project allowed her to work closely with Weapons and Complex Integration (WCI) Principal Directorate scientists and engineers, and she subsequently joined WCI in 2011 as a staff member.

In 2012, Whitley received a PECASE, which is considered the highest honor bestowed by the U.S. government on early career science and engineering professionals. The award recognized her work in applying Monte Carlo techniques to produce very accurate quantum statistical potentials for use in molecular dynamics codes. She currently works to expand the understanding of dense plasma microphysics for both stockpile stewardship and experiments at the National Ignition Facility. The award is providing her with $50,000 annually for five years to continue this research.

Whitley has been a coinvestigator on two LDRD efforts. In the first, with Graziani again as principal investigator, she applied a recently developed massively parallel molecular dynamics code to investigate the validity of specific models for plasma thermal conductivity. In the second LDRD effort, led by principal investigator physicist Robert Rudd, the molecular dynamics code is being extended to include multiscale models for more accurate simulations of transport across material interfaces.

"We're looking at the atomic level to learn about the physics of atoms, ions, and electrons with our simulations," says Whitley. "The properties of all matter depend on what happens at this level. We are using simulations to function as a virtual laboratory to achieve high-energy-density regimes difficult to attain experimentally." The research work will likely benefit stockpile stewardship by providing a better understanding of the physics underlying aging nuclear weapons. "An ideal way to improve codes is to make connections between theory, simulation, and experiment," adds Whitley.

"The LDRD process is extremely competitive. Although one must devote a great deal of energy to prepare a proposal, it is very worthwhile to receive funding," observes Whitley. "The LDRD Program provides the Laboratory with a way to bring in new talent and ideas."

When Hydrogen Becomes a Metal

Morales-Silva joined the Laboratory's equation of state and materials theory group in 2010 after earning his Ph.D. in physics from the University of Illinois at Urbana–Champaign in 2009. Morales-Silva is the principal investigator for an LDRD project focused on understanding metallic hydrogen.

Physicist Miguel Morales-Silva analyzes extreme states of hydrogen. (Photo by Alexandria Ballard.)

During graduate school, Morales-Silva worked on a promising but challenging method (quantum Monte Carlo calculations) to analyze the behavior of hydrogen at high temperatures and pressures, in particular when the element exhibits metallike behavior. Livermore's LDRD Program provided Morales-Silva the funding to pursue this method at lower temperatures (up to room temperature) and very high pressures (2 to 6 megabars). Morales-Silva's receipt of a PECASE supported his use of advanced computational techniques to study materials at extreme conditions.

Although hydrogen is the simplest element in the universe, it possesses fascinating properties that have puzzled scientists for decades. For example, the electrons of compressed hydrogen tend to delocalize—similar to a metal. "Metallic hydrogen represents the holy grail of high-pressure physics," says Morales-Silva. Despite decades of efforts from experimental groups, details are lacking about this novel state of hydrogen. "It's hard to find answers about metallic hydrogen experimentally," says Morales-Silva. "We need supercomputers for this research, but our calculation methods are lagging. We must complement experiments by improving quantum Monte Carlo methods as an alternative to first-principles calculations." He believes the LDRD results will eventually enhance the accuracy of the Livermore codes and models used in stockpile stewardship science. In addition, this research may provide scientists with a better understanding of planet formation.

Morales-Silva is coinvestigator on another LDRD effort that uses quantum Monte Carlo calculations to predict the behavior of elements heavier than hydrogen. "We're trying to push the applications of quantum Monte Carlo methods across the periodic table of elements. We want to predict, with high confidence, the properties of elements solely with simulation."

Morales-Silva says, "The LDRD Program is essential to attracting people doing basic science that will be critical in the future to Livermore programs. I am confident our work will eventually prove useful to the programs. I am doing my best science and writing my best papers." He adds, "Without the LDRD Program, for someone such as myself who is interested in basic science, the Laboratory would be much less attractive. This LDRD project has helped me become an independent researcher and has provided an important first step in my career."

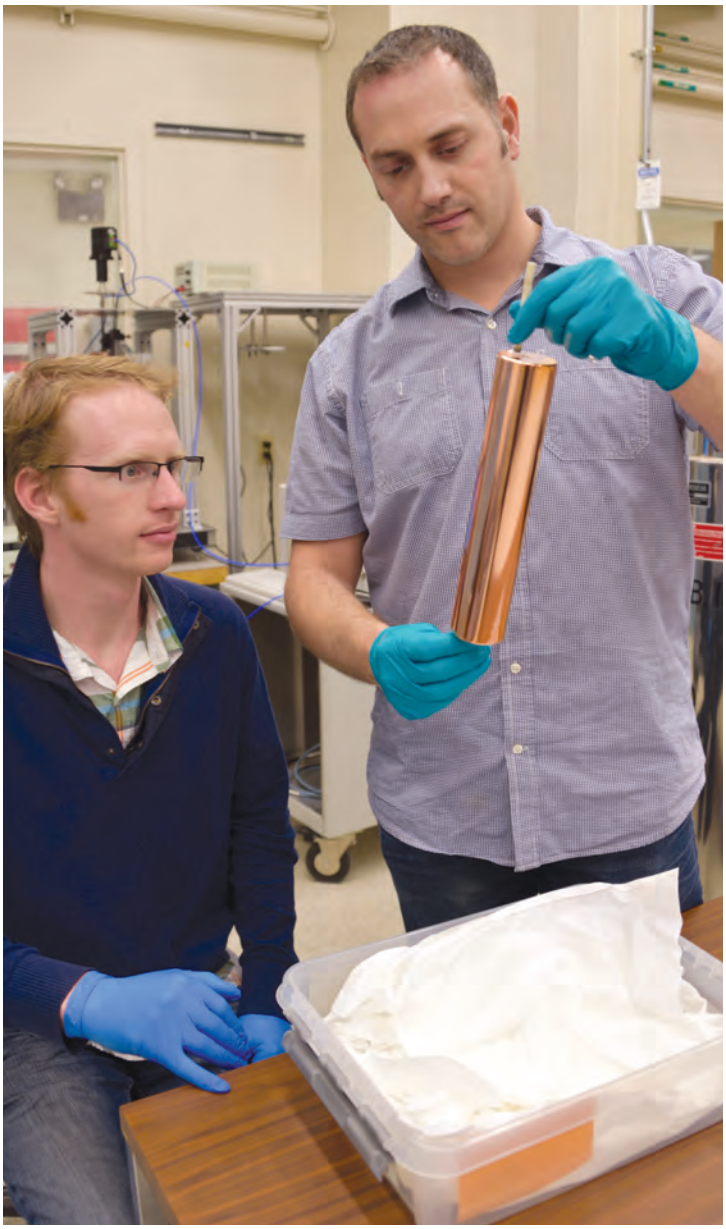
Searching for Dark Matter

Carosi, who received his Ph.D. from the Massachusetts Institute of Technology, came to the Laboratory in 2006. Carosi was coinvestigator on an LDRD project that ended in 2009, which involved the groundbreaking Axion Dark Matter Experiment (ADMX), established at Livermore with LDRD support. The experiment is now centered at the University of Washington, and Carosi is a collaborator.

The ADMX research team seeks to detect hypothetical dark-matter elementary particles called axions. Dark matter is estimated to make up about 23 percent of the energy density of the universe, while the remainder is a mysterious, repulsive "dark energy," which accounts for about 73 percent, and ordinary matter, which makes up only about 4 percent. ADMX is designed to find these dark-matter axions by measuring their decay into microwave-frequency photons in the presence of a strong magnetic field.

Because the expected signal from the decay of axions is so faint (about 10^{-24} watts), sensitive amplifiers are needed to boost the signal to a detectable level. The LDRD involving Carosi resulted in the design of microstrip superconducting quantum interference devices (SQUIDs), which are tiny rings of superconducting metal that serve as extremely low-noise amplifiers when cooled to near absolute zero. The SQUID amplifiers are designed to magnify the extremely small power signals emitted by axions in a 1-meter-tall microwave cavity structure built by Carosi. This promising approach earned Carosi a 2012 DOE Early Career Research Program Award, which consists of $500,000 annually for five years to continue this research.

"Our SQUID amplifier relies on quantum mechanics to create the quietest microwave receiver possible," Carosi says. He compares the SQUID amplifier to an ultrasensitive radio that minimizes the static hiss from background noise to allow very weak, distant stations (from the decay of axions) to be heard. Discovery of an axion would further our understanding of dark matter, the nature of quantum physics, and the force that binds atomic nuclei. SQUIDs also have potential applications in oil exploration, brain imaging, quantum computing, and secure communications.



Physicist Gianpaolo Carosi (standing) and University of California at Berkeley student Jaben Root inspect a copper tuning rod for the Axion Dark Matter Experiment apparatus. This experiment uses a tunable resonant cavity immersed in a strong magnetic field to search for axion dark matter particles converting to detectable microwaves. (Photo by Alexandria Ballard.)

Carosi was also part of another LDRD effort that was led by physicist Adam Bernstein to develop rare-event detectors for nuclear science and security. This project focused on detecting neutral particles such as neutrinos and antineutrinos emitted by nuclear materials and reactors. "We eventually would like to build a worldwide neutrino monitoring program," says Carosi. Remote nuclear reactor monitoring using advanced detectors could revolutionize global nuclear nonproliferation efforts by monitoring reactors hundreds of kilometers away and detecting fissile material from hundreds of meters away.

Carosi compares Lawrence Livermore's LDRD process to national competitions for federal research funding. The competition is stiff, and only the very best ideas are awarded funding. He says, "It's one of the most important factors that attracts postdocs, and it allows risky new ideas to percolate." Al-Ayat adds that LDRD funding allows young scientists to explore basic science questions and then move on to become an integral part of Laboratory programs important to national security. For both early career and well-established scientists, the LDRD Program continues to be prized for keeping the Laboratory's research atmosphere vital, productive, and exciting.

—Arnie Heller

Key Words: Axion Dark Matter Experiment (ADMX), Department of Energy (DOE) Early Career Research Program Award, Laboratory Directed Research and Development (LDRD) Program, Presidential Early Career Award for Scientists and Engineers (PECASE), Superconducting Quantum Interference Device (SQUID).

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Patents and Awards

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

Thermal Cycler

William J. Benett, John T. Andreski, John M. Dzenitis, Anthony J. Makarewicz, Dean R. Hadley, Satinderpall S. Pannu
U.S. Patent 8,778,663 B2
July 15, 2014
A thermal cycler includes two thermal cycler body sections, each with a face. A cavity is formed by the first and second faces, inside of which a thermal cycling unit is positioned. A heater trace unit is connected to a support section, the two thermal cycler body sections, and the thermal cycling unit. The two sections are positioned together against the support section to enclose both the thermal cycling unit and the heater trace unit.

Plasmon Resonant Cavities in Vertical Nanowire Arrays

Mihail Bora, Tiziana C. Bond, Benjamin J. Fasenfest, Elaine M. Behymer
U.S. Patent 8,780,439 B2
July 15, 2014
Tunable plasmon resonant cavity arrays in paired parallel nanowire waveguides are presented. Resonances can be observed when the waveguide length is an odd multiple of quarter plasmon wavelengths, consistent with boundary conditions of node and antinode at the ends. Two nanowire waveguides can satisfy the dispersion relation of a planar metal–dielectric–metal waveguide whose equivalent width is equal to the square-field average-weighted gap. Confinement factors of over 10^3 are possible due to plasmon focusing in the interwire space.

Nanoscale Array Structures Suitable for Surface Enhanced Raman Scattering and Methods Related Thereto

Tiziana C. Bond, Robin Miles, James C. Davidson, Gang Logan Liu
U.S. Patent 8,786,852 B2
July 22, 2014
These methods are used to fabricate and characterize nanoscale array structures for surface-enhanced Raman scattering. Nanoscale array structures may comprise nanotrees, nanorecesses, and tapered nanopillars.

Electron Beam Diagnostic System Using Computed Tomography and an Annular Sensor

John W. Elmer, Alan T. Teruya
U.S. Patent 8,791,426 B2
July 29, 2014
A system for analyzing an electron beam includes a circular electron-beam diagnostic sensor adapted to receive the electron beam. The sensor has a central axis, and connected to the sensor is an annular sensor structure that receives the electron beam. The system sweeps the electron beam radially outward from the central axis of the electron-beam diagnostic sensor to the annular sensor structure, wherein the beam is intercepted and measured.

Optical Waveguides Having Flattened High Order Modes

Michael Joseph Messerly, Raymond John Beach, John Edward Heebner, Jay Walter Dawson, Paul Henry Pax
U.S. Patent 8,798,422 B2
August 5, 2014
A deterministic methodology is provided for designing optical fibers that support field-flattened, ringlike higher order modes. The effective and group indices of these modes can be tuned by adjusting the widths of the guide's field-flattened layers or the average index of certain groups of layers. The approach outlined here provides a path to designing fibers that simultaneously have large mode areas and large separations between the propagation constants of the modes.

Harmonic Engine

Charles L. Bennett, Noel Sewall, Carl Boroa
U.S. Patent 8,807,012 B1
August 19, 2014
This engine is based on a reciprocating piston engine that extracts work from pressurized working fluid. The engine includes a harmonic oscillator inlet valve capable of oscillating at a resonant frequency for controlling the flow of working fluid into the engine. In particular, the inlet valve includes a valve head and a spring arranged together as a harmonic oscillator so that the inlet valve head is movable from an unbiased, equilibrium position to a biased, closed position to occlude the inlet. When the inlet valve is released, the inlet valve head undergoes a single oscillation past the equilibrium position to a maximum, open position and returns to a biased, return position near the closed position. In this way, it chokes the flow and produces a pressure drop across the inlet valve, causing the valve to close. Protrusions carried by either the inlet valve head or the piston head are used to bump open the inlet valve from the closed position and initiate the single oscillation of the inlet valve head. Protrusions carried by either the outlet valve head or the piston head are used to close the outlet valve ahead of the bump that opens the inlet valve.

Carbon Ion Pump for Removal of Carbon Dioxide from Combustion Gas and Other Gas Mixtures

Roger D. Aines, William L. Bourcier
U.S. Patent 8,808,433 B2
August 19, 2014
This ion pump system is designed to separate carbon dioxide from flue gas. Instead of relying on large temperature or pressure changes to remove carbon dioxide from a solvent used to absorb it from flue gas, the ion pump method dramatically increases the concentration of dissolved carbonate ion in solution. The overlying vapor pressure of carbon dioxide gas is thus increased, permitting carbon dioxide as a pure gas to be removed from the downstream side of the ion pump. The ion pumping may be obtained from reverse osmosis, electrodialysis, thermal desalination, or an ion pump system that has an oscillating flow synchronized with an induced electric field.

Fluidics Platform and Method for Sample Preparation and Analysis

W. Henry Benner, John M. Dzenitis, William J. Benett, Brian R. Baker
U.S. Patent 8,808,643 B1
August 19, 2014
Herein provided are a fluidics platform and a method for sample preparation and analysis. The fluidics platform can analyze DNA from blood samples using amplification assays such as polymerase chain reaction and loop-mediated isothermal amplification. The platform can also be used for other types of assays and analyses. In some configurations, a sample in a sealed tube can be inserted directly. The following isolation, detection, and analyses can be performed without a user's intervention. The disclosed platform may also comprise a sample preparation system with a magnetic actuator, a heater, and an air-drying mechanism. Fluid manipulation processes include extraction, washing, elution, assay detection, and cleaning after reactions and between samples.

Porous Substrates Filled with Nanomaterials
Marcus A. Worsley, Theodore F. Baumann, Joe H. Satcher, Jr., Michael Stadermann
U.S. Patent 8,809,230 B2
August 19, 2014
This composition has at least one carbon monolith, such as a carbon aerogel, with internal pores and at least one nanomaterial, such as carbon nanotubes, disposed uniformly throughout the internal pores. The nanomaterial can be disposed in the middle of the monolith. In addition, a method for making a monolithic solid with both high surface area and good bulk electrical conductivity is provided. A porous substrate with a thickness of 100 micrometers or more and macropores throughout its thickness is prepared. At least one catalyst is deposited inside the porous substrate. Chemical vapor deposition is then used to uniformly deposit a nanomaterial in the macropores throughout the thickness of the porous substrate. Applications include electrical energy storage, such as batteries and capacitors, and hydrogen storage.

Spatial Clustering of Pixels of a Multispectral Image
James Lynn Conger
U.S. Patent 8,811,754 B2
August 19, 2014
A system for clustering the pixels of a multispectral image is provided. The clustering system computes a maximum spectral similarity score for each pixel, which indicates the similarity between that pixel and the most similar neighbor. To determine the maximum similarity score for a pixel, the clustering system generates a similarity score between that pixel and each of its neighboring pixels and selects the similarity score that represents the highest similarity as the maximum similarity score. The system may apply a filtering criterion based on the maximum similarity score so that pixels with similarity scores below a minimum threshold are not clustered. The system changes the current values of the pixels in a cluster based on an average of the original values of the cluster's pixels.

Targeted Antimicrobials and Related Compositions, Methods and Systems
Paul J. Jackson, Brian E. Souza, Feliza A. Bourguet, Matthew A. Coleman
U.S. Patent 8,821,860 B2
September 2, 2014
Targeted antimicrobials are described as well as related compositions, methods, and systems.

Systems and Methods of Varying Charged Particle Beam Spot Size
Yu-Jiuan Chen
U.S. Patent 8,822,946 B2
September 2, 2014
These devices enable shaping of a charged-particle beam. A modified dielectric wall accelerator includes a high-gradient lens section and a main section. The high-gradient lens section can be dynamically adjusted to establish the desired electric fields to minimize undesirable transverse defocusing fields at the entrance to the dielectric wall accelerator. Once a baseline setting with the desired output beam characteristic is established, the beam's characteristics can be varied by slightly adjusting the electric fields established across different sections of the modified dielectric wall accelerator. The beam's shape can also be controlled by introducing intentional timing desynchronization offsets and producing an injected beam that is not fully matched to the entrance of the modified dielectric accelerator.

Passive Magnetic Bearing System
Richard F. Post
U.S. Patent 8,823,233 B2
September 2, 2014
An axial stabilizer for the rotor of a magnetic bearing provides external control of stiffness through switching in external inductances. External control also allows the stabilizer to become a part of a passive–active magnetic bearing system that requires no external source of power and no position sensor. Stabilizers for displacements transverse to the axis of rotation require only a single cylindrical Halbach array for operation and thus are especially suited for use in high-rotation-speed applications, such as flywheel energy storage systems. Eliminating the need for an inner cylindrical array solves the difficult mechanical problem of supplying support against centrifugal forces for the magnets of that array. Compensation is provided for the temperature variation in the magnetic field strength of permanent magnets in the levitating magnet arrays.

Web-Based Emergency Response Exercise Management Systems and Methods Thereof
John W. Goforth, Michael B. Mercer, Zach Heath, Lynn I. Yang
U.S. Patent 8,827,714 B2
September 9, 2014
This method simulates portions of an emergency response exercise by generating situational awareness outputs associated with a simulated emergency and sending those outputs to multiple output devices. The method also sends decisions associated with the situational awareness outputs at a decision point to a user device and receives a selected decision from the user. It then generates new situational awareness outputs based on the selected decision and repeats the sending, outputting, and receiving steps based on the new situational awareness outputs. Other methods, systems, and computer program products are included.

Method and System for Polishing Materials Using a Nonaqueous Magnetorheological Fluid
Joseph Arthur Menapace, Paul Richard Ehrmann
U.S. Patent 8,828,262 B2
September 9, 2014
A nonaqueous magnetorheological fluid includes a primarily organic carrier liquid and magnetizable particles. The fluid also includes a buffer, a stabilizer, and water, and it has a pH between 6.5 and 9.0.

Use of Carbonates for Biological and Chemical Synthesis
Gregory Hudson Rau
U.S. Patent 8,828,706 B2
September 9, 2014
This system uses carbonates, especially water-insoluble or sparing soluble mineral carbonates, to maintain or increase dissolved inorganic carbon concentrations in aqueous media. In particular, the system generates concentrated dissolved inorganic carbon substrates for photosynthetic, chemosynthetic, or abiotic chemical production of carbonaceous or other compounds in solution. In some embodiments, the invention can also enhance the dissolution and retention of carbon dioxide in aqueous media and can produce pH buffering capacity, metal ions, and heat, which can be beneficial to the preceding syntheses.

Disposable and Removable Nucleic Acid Extraction and Purification Cartridges for Automated Flow-Through Systems

John Frederick Regan
U.S. Patent 8,828,716 B2
September 9, 2014
Removable cartridges are used on automated flow-through systems to extract and purify genetic material from complex matrices. Different types of cartridges are paired with specific automated protocols to concentrate, extract, and purify pathogenic or human genetic material. Their flow-through nature allows large quantities of sample to be processed. Matrices may be filtered using size exclusion or affinity filters to concentrate the pathogen of interest. Lysed material is ultimately passed through a filter to remove the insoluble material. The soluble genetic material is then delivered past a silicalike membrane that binds the genetic material, where it is washed, dried, and eluted. Cartridges are inserted into the housing areas of flow-through automated instruments, which are equipped with sensors to ensure proper placement and usage of the cartridges. Properly inserted cartridges create fluid- and air-tight seals with the flow lines of an automated instrument.

Ultraviolet Radiation Detector and Dosimeter

Craig F. Smith, Vladimir Ryzhikov, Sergei Naydenov, Dennis Wood, Volodymyr Perevertailo
U.S. Patent 8,829,457 B2
September 9, 2014
An ultraviolet radiation dosimeter apparatus measures an individual's radiation exposure from incoming ultraviolet rays. The device includes a dosimeter body with an ultraviolet filter and a detector semiconductor substrate for detecting incoming ultraviolet rays and producing a signal. The semiconductor substrate is made of zinc–selenium(tellurium). A chip in the dosimeter body receives the signal and measures the individual's exposure from the incoming ultraviolet rays.

Three-Dimensional Boron Particle Loaded Thermal Neutron Detector

Rebecca J. Nikolic, Adam M. Conway, Robert T. Graff, Joshua D. Kuntz, Catherine Reinhardt, Lars F. Voss, Chin Li Cheung, Daniel Heineck
U.S. Patent 8,829,460 B2
September 9, 2014
Three-dimensional, boron-particle-loaded, thermal neutron detectors use neutron-sensitive conversion materials in the form of nanopowders and micrometer-sized particles, rather than other approaches such as thin films, suspensions, and paraffin. Methods are used to infiltrate, intersperse, and embed the neutron nanopowders to form two- or three-dimensional charge-sensitive platforms. The use of nanopowders enables conformal contact with the entire charge-collecting structure regardless of its shape or configuration.

Methods and Systems for Raman and Optical Cross-Interrogation in Flow-Through Silicon Membranes

Tiziana C. Bond, Sonia E. Letant
U.S. Patent 8,830,450 B2
September 9, 2014
Cross-interrogating photonic detection systems and methods are shown. A flow-through photonic crystal membrane with a surface-enhanced Raman scattering (SERS) substrate is provided with pores distributed along multiple regions. The pores of one region have walls to which a first type of target-specific anchor can be attached, while pores of another region have walls to which a second type of target-specific anchor can be attached. An optical arrangement out of plane to the SERS substrate is also provided for enhanced sensitivity and identification of target organisms.

Separation of a Target Substance from a Fluid or Mixture Using Encapsulated Sorbents

Roger D. Aines, Christopher M. Spadaccini, Joshuah K. Stolaroff, William L. Bourcier, Jennifer A. Lewis, Eric B. Duoss, John J. Vericella
U.S. Patent 8,834,605 B2
September 16, 2014
This apparatus separates a target substance from a fluid or mixture using capsules with a coating and encapsulated stripping solvents. The coating is permeable to the target substance. When the capsules are exposed to the fluid or mixture, the target substance migrates through the coating and is taken up by the stripping solvents. The substance is separated from the fluid or mixture by driving it from the capsules.

Bio-Threat Microparticle Simulants

George Roy Farquar, Roald Leif
U.S. Patent 8,835,178 B2
September 16, 2014
A biothreat simulant includes a carrier with encapsulated DNA. Steps are described for encapsulating DNA into the carrier to produce a biothreat simulant.

Mixed Crystal Organic Scintillators

Natalia P. Zaitseva, M. Leslie Carman, Andrew M. Glenn, Sebastien Hamel, Robert Hatarik, Stephen A. Payne, Wolfgang Stoeffl
U.S. Patent 8,835,865 B2
September 16, 2014
A mixed organic crystal includes a single mixed crystal with two compounds and different bandgap energies. The organic crystal exhibits a signal response signature for neutrons from a radioactive source. This signature does not include a significantly delayed luminescence characteristic of neutrons interacting with the organic crystal, relative to the luminescence that characterizes gamma rays interacting with the organic crystal. In one configuration, the organic crystal includes bibenzyl and stilbene or a stilbene derivative, and it exhibits a signal response signature for neutrons from a radioactive source.

Initiation Disruptor Systems and Methods of Initiation Disruption

Dennis W. Baum
U.S. Patent 8,839,704 B2
September 23, 2014
An initiation disruption system includes an explosive charge, a plurality of particles in a layer at least partially surrounding the explosive charge, and a fire suppressant adjacent to the particles. One method for disabling an object is to place the system near that object, initiating the explosive charge and thereby applying mechanical loading to the object so that the object is disabled. In another design, a device has a plurality of particles bound by a binder, thereby defining a sidewall with an interior for receiving an explosive, and a fire suppressant adjacent to the particles and binder.

Silica Extraction from Geothermal Water

William L. Bourcier, Carol J. Bruton
U.S. Patent 8,840,859 B2
September 23, 2014
This method produces silica from geothermal fluid containing a low concentration of the silica (less than 275 parts per million). Steps include treating the geothermal fluid by reverse osmosis, seasoning the fluid to produce a slurry with precipitated colloids that contain the silica, and separating the silica from the slurry.

Emergency Sacrificial Sealing Method in Filters, Equipment, or Systems

Erik P. Brown
U.S. Patent 8,844,938 B2
September 30, 2014
A system seals a filter or equipment component to a base and will continue to seal the filter or equipment component to the base in the event of hot air or a fire. The system includes a first sealing material between the filter or equipment component and the base, and a second sealing material between the filter or equipment component as well as the base and proximate the first sealing material. The first and second sealing materials are positioned relative to each other and relative to the filter or equipment component and the base to seal the filter or equipment component to the base. In the event of a fire, the second sealing material will be activated and will expand to seal the filter or equipment component to the base.

Real-Time System for Imaging and Object Detection with a Multistatic GPR Array

David W. Paglieroni, N. Reginald Beer, Steven W. Bond, Philip L. Top, David H. Chambers, Jeffrey E. Mast, John G. Donetti, Blake C. Mason, Steven M. Jones
U.S. Patent 8,854,248 B2
October 7, 2014

Spatially Assisted Down-Track Median Filter for GPR Image Post-Processing

David W. Paglieroni, N. Reginald Beer
U.S. Patent 8,854,249 B2
October 7, 2014
A real-time imaging system detects the presence of subsurface objects within a medium. In some embodiments, the imaging and detection system operates in a multistatic mode to collect radar return signals that travel down the surface and are generated by an array of transceiver antenna pairs positioned across the surface. The system preprocesses the return signals to suppress certain undesirable effects. The system produces synthetic aperture radar images from real aperture radar images generated from the preprocessed return signal. The system then postprocesses the synthetic aperture radar images to improve detection of subsurface objects. The system identifies peaks in the energy levels of the postprocessed image frame, which indicate the presence of a subsurface object.

Tracking Target Objects Orbiting Earth Using Satellite-Based Telescopes

Willem H. De Vries, Scot S. Olivier, Alexander J. Pertica
U.S. Patent 8,862,398 B2
October 14, 2014
A system for tracking objects in Earth's orbit uses a constellation or network of satellites featuring imaging devices. An object-tracking system includes a ground controller and, for each satellite in the constellation, an onboard controller. The ground controller receives ephemeris information for a target object and directs that information to the satellites. Each onboard controller receives ephemeris information for a target object, collects images of the object based on the expected location of the object at an expected time, identifies actual locations of the object from the collected images, and identifies a next-expected location based on the identified actual locations of the object. The onboard controller processes the collected image to identify the actual location of the target object and transmits that location information to the ground controller.

High Speed, Real-Time, Camera Bandwidth Converter

Dan E. Bower, David A. Bloom, James R. Curry
U.S. Patent 8,866,915 B2
October 21, 2014
Image data from a complementary metal-oxide semiconductor sensor with 10-bit resolution is reformatted in real time to allow the data to stream through communications equipment that is designed to transport data with 8-bit resolution. The incoming image data have 10-bit resolution. The communication equipment can transport image data with 8-bit resolution. Image data with 10-bit resolution is transmitted in real time—without a frame delay—through the communication equipment by reformatting the data.

Tethered Catalysts for the Hydration of Carbon Dioxide

Carlos A. Valdez, Joe H. Satcher, Jr., Roger D. Aines, Sergio E. Wong, Sarah E. Baker, Felice C. Lightstone, Joshuah K. Stolaroff
U.S. Patent 8,877,069 B2
November 4, 2014
This system substantially increases the efficiency of carbon dioxide capture and removal by positioning a catalyst within an optimal distance from the air–liquid interface. The catalyst is positioned within the layer determined to be the highest concentration of carbon dioxide. A hydrophobic tether is attached to the catalyst, and this tether modulates the position of the catalyst within the liquid layer containing the highest concentration of carbon dioxide.

Methods and Systems Using Encapsulated Tracers and Chemicals for Reservoir Interrogation and Manipulation

Jeffery Roberts, Roger D. Aines, Eric B. Duoss, Christopher M. Spadaccini
U.S. Patent 8,877,506 B2
November 4, 2014
This apparatus, method, and system are used for reservoir interrogation. A tracer is encapsulated in a receptacle. The receptacle containing the tracer is injected into the reservoir. The tracer is analyzed for reservoir interrogation.

Ultrafast Transient Granting Radiation to Optical Image Converter

Richard E. Stewart, Stephen P. Vernon, Paul T. Steel, Mark E. Lowry
U.S. Patent 8,879,137 B2
November 4, 2014
A high-sensitivity, ultrafast transient-grating radiation-to-optical image converter is based on a fixed transmission grating adjacent to a semiconductor substrate. X rays or optical radiation passing through the fixed transmission grating is thereby modulated and produces a small periodic variation of refractive index or transient grating in the semiconductor through carrier-induced refractive index shifts. An optical or infrared probe beam tuned just below the semiconductor bandgap is reflected off a high-reflectivity mirror on the semiconductor so that the beam double passes and interacts with the radiation-induced phase grating therein. A small portion of the optical beam is diffracted out of the probe beam by the radiation induced transient grating to become a converted signal imaged onto a detector.

System for Closure of a Physical Anomaly
Jane P. Bearinger, Duncan J. Maitland, Daniel L. Schumann, Thomas S. Wilson
U.S. Patent 8,882,786 B2
November 11, 2014
These systems are used for closure of a physical anomaly. Closure is accomplished by a closure body with an exterior surface. The exterior surface contacts the opening of the anomaly and then closes the anomaly. The closure body has a primary shape for closing the anomaly and a secondary shape for being positioned in the physical anomaly. The closure body preferably comprises a shape memory polymer.

Development of an Electronic Device Quality Aluminum Antimonide (AlSb) Semiconductor for Solar Cell Applications
John W. Sherohman, Jick Hong Yee, Arthur W. Combs, III
U.S. Patent 8,883,548 B2
November 11, 2014
Electronic-device-quality aluminum antimonide– (AlSb-) based single crystals produced by controlled atmospheric annealing are used in various configurations for solar-cell applications. The AlSb-based solar cell device provides direct conversion of solar energy to electrical power.

Nanolipoprotein Particles and Related Compositions, Methods, and Systems
Paul D. Hoeprich, Nicholas O. Fischer, Peter W. Mason, Craig D. Blanchette
U.S. Patent 8,883,729 B2
November 11, 2014
A functionalized nanolipoprotein particle uses an anchor substrate compound for binding with a corresponding anchor compound on a target molecule.

Post Polymerization Cure Shape Memory Polymers
Thomas S. Wilson, Michael Keith Hearon, Jane P. Bearinger
U.S. Patent 8,883,871 B2
November 11, 2014
This invention relates to chemical polymer compositions, methods of synthesis, and fabrication methods for devices regarding polymers capable of displaying shape-memory behavior. They can first be polymerized to a linear or branched polymeric structure and, with their thermoplastic properties, subsequently processed into a device through processes typical of polymer melts, solutions, and dispersions. They are then linked to a shape-memory thermoset polymer retaining the processed shape.

Gamma Ray Spectroscopy Employing Divalent Europium-Doped Alkaline Earth Halides and Digital Readout for Accurate Histogramming
Nerine Jane Cherepy, Stephen Anthony Payne, Owen B. Drury, Benjamin W. Sturm
U.S. Patent 8,884,233 B2
November 11, 2014
A scintillator radiation detector system, according to one embodiment, includes a scintillator and a processing device for processing pulse traces corresponding to light pulses from the scintillator, wherein pulse digitization is used to improve energy resolution of the system. A scintillator radiation detector system, according to another embodiment, includes a processing device for fitting digitized scintillation waveforms to an algorithm based on identifying rise and decay times and performing a direct integration of fit parameters. A method, according to yet another embodiment, includes processing pulse traces corresponding to light pulses from a scintillator, wherein pulse digitization is used to improve energy resolution of the system. In a further embodiment, a method includes fitting digitized scintillation waveforms to an algorithm based on identifying rise and decay times and performing a direct integration of fit parameters. Additional systems and methods are also presented.

Alkali Resistant Optical Coatings for Alkali Lasers and Methods of Production Thereof
Thomas F. Soules, Raymond J. Beach, Scott C. Mitchell
U.S. Patent 8,889,251 B2
November 18, 2014
In one embodiment, a multilayer dielectric coating for use in an alkali laser includes two or more alternating layers of high- and low-refractive index materials, wherein an innermost layer includes a layer thicker than 500 nanometers and less dense than 97 percent of a theoretical layer of the elements of alumina, zirconia, or hafnia for protecting subsequent layers of the two or more alternating layers of high- and low-index dielectric materials from an alkali attack. In another embodiment, a method for forming an alkali-resistant coating includes forming a first oxide material above a substrate and forming a second oxide material above the first oxide material to form a multilayer dielectric coating, wherein the second oxide material is on a side of the multilayer dielectric coating for contacting an alkali.

Immunostimulatory Nanoparticles and Related Compositions, Methods, and Systems
Paul D. Hoeprich, Nicholas O. Fischer, Craig Blanchette, Peter W. Mason
U.S. Patent 8,889,623 B2
November 18, 2014
Provided herein are immunostimulatory nanolipoprotein particles and related compositions, methods, and systems.

Fission Meter and Neutron Detection Using Poisson Distribution Comparison
Mark S. Rowland, Neal J. Snyderman
U.S. Patent 8,891,720 B2
November 18, 2014
This neutron detector system and method discriminates fissile material from nonfissile material, wherein a digital data-acquisition unit collects data at a high rate and in real time processes large volumes of data directly into information that a first responder can use to discriminate materials. The system comprises counting neutrons from an unknown source and detecting excess grouped neutrons to identify fission in the unknown source. Comparison of the observed neutron count distribution with a Poisson distribution is performed to distinguish fissile material from nonfissile material.

Awards

Amanda Randles, a Lawrence Fellow in Livermore's Computation Directorate, received a **Director's Early Independence Award** from the **National Institutes of Health** (NIH). This NIH Common Fund award provides funding to encourage exceptional young scientists to pursue high-risk, high-reward independent research in biomedical and behavioral science. Randles will receive approximately $2.5 million over five years, which will allow her to combine personalized, massively parallel computational models and experimental approaches to develop a way of predicting likely sites for cancer to metastasize. The goal of the project is to develop a method to simulate the flow of realistic levels of cells through the circulatory system, thereby gaining insight into mechanisms that underlie disease progression and localization. Randles is one of 85 recipients of the 2014 NIH Common Fund grants.

Livermore engineer **Scott Couture** received an award for **Meritorious Civilian Service** from the **U.S. Air Force** for his work as principal adviser for nuclear plans and policies to the Under Secretary of the Air Force, Eric Fanning. Couture, who works in the Laboratory's Weapons and Complex Integration (WCI) Principal Directorate, served as principal adviser from May 2012 until May 2014. Since joining Lawrence Livermore in 1992, Couture has worked on robotics for nuclear waste handling and on precision machine tools for the National Ignition Facility. More recently, for WCI, he has contributed to weapons surveillance, annual assessments, and plutonium shipping containers.

Radoslav Radev received the **International Electrotechnical Commission**'s (IEC's) **1906 Award** for his work on developing international standards for radiation detection instrumentation. Radev has served as an expert on the Nuclear Instrumentation Technical Committee and its Radiation Protection Instrumentation Subcommittee since 2002. He received this recognition for his exceptional contributions to the development of more than a dozen international standards for radiation protection instruments and for border control instrumentation preventing illicit trafficking of radioactive and special nuclear material. The IEC 1906 Award also distinguished Radev for being the project leader for the major revision of the IEC 61005 "Neutron Ambient Dose Equivalent (Rate) Meters" standard, published in 2014.

Founded in 1906 and based in Geneva, Switzerland, the IEC is the world's leading organization for developing and publishing international standards for all electrical, electronic, and related technologies. More than 10,000 experts from industry, commerce, government, research labs, and academia participate in IEC's standardization work.

Harold Conner, **Jr.**, associate director of Facilities and Infrastructure (F&I) within the Laboratory's Operations and Business Principal Directorate, received the **Alumni Professional Achievement Award** from his alma mater, the **University of Tennessee at Knoxville**. This award recognizes alumni who have achieved a high level of success in their field and who have a record of notable career accomplishments and a history of outstanding contributions to their profession.

Conner has a long list of career accomplishments. Prior to joining Livermore in 2007 as the associate director of F&I, Conner logged 40 years of experience with the Department of Energy and National Nuclear Security Administration (NNSA) leading nonnuclear, nuclear, low-hazard, and high-hazard operations. He built an extensive record of safely and cost-effectively managing and revitalizing facilities and infrastructure at the Savannah River Site, Oak Ridge Y-12, Oak Ridge K-25, and Idaho National Engineering and Environmental Laboratory.

Lawrence Livermore members of **NNSA**'s **Advanced Manufacturing Road Map Development Team** (AM Team) received the **NNSA**'s **Defense Programs Award of Excellence** for their work performed in support of the Stockpile Stewardship Program in 2014 (see the article beginning on p. 4). The award honors significant achievements in quality, productivity, cost savings, safety, or creativity in support of the nuclear weapons program. The Livermore-led AM Team includes 62 researchers from Livermore, Kansas City National Security Campus, Y-12 National Security Complex, Pantex Plant, Savannah River Site, and Los Alamos and Sandia national laboratories. The multidisciplinary team worked together to perform a thorough assessment of the AM technologies that could be used to transform the nuclear security enterprise, and produced a detailed reference document and road map that laid out a path forward for the Defense Program's investment in this area.

The Lawrence Livermore members of the AM Team include **Melissa Marggraff**, **Robert Maxwell**, **Alexander Gash**, **Jon Maienschein**, **Wayne King**, **Daniel Orlikowski**, **Joshua Kuntz**, **Thomas Wilson**, **Mark Bronson**, **Brandon Chung**, **Geoffrey Campbell**, **Diane Chinn**, **Gilbert Gallegos**, **Eric Duoss**, **Christopher Spadaccini**, **Mona Dreicer**, **Steven Peterson**, **Cynthia Brandt**, **Cary Spencer**, and **George Anzelon**.

Abstracts

Next-Generation Manufacturing for the Stockpile

Additive manufacturing (AM), often called three-dimensional printing, offers the National Nuclear Security Administration (NNSA) a new avenue for creating replacement nuclear weapons parts and related stockpile materials. Lawrence Livermore is collaborating with other NNSA laboratories and production plants to expand the range of materials and component types compatible with AM, develop a better fundamental understanding of the materials involved in AM, and exploit the flexibility of AM processes to enhance the properties and performance of components. NNSA's AM experts envision broad application for the technology across the weapons complex, from tools and foam cushions to metal lattice structures to more advanced materials such as high explosives and nuclear components. In time, AM could profoundly change how the nuclear weapons complex produces parts by shrinking the manufacturing production footprint and modernizing infrastructure, resulting in a more cost-effective and responsive stockpile.

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Building the Future: Modeling and Uncertainty Quantification for Accelerated Certification

In many industries, qualifying a new material for inclusion in a complex system is a multimillion-dollar, decade-long endeavor. With the advent of new manufacturing techniques, such as additive manufacturing (AM), that offer a faster, more flexible approach to producing complex components, developing alternative approaches to qualification becomes more urgent. Such matters are of great interest to Lawrence Livermore's vital and expanding AM research effort. With Laboratory Directed Research and Development Program funding, Livermore modeling experts are exploring how modeling and simulation, carefully chosen experiments, and uncertainty quantification can accelerate additively manufactured component qualification and address some of the quality challenges with which AM users are grappling. Metal AM methods, such as selective laser melting, sometime produce parts with distortions, too many pores, residual stresses that threaten part integrity, or surface-finish issues. Using data mining and multiscale modeling, powered by Livermore's parallel codes and massive computer resources and validated by experiments, the researchers have demonstrated their ability to predict and in some cases efficiently correct such problems. These early results suggest that this approach could help to streamline part qualification, which would benefit AM work and the national security initiatives it supports at the Laboratory.

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U.S. Government Printing Office: 2014/570-075-10008

Expanding Access to High-Performance Computing

At the Livermore Valley Open Campus, the High Performance Computing Innovation Center is partnering with private companies to further the Laboratory's missions and strengthen the nation's economic competitiveness.

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- *A new reactive transport model helps assess aging nuclear weapons.*
- *Upgrades at the National Ignition Facility set the course for more experiments and stronger partnerships.*

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P.O. Box 808, L-664
Livermore, California 94551

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