

November/December 2021

Science & Technology

REVIEW



Light-Source Experiments around the World

Also in this issue:

Polymer Production Enclave

Hydrodynamic Experiments

Early and Mid-Career Recognition Update

About the Cover

Multidisciplinary teams of Lawrence Livermore researchers are utilizing some of the largest, most complex machines on the planet—synchrotron radiation facilities that generate the world’s fastest, brightest x rays—to observe how elements react at the atomic scale under extreme conditions.

As the article on p. 4 describes, determining when a substance will shift between states plays a significant role in the materials and modeling simulation codes that the Laboratory uses to verify the safety, security, and effectiveness of the nation’s nuclear weapons stockpile.



Cover design: Mary J. Gines

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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Predatory Bacteria Impact Microbial Food Web

The word “predator” may conjure images of leopards killing and eating impala on the African savannah or great white sharks attacking elephant seals off the coast of California. Some microorganisms are also predators that kill and eat other bacteria. Just like their microbiology counterparts, bacteria belong to intricate food chains but until recently, it has been challenging for scientists to document their ecological significance.

A Lawrence Livermore-led research team discovered that predatory bacteria grow faster and consume more resources than nonpredatory bacteria. The team quantified the growth of predatory and nonpredatory bacteria in soils (and one stream) by tracking isotopically labeled substrates into newly synthesized DNA. Their findings were published in the April 27, 2021, issue of the journal *mBio*, published by the American Society for Microbiology.

The scientists studied three types of bacteria in soil—nonpredators, obligate predators, and facultative predators—and found that obligate-predatory bacteria grew 36 percent faster and assimilated carbon at rates 211 percent higher than nonpredatory bacteria. Livermore scientist Jennifer Pett-Ridge, a co-author of the paper, says, “These unique, quantitative measures of predator activity suggest that predatory bacteria—along with protists, nematodes, and phages—are active and important in microbial food webs.”

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Theoretical Laser-Driven Semiconductor

Engineers at Lawrence Livermore in collaboration with the University of Illinois Urbana-Champaign have designed and simulated a theoretical, laser-driven photo-conductive semiconductor switch (PCSS) that could support communication systems faster and more powerful than fifth-generation wireless technology. If realized, the device could achieve faster speeds at higher voltages than existing photoconductive devices and transfer more data over longer distances. The research, funded by the Laboratory Directed Research and Development Program, appeared in the May 5, 2021, issue of *IEEE Journal of the Electron Devices Society*.

Using experimental data and simulations, the team proposed that under extreme electric fields, the new, unique device could generate an electron-charged cloud in the base semiconductor material, gallium nitride (GaN). Unlike normal semiconductors, whose electrons move faster as the applied electrical field increases, gallium nitride, a wide bandgap material, generates a phenomenon called negative differential

mobility (NDM), where an electron cloud slows down, allowing the device to create extremely fast pulses and high-voltage signals at frequencies approaching one terahertz (10^{12} hertz) when exposed to electromagnetic radiation. This work represents the first attempt to use NDM to push the power-frequency bounds of a GaN PCSS toward the sub-terahertz regime—the frequency range of 500 to 1,000 gigahertz.

“The goal was to build a device significantly more powerful than existing technology but also capable of operating at very high frequencies,” says Livermore engineer Lars Voss. “The output pulse is shorter than the laser’s input pulse and acts like a compression device. You can compress an optical input into an electrical output, potentially generating extremely high-speed, high-power radio frequency waves.”

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Livermore Device Records Neuroscience Breakthrough

Brain activity in the hippocampus, a region responsible for memory and other cognitive functions, was previously thought to travel in one direction. A newfound phenomenon discovered using film-like electrodes developed at Lawrence Livermore suggests, however, that brain waves travel up and down the hippocampus, like a two-way street. The electrodes that recorded this never-before-seen brain activity were funded by the Defense Advanced Research Projects Agency’s Systems-Based Neurotechnology for Emerging Therapies Program, which aims to improve treatments for neuropsychiatric illnesses in military service members. The team’s findings were published in the May 12, 2021, issue of *Nature Communications*.

The device, smaller than a dime and consisting of a 32-channel, multielectrode array, was used by surgeons at the University of California at San Francisco to record electrical signals of conscious patients undergoing epilepsy-related surgery. When patients were given a cognitive test, their brain waves traveled toward the front of their hippocampus, and when they waited for the next test question, the waves reversed. This potentially indicates that brain wave direction may reflect distinctive cognitive processes.

Livermore’s Implantable Microsystems group leader Razi Haque says, “This research required the creation of novel, conformable, and higher density electrodes that could wrap around specific regions deep in the brain.” The team also used machine learning to reveal that certain areas of the hippocampal surface activated depending on the direction of the waves. Leveraging years of microfabrication capabilities and infrastructure, the research group is working toward obtaining accreditation from the U.S. Food and Drug Administration to build human-grade devices and exploring development of sub-chronic implants that could remain in the brain for up to 30 days.

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Collaborations Enable **A BRIGHT FUTURE**



LAURENCE Livermore National Laboratory is home to cutting-edge research and some of the world's most innovative technology, including the world's most energetic laser and some of its fastest supercomputers. We consistently invest in new instruments and capabilities to support our national security research, but we cannot site every tool we need on our one-square-mile main campus. One key to the Laboratory's success involves its collaborations with other research institutions and experts, nearby and across the globe. The complexity and cost of modern experimental capabilities require that broad research directions and investments be set by research communities, not individual institutions. Cultivating relationships with other research centers enables the creation and supports the success of ambitious experimental facilities and allows us to work together to tackle complex scientific challenges that would be difficult or impossible for a single research group or institution.

As described in the feature article beginning on p. 4, Livermore researchers conduct experiments using some of the world's brightest x-ray sources. Many of these sources are located in the United States and are funded by the Department of Energy (DOE), for which the construction and operation of large-scale scientific user facilities have been integral to the mission of the DOE Office of Science from its earliest days. Others are located at research facilities in Europe and Asia, some of which are newer partners for us. For instance, Pohang X-ray Free Electron Laser, where our researchers have performed remarkable shock-compression experiments on iron, is located in South Korea, where we have been growing our research relationships over the past decade with several universities, particularly in the area of clean energy technology.

Of course, collaborations are about more than working together to build, operate, and use the biggest and newest scientific facilities. By collaborating with researchers from other institutions, we inject different perspectives and approaches into our scientific investigations and many times come up with new and better solutions. The value and ubiquity of collaborations in our work is apparent when you look at our publication statistics on peer-reviewed, unclassified journal articles published. For example, in the Physical and Life Sciences (PLS) Directorate, where roughly 1,000 such scholarly papers a year are authored

or co-authored, more than 80 percent of published papers are the product of collaboration between PLS researchers at the Laboratory and other institutions. In fact, close to 40 percent of PLS's scholarly output involves international collaboration.

Ensuring the nation's security and prosperity by delivering leading-edge basic and applied science and technology is far too large a mandate for us to fulfill alone. Collaborations with other national laboratories and with a diverse collection of universities and other research institutions help us accomplish the mission. Collaborations also serve an important recruiting function, exposing the next generation of engineers, scientists, and technicians to Livermore people, resources, and research challenges. Like any productive relationship, though, research collaborations take time, effort, and mutual understanding to generate meaningful results. It is vital that we keep these research relationships vibrant, especially now and over these past two years, when travel to other facilities has often proven challenging due to the pandemic.

One pandemic-era collaboration success story is detailed in the article starting on p. 12. Lawrence Livermore and the Kansas City National Security Campus partnered to create a polymer production enclave, sited at the Laboratory, to better integrate polymer design activities—performed by Livermore staff—with polymer parts production—performed by Kansas City staff—for the national security enterprise. Working side by side, researchers and technicians from the two DOE facilities have already achieved several technical breakthroughs.

Collaboration is also the theme for the second highlight in this issue. The article beginning on p. 16 explains how multidisciplinary teams composed of skilled Livermore designers, engineers, and technicians devise and diagnose hydrodynamic experiments that help ensure that the nation's nuclear stockpile remains safe, secure, and effective.

The third highlight starting on p. 20, focuses on the work performed by emergent, extraordinary scientists and engineers, and how a relatively new awards program pays dividends for both awardees and the Laboratory. After all, great people are central to Livermore's formula for success.

■ Glenn A. Fox is associate director for Physical and Life Sciences.

Extremely BRIGHT Incredibly FAST

Multidisciplinary teams of researchers are leading cutting-edge experiments at world-class, light-source facilities to observe how materials change under extreme conditions.

WHAT began as a ten-centimeter contraption made of wire, glass, and red sealing wax that used electrical and magnetic fields to accelerate protons in a spiral-shaped path before they collided with a target—the first cyclotron—spawned larger, more powerful devices for groundbreaking discoveries; unlocked the secrets of the atom; and revealed new elements, isotopes, cosmic particles, and antiparticles. Upon receiving the 1939 Nobel Prize in Physics for the invention and development of the cyclotron, Ernest O. Lawrence anticipated that his “proton merry-go-round” was still in its nascent stage. He explained, “We have been looking towards the new frontier in the atom, the domain of energies above a

hundred-million volts, for we have every reason to believe that there lies ahead for exploration a territory with treasures transcending anything thus far unearthed. To penetrate this new frontier will require the building of a giant cyclotron, perhaps weighing more than 4,000 tons... We have been working on the designs of such a great instrument and are convinced that there are no insurmountable technical difficulties in the way of producing atomic projectiles of energies well above one hundred million volts.”

More than 80 years later, some of the largest, most complex machines on the planet—synchrotron radiation facilities that generate the world’s brightest x rays—stand as a legacy of Lawrence’s work

and the result of progressive scientific discoveries yielding more powerful cyclotrons, particle accelerators, and x rays. These synchrotron radiation light sources produce “hard” x rays at the high-energy, short-wavelength band of the electromagnetic spectrum as well lower energy “soft” x rays. At wavelengths of 0.10 to 0.01 nanometers, comparable to interatomic distances, hard x rays are ideal for studying atoms; soft x rays measure about 1 nanometer in length and are perfect for studying biological samples, nano structures, and energy science in general. Their brilliance—which varies depending on the beamline and the facility—allows them to penetrate matter and interact with atoms, producing x-ray diffraction,

imaging, and spectroscopy patterns that researchers examine to understand how elements react under extreme conditions. Meeting the Laboratory's missions requires that researchers understand how materials behave under high pressure or forces, specifically, how their atomic structure changes, how quickly, if kinetics is involved in those changes, and what new material properties emerge. "The truth is, how a big, giant bomb behaves depends directly on the behavior of infinitesimal atoms," says Livermore materials scientist Mukul Kumar. Laboratory researchers work at the atomic scale on time-resolved, light-source experiments to observe how materials transform under extreme conditions. Determining when a substance will shift between states of solid, liquid, gas, or even plasma in some cases plays a significant role in the materials and modeling simulation codes the Laboratory uses to verify the safety, security, and effectiveness of the nation's nuclear weapons stockpile in the absence of testing. The goal of these experiments is to capture the data needed to validate the physics models in the simulation codes, and Livermore's scientists interrogate and resolve the discrepancies. "The predictions are only as good as the underlying science; the physics must be right. These light-source experiments are the proving ground, and the Laboratory's modeling and simulation capabilities provide the connective tissue that informs our large-scale hydrodynamics testing, our detonation science, and materials deformation studies."

"No matter the specifics of the experiment, we're always pushing these materials into extreme conditions to see how they change on timescales from microseconds to nanoseconds—100 billionths of a second. To observe what's happening, we need x rays that have short pulse lengths, appropriate energies, and sufficient intensities to capture and document those changes just as fast," says Trevor Willey, physicist in the Materials Science Division at the Laboratory. Some light-source experiments involve shock

compression using a gas gun, some involve a laser or laser-shock compression in combination with a diamond anvil cell (DAC), and some experiments involve detonations. "Each of these light sources, beamlines, and even experimental hutches along the beamlines produces experiments with specific flavors," says Willey.

The Right Flux

"One of the biggest challenges with these experiments is that atoms react in nanoseconds. The light-source facility needs to produce x rays at that same speed. The flux of photons—the number of photons per second in a given area—needs to rise above the background noise of the system in order for us to document that reaction. The flux of photons must be good enough to capture the behavior of the atoms," says Kumar. The flux at the Advanced Photon Source (APS) at Argonne National Laboratory (ANL) outside of Chicago, Illinois, is well-suited for a variety of experiments designed by Livermore researchers and scientists.

Ultrabright, high-energy, storage-ring-generated x-ray beams arrive at "sectors" distributed across APS. One of those sectors is the High-Pressure Collaborative Access Team (HPCAT) at Sector 16 where four simultaneously operational beamlines have been established with an array of x-ray probes and diagnostics optimized for high-pressure research using x-ray diffraction, x-ray spectroscopy, and x-ray imaging techniques. Lawrence Livermore, Los Alamos, and Sandia national laboratories and the Stewardship Science Academic Alliances Program are principal stakeholders in the HPCAT team; the National Nuclear Security Administration (NNSA) is the primary sponsor. "Before the COVID-19 pandemic, HPCAT hosted about 750 on-site experimental users annually, and 50 percent of these experimenters were academics, students, and postdoctoral researchers from around the world, many of whom wind up working for the national labs," says Nenad Velisavljevic, director of HPCAT and a Livermore employee. "Over the last two years, HPCAT implemented



The first successful cyclotron (above) built by Ernest O. Lawrence (below) accelerated a few hydrogen ions to an energy of 80,000 electronvolts. The device earned Lawrence \$500 from the National Research Council towards the construction of a machine that might be useful for nuclear physics. (Images courtesy of University of California, Lawrence Berkeley National Laboratory.)



critical and necessary adjustments and now hosts remote-user operations as well. HPCAT continues to provide critical capabilities for NNSA laboratories even with the ongoing COVID restrictions.”

Livermore physicist Samantha Clarke has utilized HPCAT’s high flux to enable more accurate safety and performance modeling of nitroamine CL-20, a powerful explosive important to weapons research, by probing CL-20’s structural properties under extreme conditions. Clarke and her team determined that the compressibility of the molecule along each axis is consistent across the entire pressure range, potentially due to the molecule’s cagelike structure. Based on the diffraction data captured, which matches calculated values, the team identified novel

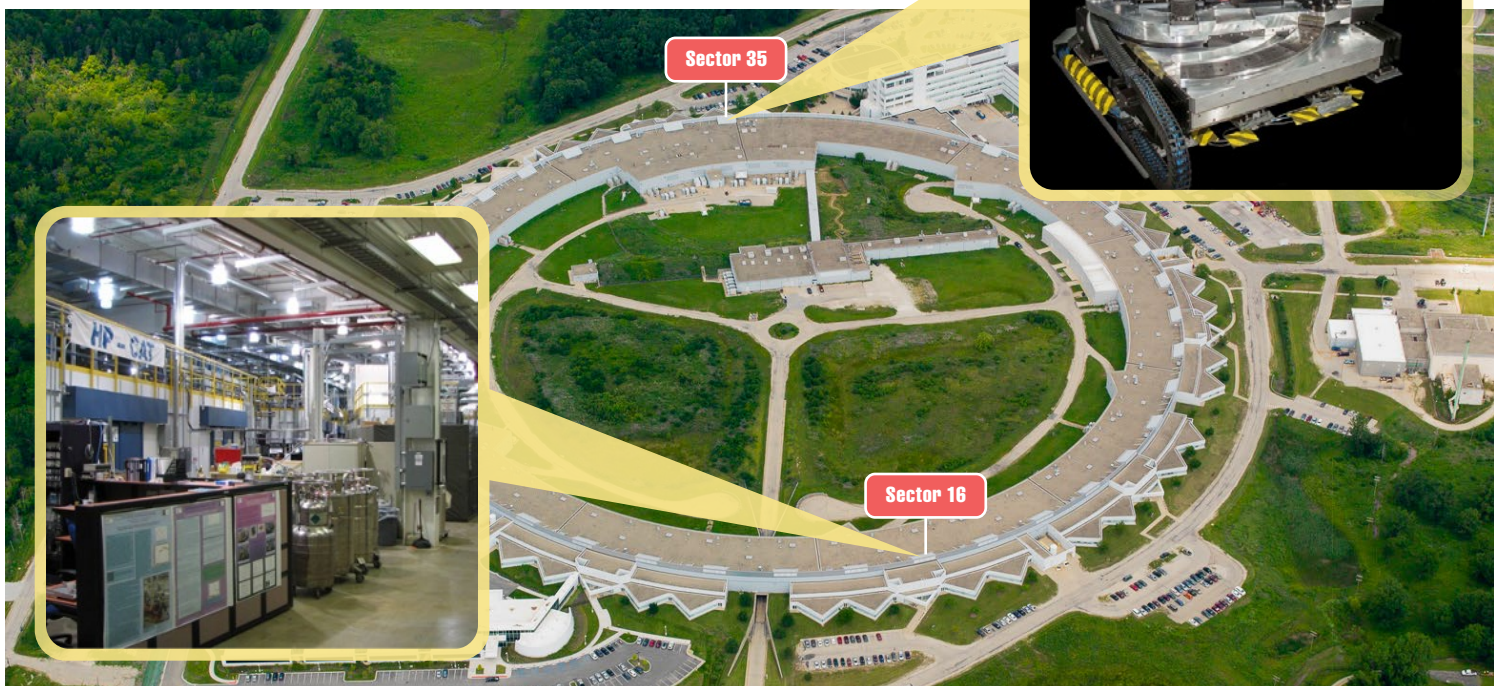
experimental equation-of-state parameters describing how CL-20 changes under different conditions. “The experiments at HPCAT allow us to analyze high-pressure and temperature states of matter that no one in the world has ever investigated with such high resolution. For many of these experiments, we are observing never-before-seen phases,” says Clarke.

Research Hutches

APS’s Dynamic Compression Sector (DCS) consists of a series of hutches at Sector 35 where Livermore scientists perform a variety of powder gun, gas gun, and laser-driven research using permanently installed drivers. The user-defined DCS B Station has offered Livermore scientists the flexibility to explore aspects of

high-explosive detonation physics over the last seven years. Conventional high explosives usually have some excess carbon, and under the extreme temperatures and pressures of detonation, a Livermore team has observed the formation of carbon nanoparticles in diamond, graphitic, and even liquid carbon phases depending on the pressures and temperatures attained. In one case, analysis of time-resolved, small-angle, x-ray scattering data during detonation of a hydrogen-free explosive, dinitrofurazanfuroxan, yielded dynamic measurements of liquid-carbon condensation and solidification into nano-onions—concentric series of spherical carbon shells roughly 30 nanometers in diameter—in just over 200 nanoseconds. (See *S&TR*, July 2017, pp. 12–15.)

At the Advanced Photon Source at Argonne National Laboratory in Lemont, Illinois, four simultaneously operational beamlines with an array of x-ray probes optimized for high-pressure research support a variety of Livermore light-source experiments at the High-Pressure Collaborative Access Team station in Sector 16. The Dynamic Compression Sector (DCS) Laser System at Sector 35 provides researchers with flexible, temporal pulse-shaped lasers that drive shocks into condensed matter, which are then probed by x-ray pulses from the synchrotron source that intersect in the DCS target chamber (top right).



Observing the type of carbon produced and how quickly it forms over hundred-nanosecond timescales provides both empirical input and validation of detonation codes essential to stockpile stewardship. “Using small angle scattering, we can observe the emergence and aggregation of these particles during detonation,” says Willey. “One of the most fascinating and technologically promising class of particles we’re looking at is nano diamonds. One of the most common methods used to produce nano diamonds is through high-explosive detonations, where the temperature and pressure is intense enough to form diamond. Contrary to what’s out there in the scientific literature, these nano diamonds aggregate during detonation nearly as fast as they form in this hot carbon soup. Understanding how these detonations produce nano diamonds may inform how we tweak their properties.” These nano diamonds have several technological applications. Nano diamonds can absorb substantial heat, efficiently emit electrons, and are also inert and nontoxic. Rigid-yet-tunable nano diamonds come in a variety of shapes and sizes and have the potential to revolutionize pharmaceuticals, fuel additives, material coatings, other nanotechnologies, and even quantum computing. (See *S&TR*, March/April 2008, pp. 14–16.)

The DCS C-Hutch at APS houses high-energy lasers that Livermore scientists use to shock-compress materials. Dynamic compression experiments occur on nanosecond timescales and require a light source that can generate extremely bright short-pulsed x rays so scientists can take a “snapshot” of the sample in its extreme state. For one such experiment, Livermore physicist Richard Briggs proposed shock-compressing gold, which had no expected phase transitions but the test would provide a strong signal from the scattered x rays. To the team’s surprise, the sample’s crystal structure changed at close to 200 gigapascals (GPa)—almost

two-thirds the pressure at the center of the Earth—the first time this phase had ever been observed in gold. The team’s findings led to additional experiments designed to investigate high-pressure phase transitions in materials regularly used at Lawrence Livermore’s National Ignition Facility and at the University of Rochester’s Omega Laser Facility in Rochester, New York. “At DCS, we’ve laid the groundwork for performing these experiments and developed unique techniques that apply the Laboratory’s mission for understanding materials response relevant to stockpile stewardship. And we’re still finding new surprises!” says Briggs.

Nanosecond Laser Compression

“What we really want to know about material behavior is how quickly the products form and what happens to them,” says high-energy-density physicist Jon Eggert. Light sources like the Linac Coherent Light Source (LCLS) in Menlo Park, California, an Office of Science User Facility operated for the U.S. Department of Energy by Stanford University, allow Livermore scientists to directly measure material behavior under laser-driven dynamic compression and answer these questions in unprecedented detail. “LCLS produces a different flavor of x rays—shorter, more intense, more monochromatic, more coherent, but with a slower repetition rate,” says Willey. The LCLS delivers 120 x-ray pulses per second, each lasting one quadrillionth of a second (femtoseconds), the rate at which atomic movements can be tracked and measured. These measurements help constrain material behavior models used by the programs in several Laboratory applications including weapons design,



Livermore scientists (left to right) Federica Coppari, Amalia Fernandez Panella, Amy Coleman, and Samantha Clarke at the Dynamic Compression Sector of the Advanced Photon Source.

advanced materials and manufacturing, and computer modeling and simulations.

At the Matter in Extreme Conditions End Station at LCLS, Livermore physicists Martin Gorman, Samantha Clarke, Jon Eggert, and Ray Smith have teamed up with other experimentalists from around the world to subject zirconium samples to laser-driven shock compression to 22 GPa so they transition to the high-pressure *omega* phase that forms in zirconium alloys with most transition metals. For each experiment, a laser beam 500-micrometers in diameter drove a shock wave into zirconium samples using a 10-nanosecond flat-top laser pulse. The extreme pressures produced by the laser-driven compression shock exceed pressures produced by static compression methods or dynamic compression using gas guns, generating novel structures. “By using one of the fastest, brightest x-ray sources in the world, we can collect atomic snapshots of

samples after they have been compressed by a laser-induced shockwave. The x-ray snapshots indicate if the sample has transformed to a new phase at high pressure, which may have vastly different material properties to the ambient material,” says Gorman. “This opens the door to recovering novel phases of matter with functional properties. Crucially, nanosecond laser compression allows access to vast regions of phase spaces that cannot be studied using other recovery techniques.”

Livermore physicist Amy Coleman led a team that developed a new way of housing potassium in a target package for light source experiments so they could study potassium under dynamic compression at LCLS without it reacting, either with the air or the other target components. Very reactive and difficult to study using static compression techniques, potassium can eat away at the diamonds in DACs causing experimental failure. Potassium also melts at a relatively low temperature, so much of the collected diffraction data describes its liquid state. Analysis of liquid diffraction is complex and requires diffraction data of the highest quality. “At LCLS we are able to probe the liquid structure of potassium at pressures and temperatures that had never been accessed. The breadth of the detectors, the high brilliance, and the short duration of the x rays allow us

to obtain data of high-enough quality to perform quantitative analysis on liquids via dynamic compression. We are paving the way to obtaining structural information and measurements of density for a wide range of materials in the liquid state and broadening understanding of myriad extreme condition liquid systems such as planetary interiors,” says Coleman.

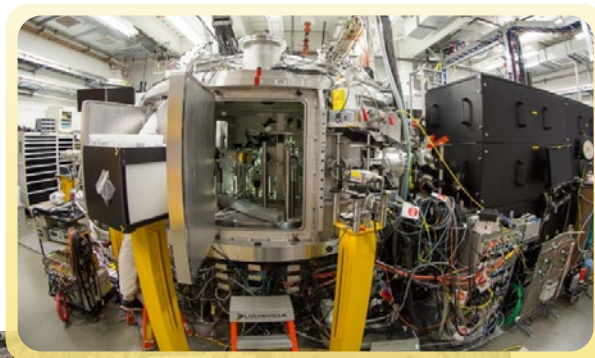
Transformative Tools

In 2007, Livermore physicist Will Evans and his team pioneered the invention of a device for studying the dynamic-pressure properties of materials—the dynamic diamond anvil cell (dDAC)—that repetitively applies time-dependent load and pressure to a sample by adapting electromechanical piezoelectric actuators to a conventional diamond anvil cell. The dDAC allows the study of phase transition kinetics and metastable phases at strain rates of up to 500 GPa per second through precise specification. Initially, the dDAC was used with laboratory-based optical spectroscopy diagnostics and optical imaging techniques because extant x-ray light sources and detectors had slow frame rates, which produced poor time resolution. Then, in 2019, Livermore physicist Zsolt Jenei and his team in the Lawrence Livermore High-Pressure Physics Group,

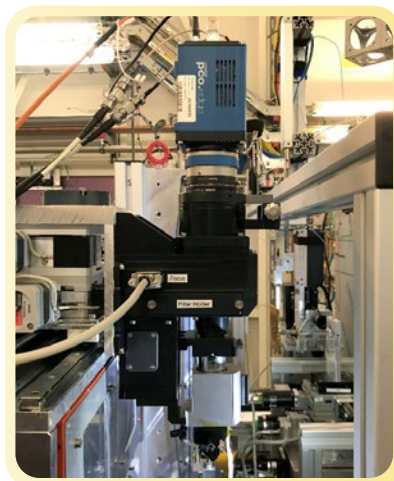
along with scientists from Deutsches Elektronen-Synchrotron (DESY), the European Synchrotron Radiation Facility, and the universities of Oxford, Bayreuth, and Goethe developed a next-generation dDAC that can compress samples faster than any other previous DAC—1.6 billion atmospheres per second. (See *S&TR*, July/August 2019, pp. 20–23.)

The improved dDAC characterizes the response of a sample under well-controlled fast compression. “Our technique can dial in different compression rates from slow to fast, which cannot be done with laser compression or a gas gun,” says Jenei. “This allows us to bridge the gap between traditional static and shock compression and investigate compression-rate-dependent phenomena across orders of magnitude, but we also need an x-ray source with enough photons to capture the diffraction and sensitive enough to detect changes at almost the exact same speed.” Since the invention of the dDAC, one challenge has been conducting fast-diffraction experiments due to the lack of photon flux—the number of photons per second, per unit area—and fast, highly sensitive, high-energy x-ray diffraction detectors.

The Matter in Extreme Conditions experimental hutch (right) at SLAC’s Linac Coherent Light Source (LCLS) in Menlo Park, California (below), allows Livermore scientists to directly measure material behavior under laser-driven dynamic compression using 120 x-ray pulses that last one quadrillionth of a second, the rate at which atomic movements can be tracked and measured.



With the arrival of a high-brilliance third-generation synchrotron radiation source at DESY's PETRA III, outside of Hamburg, Germany, the biggest and most brilliant light source in the world, and the development of the gallium-arsenide (GaAs) LAMBDA detector, Livermore scientists can collect diffraction images with adequate short exposure times and temporal resolution. Using next-generation dDAC and the Extreme Conditions Beamline, the team has achieved compression rates of up to 160 terapascals per second on a sample of gold. More recently, the team explored the effect of kinetics related to nucleation and growth of different high-pressure phases of bismuth at various compression rates. They used time-resolved x-ray diffraction with first-time 0.25 millisecond time resolution to accurately determine phase-transition pressures at compression rates spanning five orders of magnitude while compressing a sample of bismuth. "In the relatively low pressure and temperature region, bismuth has a complex phase diagram. Under dynamic compression from the ambient state, the incommensurate phase III of bismuth has not been observed. We were surprised to see that an overpressurization of bismuth's third and fourth phase boundary happens at



Using a next-generation dynamic diamond anvil cell, the LAMBDA detector (left), and the Extreme Conditions Beamline at PETRA III (right), the Livermore team has achieved unprecedented compression rates of up to 160 terapascals per second on a sample of gold.

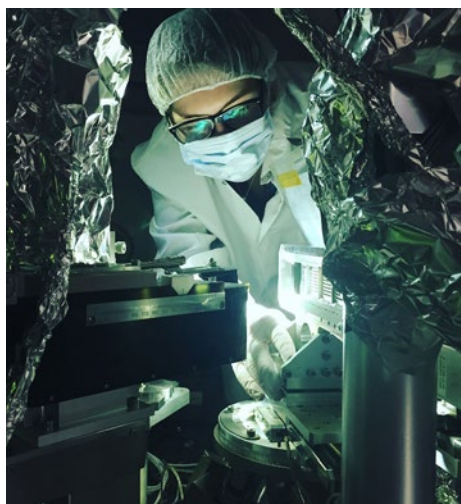
fast compression rates for different bismuth samples and stress states," says Jenei.

These surprising findings also uncover new avenues for future studies of transition kinetics at previously inaccessible compression rates. One of the challenges of these experiments is combining techniques so that they work simultaneously with the dDAC. "On their own, each technique is relatively straightforward, but setting everything up to start at the exact same moment can be challenging," says Earl O'Bannon, a Livermore staff scientist in the High-Pressure Physics Group who prepares the samples and runs the experiments on the DESY PETRA III Extreme Conditions Beamline. "It's exciting to be constantly pushing the edge of what's possible with the diamond anvil

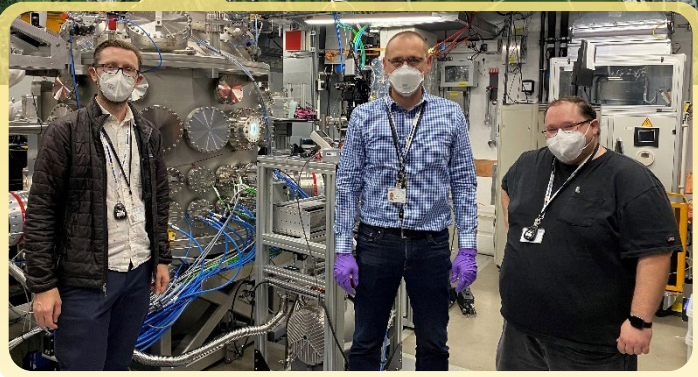
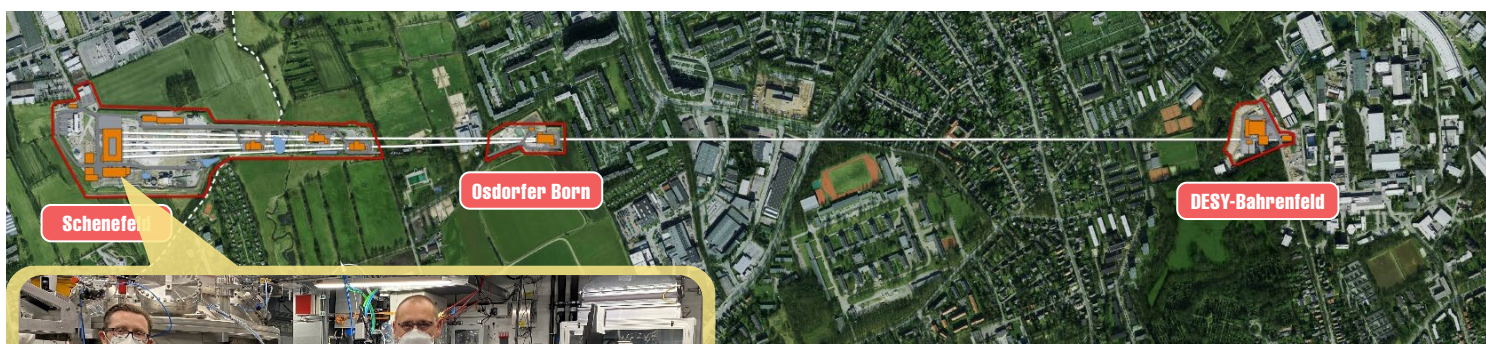
cell. We are now able to use the x rays to obtain structural information and directly image opaque metal samples using x-ray imaging techniques while achieving millisecond time resolution. We also get to see ideas go from the drawing board to reliable tools and techniques that support the Laboratory's stockpile stewardship mission, find widespread use in the high-pressure community, and maintain Livermore's leading role in high-pressure science," says O'Bannon.

Unexpected Changes

Using a unique combination of a short-pulse optical laser and an ultrashort, free-electron laser pulse at the Pohang Accelerator Laboratory X-ray Free Electron Laser in South Korea, Livermore physicist Hyunchoe Cynn and his international colleagues recorded the atomic structural evolution of shock-compressed iron at the remarkable time resolution of 50 picoseconds under a high-strain rate. The team documented a three-wave temporal evolution of the elastic, plastic, and deformational phase transitions to the second phase, followed by post-compression phases. Their experiment was the first direct, complete



Livermore physicist Amy Coleman loads a target mount into the vacuum chamber at the LCLS. The experiments are typically conducted under vacuum to avoid unwanted effects from the presence of air during laser ablation of the targets. Researchers typically load several cartridges at a time so that they can shoot around 200 targets before the chamber is vented and new targets are put in place.



Livermore scientists (left, from left to right) Earl O'Bannon, Zsolt Jenei, and Daniel T. Sneed stand in front of the high-energy-density (HED) instrument at the European X-ray Free Electron Laser (Eu-XFEL) facility in Schenefeld, Germany (above). The team performed the first dynamic diamond anvil cell experiments on the HED instrument at the Eu-XFEL supporting a team of more than 50 international scientists.



The Advanced Light Source at Lawrence Berkeley National Laboratory in Berkeley, California. (Photo credit: University of California, Lawrence Berkeley National Laboratory.)



Lawrence Livermore materials scientist, Holly Carlton (above), prepares a sample at the Advanced Light Source at the Lawrence Berkeley National Laboratory beamline 8.3.2.



The Pohang Accelerator Laboratory X-ray Free-Electron (PAL-XFEL) Laser (above) in Pohang, South Korea outside of Seoul provides XFEL radiation in a range of 0.1 to 6 nanometers. (Photo credit: POSTECH.)

observation of shock wave propagation associated with crystal structural changes captured by high-quality x-ray diffraction data. The experiment also demonstrated the ability to measure atomistic evolution during the lattice compression and release processes at unprecedented time and strain rate. “Pohang is an exceptional facility that combines shock compression of materials using an optical laser at the picosecond range that is able to accurately capture and measure high-resolution data. We really didn’t expect to see so many changes in such a short time,” says Cynn.

Cynn joined Livermore colleagues, Jenei, O’Bannon, Evans, and Magnus Lipp to explore the structural evolution of tantalum at high pressure and temperature by irradiation using the x-ray free electron laser (XFEL) Beam at European XFEL (Eu-XFEL) in Schenefeld, Germany. Their approach used the x rays to directly heat tantalum under extreme pressures in a DAC. The applied XFEL beam also provided x-ray diffraction information and density of tantalum as a function of pressures and temperatures. The XFEL’s brilliance allowed the team to measure a dynamic material response within a 10-femtosecond x-ray pulse. Due to the ultrashort x-ray pulse structure at Eu-XFEL, material change—lattice expansion, melting, and chemical reaction—induced by the first pulse was probed and recorded from the second pulse after 440 nanoseconds. In addition to the lattice response, liquid tantalum scattering was measured for the first time under extreme conditions.

Ongoing Innovation

Near the site where Lawrence’s four-meter synchrotron once rocketed atomic particles to 100 megaelectronvolts, the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory in Berkeley, California, now generates 1.9 gigaelectronvolts traveling at nearly the speed of light while emitting infrared, ultraviolet, and x rays through 40 beamlines. Since it first opened in 1993, Livermore scientists have used ALS for a range of

in situ, time-resolved experiments. The 8.3.2 beamline at ALS uses x rays between 6 and 43 kiloelectronvolts (0.2 to 0.03 nanometers) and produces nondestructive 3D imaging of solid objects at a resolution down to 1 micrometer via computed tomography—the process of capturing a series of layered digital images of an object. Combining ALS’s synchrotron radiation microtomography and in situ uniaxial compression testing, Livermore scientists Holly Carlton, Nickolai Volkoff-Shoemaker, Mark Messner (now at ANL), Nathan Barton, Jon Lind, and Kumar have recently uncovered local microstrain deformations and failure modes of additively manufactured metal-lattice structures including the octet-truss, the rhombic-dodecahedron, and isotruss with different densities. They also utilized in situ computed tomography to incorporate 3D-defect distributions of lattice structures into model predictions for more detailed understanding of how these structures deform. “In the last decade, additive manufacturing or 3D printing has made a real impact on how we approach component development for the life-extension programs. We can design and build these complex, additively manufactured structures, but we need to know how they will respond under a range of conditions. Using high-resolution computed tomography at the ALS, we can map out defects, see how materials and configurations deform in real time, and use those findings to inform our design process and computational modeling,” says Lind, a Livermore physicist who has contributed to both quasi-static and dynamic testing.

Just as Lawrence knew that his “atom smasher” would be eclipsed by future technological innovations, contemporary light-source facilities continue to pursue and refine the next generation of tools that will uncover the secrets of the atomic world around us. ALS is currently undergoing an upgrade to produce highly focused soft x rays that

will be at least 100 times brighter than the current beams. In 2024, APS will undergo a major, three-year upgrade to improve its capabilities, helping to keep the United States at the forefront of hard x-ray science. When completed, APS will produce the world’s brightest hard x rays and allow researchers to observe individual atoms moving and interacting in real time. LCLS at Stanford University is also preparing for a major upgrade—LCLS-II—which will increase its x-ray pulse repetition rate from 120 pulses per second to 1 million pulses per second and revolutionize how scientists study rare chemical events, quantum materials, and biological systems.

“We explore the behavior of materials at never-before-seen conditions, and Livermore teams have, in several instances, been the first to observe interesting behaviors, even in materials once thought to be well studied or boring,” says Gorman. “My colleagues and I are excited to know we might be able to synthesize novel materials or develop tools that could change the world.” Evans adds, “These x-ray light sources are an important, dramatically enhanced capability that are transformative for science around the world and for Livermore research.”

—Genevieve Sexton

Key Words: Advanced Light Source (ALS), Advanced Photon Source (APS), copper, cyclotron, Deutsches Elektronen-Synchrotron (DESY), dynamic diamond anvil cell (dDAC), Dynamic Compression Sector (DCS), European XFEL (Eu-XFEL), gold, hard x rays, High-Pressure Collaborative Access Team (HPCAT), Linac Coherent Light Source (LCLS), nano diamond, nitroamine CL-20, Pohang Accelerator Laboratory X-ray Free-Electron Laser (PAL-XFEL), potassium, synchrotron, x-ray free electron laser (XFEL), zirconium.

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POLYMER PRODUCTION ENCLAVE

Puts Additive Manufacturing on the Fast Track

SINCE its establishment, Lawrence Livermore has played a critical role in designing components for the Nuclear Security Enterprise (NSE), and more recently, in developing additively manufactured polymer parts to replace aging weapons stockpile parts. Additive manufacturing (AM)—the layer-by-layer technique of printing 3D objects from a digital model—gained traction at Livermore in 2009 after a series of Laboratory Directed Research and Development investments led by Chris Spadaccini, division leader of Livermore’s Materials Engineering Division. (See *S&TR*, March 2012, pp. 14–20.) “Advancing additive manufacturing requires multidisciplinary teams of engineers, physicists, chemists, computer scientists, and production-line experts, and the Laboratory was an ideal place to do that,” says Spadaccini. Even at an early stage of AM research and development, the potential for polymeric components in the weapons program, specifically in support of the W80-4 Life-Extension Program (LEP) and W87-1 Modification Program, generated enthusiasm across NSE. (See *S&TR*, January/February 2015, pp. 4–11.)

Livermore and the Kansas City National Security Campus (KCNSC), which has decades of experience as a production facility for the NSE and in meeting the extremely rigorous qualification standards for stockpile component production, recognized the potential for AM polymers and began to explore an improved, concurrent design and development process. “When the AM team first came to the weapons program, we could print a 2D silicone doily. Now, we can print complex parts with completely arbitrary shapes, and we’re integrating machine learning and high-performance computing. It’s remarkable how far additive manufacturing has evolved in such

a short time,” says program leader and materials scientist Bob Maxwell. While there have been tremendous breakthroughs for polymer parts over the last decade, the overall design, production, and deployment process has been slow, taking years to design, produce, approve, and deliver a single viable part.

In 2019, the need to revamp the Livermore–KCNSC partnership became apparent, and a vision for a Polymer Production Enclave came into focus. “After looking at how many 3D-printing machines we would need to create stockpile components for the LEPs, we realized we had to change the way we collaborate and that led to the current Polymer Production Enclave,” says Maxwell. The previous design and production process entailed Livermore’s weapons designers conceptualizing and prototyping components and then sending their blueprints to the production team in Kansas City, Missouri. To simultaneously advance design and production capabilities and reduce timescales and costs, Lawrence Livermore and KCNSC embarked on a more fully integrated model that features a newly constructed, state-of-the-art polymer design and production facility at the Laboratory—and something of a historical return to the time when physicists would walk the floors of a production facility to see their prototypes realized in a production setting.

In September 2020, former Laboratory Director William Goldstein, current Laboratory Director Kim Budil, former National Nuclear Security Administration Administrator Lisa E. Gordon-Hagerty, and Livermore Field Office manager Pete Rodrik dedicated a new Applied Materials Engineering campus at the Livermore site, which features the new Polymer Production Enclave. (See *S&TR*, January 2021, pp. 4–11.) The



Laboratory's Weapons and Complex Integration Principal Directorate's Infrastructure and Operations team constructed and outfitted the new facility in a little over one year during the COVID-19 pandemic. To launch the Polymer Production Enclave, KCNSC worked closely with Livermore to specify and procure identical machines, tools, and other production equipment to be housed at both the Livermore and Kansas City sites so that both partners can access the same resources in parallel. The Livermore facility now hosts 10 additive manufacturing machines, while there will ultimately be 15 or more in Kansas City. The Livermore facility also features a materials-mixing laboratory, a post-manufacturing evaluation space, and offices and conference rooms for real-time exchanges with KCNSC and other stakeholders. Now, the collaborators can simultaneously complete multiple production phases—such as ink processing, printing, materials characterization, and quality control—and immediately incorporate their findings into upcoming rounds of development and testing. “This approach allows both sites to view the design and production processes through the other’s lens. We’re learning more about the considerations and challenges facing the designers, and the designers are becoming more familiar with the production challenges we face. We’re already seeing the benefits of partnering closely, sharing information seamlessly, and leveraging expertise from both sites,” says Jessica Bailey, leader of the KCNSC team. Maxwell adds, “We’re having more detailed dialogues. We’re coming up to speed on production process realities so we can anticipate what roadblocks new concepts might run into on the production floor. We’re joining

Additive manufacturing is a multidisciplinary field, and the Polymer Production Enclave engages experts from the engineering, production, and scientific spheres to support national stockpile stewardship. The Kansas City National Security Campus and Lawrence Livermore teams pictured above bring together a variety of expertise and skill sets to expedite progress in advanced additive manufacturing.

forces as early as possible to co-develop new technologies and accelerate production. Instead of designing, producing, and deploying a part in eight years, we hope to do so in four.” Dan Bowen, chief scientist at KCNSC, says, “At its heart, the Polymer Production Enclave isn’t just a building; it is an extremely close, transparent collaboration that increases our agility and ability to significantly improve development time.”

Early Wins

The most common method for producing polymer AM components is direct ink writing (DIW), which involves extruding a silicone resin ink through a nozzle onto a substrate creating a series of intricate lattice structures. The substrate or mandrel moves during the extrusion process following a digital design dictating its path. “Working with DIW is challenging. You can always design the ideal part, but you plug that design into a computer, push the button, and you might end up with spaghetti instead of a nice, cohesive 3D part,” says Tom Wilson, polymer scientist in Livermore’s Materials Science Division.

The Polymer Production Enclave team has already realized several important early wins, including the ability to tailor an



ink's response to different loading conditions and move from isotropic legacy foams, which exhibit the same properties, such as stiffness or porosity, in all directions to more dynamically responsive foams. "Typically, these parts were springy in one direction like a shoe insert, but these component materials experience multidimensional stresses, not just up or down, but also side-to-side with a lot of shear forces, so we have to account for that. Now, we can design to accommodate multidimensional stress and strain for different components," says Maxwell.

The polymer team has also developed customized methodologies to correct the tool path of printing components. For such complex parts, the polymer team needs the printing nozzle to align within tens of micrometers—thinner than a strand of human hair—of the substrate, but typical machining for substrates might be plus or minus 50 micrometers—the thickness of a sheet of paper. By collecting optical and interferometric measurements of the substrate's geometry relative to the ideal location of the substrate and applying the machine's inverse kinematics (the reverse-engineered calculations used to determine the desired endpoint of a series of robotic movements), the researchers kept the substrate and nozzle precisely aligned, ensuring the target architecture was produced. Combined with the kinematic mandrel mount, the team's calculations also reduce the time needed to reset the machines after printing each part. The polymer team has also invented a 3D-printing platform with

enhanced movement along both linear and rotational axes. "We're now able to 3D print onto 3D objects with spatial registration of composition and structure of the part with respect to the substrate," says Livermore materials scientist Eric Duoss.

Once a part has been printed, researchers must examine it in a noninvasive manner for potential flaws that might compromise its integrity. Chuck Divin, a nondestructive evaluation (NDE) engineer at Livermore, has led a team of engineers and scientists at the Polymer Production Enclave in developing new NDE methods of inspection that allow researchers to determine the as-built structure and composition of a part with greater precision and accuracy, reducing uncertainties to less than 0.2 percent without disassembling a part. KCNSC and Livermore worked together to modify the NDE system to be more practical, robust, and user-friendly, ensuring that technicians can reliably evaluate parts.

Collaboration is Key

Created to enhance and expand capacity, the Polymer Production Enclave has also attracted next-generation engineers and materials scientists. Toward the end of his undergraduate studies, Dominique Villacarte, characterization engineer for the polymer AM team, started to research his career options and began at the Laboratory in March 2020 as a chemistry and materials science technologist for the Laboratory's Ceramics and Polymers Engineering and Plastics group. "Being able to help our country through the Laboratory's mission appealed to me. I love working in a team setting and learning from my colleagues at the enclave is great. We all come from different educational backgrounds, learn from each other, and complement our different strengths. Our team works hard, and we continually strive to make our processes the best they can be," says Villacarte. "The younger members of the team are motivated to work for the National Security Enterprise and recognize the benefits to the mission. Engaging this new generation of materials scientists and engineers who possess cutting-edge skills and knowledge is a boon to how we approach and solve these challenges," says Wilson. Duoss adds, "The Enclave is so important to rethinking design and production. We are seeing our technologies deployed in a dynamic, accelerated way and the key to that is collaboration."

—Sheridan Hyland

Key Words: 3D printing, additive manufacturing (AM), direct ink writing, high-performance computing, inverse kinematics, Life-Extension Program (LEP), nondestructive evaluation (NDE), Nuclear Security Enterprise (NSE), polymer, silicone.

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(a) The fabrication room in the Polymer Production Enclave features new machines and tools identical to those in use on the Kansas City National Security Campus's production floor. The Livermore Weapons and Complex Integration Principal Directorate's Infrastructure and Operations team completed the repurposing of the facility and installation of equipment in just over a year.

(b) Direct ink writing techniques used for additive manufacturing (AM) within the Polymer Production Enclave allow researchers to produce highly intricate and precise lattice structures, including helicoidal or flat spiral structures. The newly developed abilities to mix materials across parts provide a range of characteristics and features not previously available for weapons components using legacy foams.

(c) Dominique Villacarte, a characterization engineer for the polymer AM team, uses the Optical Gaging Products Smartscope Quest 450—a highly sensitive and accurate coordinate measurement system that incorporates optical, touch probe, microprobes, and a patented TeleStar® telecentric Through-the-Lens laser—to assess the quality of parts.

(d) Livermore staff scientist and formulation chemist Jeremy Armas uses a rheometer—an instrument that characterizes the flow of a substance in response to forces—on a silicone ink formulation to ensure its suitability for direct-ink-write applications used at the Polymer Production Enclave.

HYDRODYNAMIC EXPERIMENTS SUPPORT Stockpile Stewardship

INSIDE a heavily shielded chamber with 1.8-meter-thick concrete walls, high explosives detonate around a mass of inert test material. Subjected to an intense shock wave, the material briefly acts like a liquid. Advanced diagnostic equipment installed throughout the chamber captures thousands of data points and x-ray images from almost every angle in a split second. The hydrodynamic test—so named for the equations that explain how liquids in motion behave—which took months to plan and a 50-person team of skilled designers, engineers, and technicians to orchestrate and execute, lasted just 100 microseconds. Now, the copious data gathered from that brief test will inform critical weapons design decisions in the service of keeping the nation's nuclear deterrent safe, secure, and effective.

Lawrence Livermore has carried out hundreds of hydrodynamic tests over the last six decades in support of the Stockpile Stewardship Program's goals in the absence of full-scale nuclear testing, which came to an end in 1992. With the advent of the National Nuclear Security Administration's

life-extension programs (LEPs) and modification programs (see *S&TR*, October/November 2018, pp. 4–11), the need for and pace of hydrodynamic tests at the Laboratory's Site 300 have increased.

In 2007, Livermore's hydrodynamic testing program was addressing a variety of scientific queries, but the main objective was enabling the design and stewardship of the nation's nuclear stockpile by verifying the performance and safety of the nuclear explosives package—work typically accomplished through empirical testing in conjunction with physics model development and high-performance computing simulations (see *S&TR*, September 2007, pp.4–11). Integrated weapons experiments (IWEs), a key focus of the hydrodynamic tests at Site 300, study weapon systems, including the components that comprise a nuclear device. "IWEs are complex experiments that involve different physics and different measurement scales," says experimental physicist Reed Patterson. "In a hydrodynamic test, many things occur—physical and chemical reactions, debris dispersal,



Principal investigator Cliff Mortensen (left) stands behind a tank filled with foam and water that will slow but not deform fragments produced in an experimental explosion while high-voltage, high-intensity flash lamps (above) illuminate the experiment for high-speed cameras that will record the breakup of the device.

interactions of different components. We examine the entire integrated system and compare the results of the hydrodynamic tests with simulations to provide more accurate assessments of the conditions that trigger a nuclear device's primary—the mass of plutonium that initiates full detonation.”

Teaming Up for Success

“Every IWE starts with questions a weapons designer wants to answer. ‘How will this react?’ ‘How will this material impact a device?’ ‘What happens when we alter this mechanism?’ The members of the Laboratory’s hydrodynamic test program do everything they can to help the weapons designers answer those questions with as much detailed data as possible,” says Patterson. To do so, several multidisciplinary teams—ramrods, engineers, and diagnosticians—collaborate and devise the hydrodynamic experiments that produce data to yield those much-needed answers. During the engineering phase of a hydrodynamic experiment, the Laboratory’s ramrods—named after the cattle hands responsible

for ensuring herds arrived on time—evaluate the design of the experiment, configure the components with the engineering and diagnostics teams, and liaise with principal investigators to address emerging challenges. “You don’t get a second chance,” says ramrod and program group lead for hydrodynamic testing, Steve Bosson. “The test must be a success.”

The Diagnostics Development Group works with the experiment designers and ramrods to determine which diagnostics to use, develop customized instrumentation, and provide technical and field support for existing diagnostics and data analysis. “We develop novel diagnostics when the design team wants to measure something new. It’s our job to push the boundaries of what’s possible,” says program group leader Kerry Krauter. “We also troubleshoot and upgrade diagnostics and assist with data analysis.” These diagnostics gather sophisticated data describing the debris generated by a detonation including debris velocity and position, the shape of the device as it deforms, and the resulting temperature and density of the blast material. “The weapons designers need to know



Inside Livermore's Site 300 Contained Firing Facility (CFF), Clif Mortensen (right) aligns a mirror that will reflect the experiment toward cameras as they capture the experiment while former Livermore technicians, Brian Pepmeier (left) and Ashley Swan (center) inspect camera ports and ensure that debris will not interfere with data collection. Mortensen (far right) examines a unit that allows researchers to control the temperature of a hydrodynamic test.

more than the position, velocity, and shape of the debris. They want to know how the temperature changed during the blast, as well as how the density of the device changed. These data are challenging to measure directly during the microsecond duration of the test, so we make inferences and compare them with the Laboratory's simulations to fine-tune our findings and improve their fidelity," says Krauter.

Over the years, the Laboratory's hydrodynamic test diagnostics have yielded technologies specially developed by the Laboratory. Photonic doppler velocimetry measures the velocity of the device's destruction by recording the slight shift in the frequency of light reflected from it, also known as the Doppler effect. The surfaces of the device are tracked using broadband laser ranging (BLR), a technique also developed by researchers from several national

laboratories including Livermore. BLR works by training a laser pulse on the device's surface that reflects back to an interferometer, which merges two or more light sources to create an interference pattern indicating the movement of fragments during the detonation. The hydrotest diagnostics also include x rays. Until recently, these x rays were captured on film, but researchers are now transitioning to digital media. "These improvements have increased spatial resolution," says Krauter. "Now, we can achieve incredibly precise, accurate measurements." With 160 data channels for determining position and velocity, new flash x-ray capabilities (see *S&TR*, July/August 2018, pp.12–15), and improvements in the coordination and execution of hydrodynamic tests, the Laboratory's ever-evolving diagnostic capabilities represent a substantial improvement over the last 15 years and have contributed to a quickening pace to meet the expanded demand for tests in support of the W80-4 LEP and the W87-1 Modification Program.

Subcritical Program Support

The hydrodynamic test program also now supports preparations for subcritical tests, which are similar to hydrodynamic tests except instead of inert material, they utilize plutonium, the fissile material in a nuclear device. A limited number of neutrons are released during a subcritical test to prevent a self-sustaining chain reaction. "Since



2007, we've doubled the number of ramrods to eight. Our heavy involvement in subcritical testing presents a big shift for the teams. Hydrodynamic testing ensures the subcritical program's success," says Patterson.

Use of hydrodynamics experiments and simulations provide a high degree of fidelity for comparison with subcritical tests even though plutonium behaves differently than the inert materials in the preparatory tests. A single subcritical experiment costs tens of millions of dollars, requires three to five years to plan, and involves hundreds of people with a broad range of expertise in physics, engineering, explosives, safety, chemistry, and materials science, as well as support staff to coordinate and execute the administration, classification, procurement, shipping, transportation, materials management, and information technology required to support an experiment. To assure that a subcritical test will succeed, Livermore's hydrodynamic test group will perform as many as half a dozen experiments to verify that the experimental setup planned for the subcritical tests will successfully record the data needed. Three major series of subcritical tests are in planning stages, the first of which, Nimble, is scheduled for 2022 and will take place at the U1a Complex at the Nevada National Security Site.

"To give the subcritical teams better confidence, we do a series of hydrodynamic experiments," says Jeff Florando, the associate

program director for hydrodynamic and subcritical experiments. "One experiment might test the fragment mitigation strategy within its confinement vessel. You need to know what fragments will result after detonation, what kind of damage they cause, and how to decrease damage to the vessel and diagnostic equipment from a particular configuration." Other hydrodynamic tests ensure the timing of diagnostics measurements will be perfect. Getting the timing right is crucial because the tests and the opportunity to collect data lasts just nanoseconds. Patterson says, "Our mission demands that we work with a variety of hazards, including toxic and radioactive materials and high explosives. We do so in a safe and secure manner, making sure that we deliver the highest quality product to our customers, and that the test data we produce provides the answers they seek."

—Allan Chen

Key Words: Broadband laser ranging (BLR), Contained Firing Facility, flash x ray, hydrodynamic test, integrated weapons experiment (IWE), life-extension program (LEP), Nevada National Security Site, radiography, Site 300, subcritical test, W80-4 Life Extension Program, W87-1 Modification Program.

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DELIVERING EXCEPTIONAL PROMISE

An Update on Early and Mid-Career Recognition Award Recipients

LAURENCE Livermore's Early and Mid-Career Recognition (EMCR) Program acknowledges the exceptional scientific, technical, and engineering contributions of individuals 4 to 16 years into their professional careers who have made significant mission-critical contributions at the Laboratory. Since the inception of the EMCR Program in 2015, every year about a dozen distinguished Livermore scientists and engineers receive a take-home cash award and one year of institutional funding for up to 20 percent of their time to pursue technical activities in support of the Laboratory's mission in their areas of interest. Candidates must be nominated and then evaluated by a committee empaneled by the deputy director for science and technology.

Funding provided by EMCR helps jumpstart research projects and new technologies and puts the recipients on a fast track to achieve their career objectives. Upon receipt of the award, recipients submit proposals for their chosen projects. "When the EMCR Program was established, the original goal was to recognize our early and mid-career staff for their past successes, as well as prepare and motivate them to take on leadership roles. If you look at awardees over the past seven years and the contributions they have made, everyone would agree that the goal of this award continues to be fulfilled," says EMCR chairperson Eric Schwegler.

FÉLICIE ALBERT

EMCR 2015 recipient and scientist Félicie Albert joined the Laboratory in 2008 as a postdoctoral researcher and has performed experiments at premier light-source facilities around the world. Albert used her EMCR funding for beamtime at the SLAC National Accelerator Laboratory using the world-class Linac Coherent Light Source (LCLS) free-electron laser. "Experimentation can provide new diagnostic techniques and help scientists explore different states of matter existing only in the center of stars, giant planets, and exploding nuclear weapons. High-energy-density science and the Laboratory's mission to maintain the nation's nuclear weapons through its Stockpile Stewardship Program rely on this research," says Albert. LCLS delivers 120 x-ray pulses per second, with each pulse length as short as one quadrillionth of a second. Such pulses drive a material to extreme temperatures



Past Early and Mid-Career Recognition (EMCR) Award recipients: (from left) Félicie Albert, Crystal Jaing, Hui Chen, Dan Haylett, Andrew Pascall, Carlos Valdez, Marcus Worsley, and Todd Gamblin. (Photo by Garry Mcleod.)

and change its atomic structure. Albert explains, “LCLS is a one-of-a-kind laser, and its ability to bring matter to extreme temperatures and create states otherwise impossible to produce is extraordinary—there are few lasers like it in the world.”

With her beamtime, Albert performed experiments on aluminum, silicon oxide, and iron samples, heating them with the laser to alter their atomic structure, and then probing them with betatron radiation. The probe was produced by a separate, optical laser next to the sample, which irradiated helium gas to create a plasma, stripping electrons from the helium atoms and generating an electron-plasma wave that the trapped electrons could “surf on” and accelerate to relativistic energies. These electrons then rapidly wiggled back and forth about their propagation axis, producing the betatron x-ray radiation needed to probe the sample and capture the matter’s reaction to the LCLS irradiation with ultrafast precision. Albert’s combination of LCLS’s x-ray and optical laser beams, together with betatron radiation, was unprecedented.

As deputy director for Livermore’s High Energy Density Science Center and the Jupiter Laser Facility, Albert continues to explore novel techniques and expand her research to include x-ray sources with photon energies necessary for the radiography of dense materials.

CRYSTAL JAING

After receiving an EMCR in 2016, Crystal Jaing enrolled in the post-master’s certificate program in genomics and DNA sequencing at Johns Hopkins University in Baltimore, Maryland. The program provides scientists, like Jaing, who have an extensive background in biochemistry and molecular and cell biology, with additional bioinformatics skills so they can delve into more complex experimental designs and data analysis. “When I received the award, one of my colleagues was enrolled in the program at Johns Hopkins, and his studies in bioinformatics during that time aligned with our ongoing projects. I knew this real-world application would equip me with the skills to oversee broader efforts in large-scale DNA sequencing and data analysis at the Laboratory,” says Jaing.

Since 2016, Jaing has taken on additional leadership roles for bioinformatics-related projects. As principal investigator



for testing and evaluation of the Functional Genomic and Computational Assessment of Threats project, an initiative within the Intelligence Advanced Research Projects Activity, she utilized bioinformatics to assess the threat of a DNA fragment and its potential use as a bioterrorism agent. Jaing’s recent research with the Laboratory’s Bioscience and Biotechnology Division has helped predict and detect future pathogen outbreaks, whether natural or malicious, and her studies at Johns Hopkins have proven vital during the COVID-19 pandemic for public health and biosecurity, and especially for accurate, fast diagnostics.

Over the last year, Jaing’s team has examined the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), analyzing clinical nasal swabs on the Lawrence Livermore Microbial Detection Array, a technology developed by her team for early viral and bacterial detection to determine which co-infecting viral and bacterial pathogens are present in samples, indicating a potentially higher morbidity. By identifying COVID-19 co-infections, appropriate antibiotics can be administered in addition to COVID-19 treatment protocols. On the other hand, if a COVID-19 patient is infected with another virus such as the flu, this data can help track the spread of SARS-CoV-2 during flu seasons. Understanding the overlap of SARS-CoV-2 with other co-infections reveals disease severity and impact, supports clinical decisions, and helps doctors triage patient management. Says Jaing, “The additional education makes all of this research possible, enables more complex biological data analysis, grows the Laboratory’s biodetection capabilities, and allows me to take on additional leadership roles.”

TODD GAMBLIN

Scientific simulations that support the Laboratory’s mission run on supercomputers using hundreds of external software libraries, also called packages or dependencies. Various high-performance computing (HPC) applications need different versions or configurations of the same dependencies to work correctly on high-performance computer systems, so selecting the right dependency becomes essential to application performance. Traditionally, users, developers, and HPC support staff spend hours building codes and libraries by hand to obtain the ideal dependency configuration.

In 2013, computer scientist Todd Gamblin created the open-source package manager Spack (supercomputer package manager) to address this problem and speed up time to delivery. Spack automates



the scientific software installation process by managing complex dependency networks—choosing from different versions, compilers, and other configuration options to ensure compatibility across an application’s built-in dependencies. The tool caught on at the Laboratory as well as externally, and the Spack team at Livermore has grown to include six computer scientists and software developers to support demand for the software.

Receiving the EMCR award in 2017 gave Gamblin the opportunity to expand Spack’s features and improve its methods for automatically configuring a set of libraries. He optimized the way Spack solves dependency conflicts among every potential combination, allowing the Spack ecosystem to handle even more complex package configurations. In 2019, Spack won an R&D 100 award in the Software/Services category and was an R&D Special Recognition medalist in the Market Disruptor–Services category. Today, Spack manages more than 5,900 software packages, and its open-source community includes hundreds of users and contributors globally.

Gamblin says, “The EMCR project laid the groundwork for Spack’s new answer-set programming solver in 2020. My research continues to help the Spack and HPC community solve complex package problems.” With Spack’s new logic solver, Laboratory scientists and physicists can install their software faster than ever with minimal downtime. Gamblin’s latest initiative is the Binary Understanding and Integration Logic for Dependencies project, funded by the Laboratory Directed Research and Development Program, which aims to develop a machine-verifiable model of package compatibility within Spack for automated software integration on existing and future HPC systems.

ANDREW PASCALL AND MARCUS WORSLEY

Chemical engineers Andrew Pascall and Marcus Worsley combined their 2019 EMCR to create next-generation ceramic–metal (cermet) composite armor, which combines the high hardness of ceramic, increasing the armor’s resistance to penetration, with the toughness of metal, increasing its ductility. Pascall and Worsley’s cermet armor includes an internal metal lattice for reinforcement, like rebar inside of concrete. Together, the cermet materials and lattice design



could increase performance, operational supportability, and durability of armor used for military personnel and vehicles—making significant progress in the field of cermet armor.

Pascall and Worsley worked with Laboratory postdoctoral researchers Amy Wat and Jesus Rivera utilizing a software program called “nTopology” to design the lattice and adjust its parameters—such as the shape of the lattice (cubic lattice, octet truss, and helicoidal for example) and strut thickness. The lattice is then printed in wax using a 3D printer and embedded into an ultrahard, lightweight ceramic called boron carbide, referred to as a “green body.” When heated, the wax melts away from the green body, leaving empty channels in the shape of the lattice. Finally, the green body is placed on a piece of aluminum, which is then heated and wicks into the empty lattice channels, bonding with the porous ceramic, in a process called molten metal infiltration.

The two awardees are characterizing the mechanical properties of the different lattice designs for fracture toughness and tensile strength. Once they determine the ideal lattice combination, they will begin creating larger armor parts that can be tested to assess its strength. Pascall says, “The EMCR award, along with Marcus’s heat treatment expertise and my ability to design the initial armor pieces, made this project possible.” Worsley adds, “Our complementary skill sets allow us to cover different angles of problems and solutions.”

HUI CHEN

Internationally acclaimed physicist and 2017 EMCR recipient Hui Chen used her award to design a course to train new Laboratory employees on the use and application of high-energy-density (HED) science technology at Livermore’s National Ignition Facility and Jupiter Laser Facility. Chen explains,

“Many individuals, myself included, come to Livermore with a background in other areas of physics, and HED experiments at the Laboratory’s laser facilities require specialized training.” HED experiments performed at these facilities study and replicate matter and energy under extreme conditions and temperatures typically found at the center of giant planets and stars. With the course, Chen hoped to make the learning curve easier for new Laboratory employees who have been researching other areas of physics.

The course, “Introduction to HED Laser–Plasma Experiments and Diagnostics,” consists of six one-hour-long lectures with topics that include principles of laser-driven HED experiments and techniques, diagnostic principles, and current HED experiments using lasers. Chen says, “The short course had an attendance of



around 160 participants and turned out to be a huge success.” She adds, “With the support of the High Energy Density Science Center’s director, Frank Graziani; professor Farhat Beg at University of California San Diego (UCSD); and Joe Kilkenny of General Atomics, I expanded the introductory course into a full 20-lecture series on HED diagnostics for the center and UCSD, which has had two sessions with an attendance of about 300 attendees each time.”

In addition to HED instruction, Chen has led many experimental studies with national and international collaborators and made important contributions to several areas of plasma physics, most notably in the field of relativistic positron generation via intense laser-matter interactions, novel sensors for gated x-ray imaging, and x-ray spectroscopy of highly charged ions.

DAN HAYLETT

Livermore physicist Dan Haylett developed a course for new Laboratory employees in the Weapons and Complex Integration (WCI) Principal Directorate with his 2017 EMCR funding. The course, Modern Primary Design, offers a deep dive into physics as well as advancing the Laboratory’s ongoing nuclear weapon modernization efforts. This research supports Livermore’s Stockpile Stewardship Program of maintaining the nuclear stockpile without relying on testing.

The concepts behind the course stem from Livermore’s legacy of weapons design and the incorporation of advanced simulation and computing tools that bring these concepts to life. More specifically, Haylett teaches design fundamentals for the “primary,” or trigger in the fission bomb component of a thermonuclear weapon and studies the factors that affect its design. Haylett hopes to share his expertise in primary science, design, and construction with WCI designers. Haylett explains, “My course offers an array of alternative designs, some of which incorporate safer materials, the latest technologies, and modern security methods. Many of my former participants say the class has helped them advance their programmatic work. The Laboratory’s continued mission fulfillment relies on a thorough transfer of knowledge to the next generation of designers.”

CARLOS VALDEZ

Synthetic chemist at the Laboratory’s Forensic Science Center (FSC) Carlos Valdez and his team used his 2019 EMCR award to overcome the limitations of gas chromatography-mass spectrometry (GC-MS) in detecting synthetic opioids such as



fentanyl. The ability to accurately detect synthetic opioids could help the Laboratory, other government agencies, and law enforcement combat these lethal substances by controlling their production and developing medical countermeasures or antidotes.

GC-MS can only detect highly volatile substances, meaning substances easily vaporized by gas and heat. Due to the low volatility of fentanyls in their native salt form, these substances are virtually undetectable by GC-MS. To address this problem, Valdez’s team developed a novel method utilizing a compound, trichloroethoxycarbonyl chloride, which reacts with the fentanyl, generating two new molecules detectable by GC-MS.

With this information, scientists can now confirm the presence of a given fentanyl in urine or blood collected from an overdose victim. In addition, this technology can be utilized in the field during an illegal narcotics seizure to alert law enforcement or emergency personnel when a fentanyl is present. “The FSC staff assists government agencies like the U.S. Drug Enforcement Agency with this critical technology so they can detect opioids in real-life cases. EMCR awards catalyze potential scientific and technical advancements that otherwise may never see the light,” says Valdez. Valdez continues to make advancements in fentanyl research and in the development of antidotes against nerve agents as the principal investigator for three projects funded by the Defense Threat Reduction Agency.

The EMCR Program provides Laboratory leadership with the opportunity to learn about exceptional scientists and engineers making an impact in support of the Laboratory’s mission and who exhibit leadership potential. Says Schwegler, “It’s been a real pleasure to be involved in this award program, which is an essential investment in the Laboratory’s future.”

—Shelby Conn



Key Words: Aluminum, answer-set programming, beamtime, betatron x-ray radiation, boron carbide, ceramic-metal (cermet) armor, DNA sequencing, Drug Enforcement Agency (DEA), electrons, Early and Mid-Career Recognition (EMCR), fentanyl, free-electron laser, gas chromatography-mass spectrometry (GC-MS), genomics, green body, high-energy-density (HED), high-performance computing (HPC), Jupiter Laser Facility, Linac Coherent Light Source (LCLS), National Ignition Facility (NIF), nucleus, package manager, pathogens, SLAC National Accelerator Laboratory, software, solver, Spack, synthetic opioids.

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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. For the full text of a patent, enter the seven- or eight-digit number in the search box at the U.S. Patent and Trademark Office's website (uspto.gov).

Patents

Method of Manufacturing a Complex Product by an Additive Manufacturing Process

Andrew Pascall, Hanna Coe, Julie Jackson, Susant Patra
U.S. Patent 11,053,603 B2
July 6, 2021

Automated Control of Microfluidic Devices Based on Machine Learning

Brian Giera, Eric B. Duoss, Du Nguyen, William Smith, Sachin Subhash Talathi, Aaron Creighton Wilson, Congwang Ye
U.S. Patent 11,061,042 B2
July 13, 2021

Biodegradable Surfactants and Related Compositions, Methods, and Systems

Mathew Lyman, Lawrence Dugan, Roald Leif, Bonnee Rubinfeld, Brian Souza, Carlos Valdez
U.S. Patent 11,066,359 B2
July 20, 2021

System and Method for Stimulated Emission Depletion Projection Stereolithography

Ryan Hensleigh, Bryan D. Moran, Julie A. Jackson, Eric Duoss, Brett Kelley, Maxim Shusteff, Hayden Taylor, Christopher Spadaccini
U.S. Patent 11,072,160 B2
July 27, 2021

Preventing Stent Failure Using Adaptive Shear Responsive Endovascular Implant

Erik V. Mukerjee, Jane A. Leopold, Amanda Randles
U.S. Patent 11,083,604 B2
August 10, 2021

Optimal Toolpath Generation System and Method for Additively Manufactured Composite Materials

James Lewicki, William Compel, Daniel Tortorelli, Felipe Fernandez-Ayala
U.S. Patent 11,084,223 B2
August 10, 2021

Ultra-Compact System for Characterization of Physical, Chemical and Ignition Properties of Fuels

Matthew J. McNenly, Geoffrey M. Oxberry, Ahmed E. Ismail, Nicholas Killingsworth, Daniel L. Flowers
U.S. Patent 11,085,910 B2
August 10, 2021

Liquid Tamped Targets for Extreme Ultraviolet Lithography

Yechiel R. Frank
U.S. Patent 11,086,226 B1
August 10, 2021

System and Method for Laser System Having Non-Planar Thin Disc Gain Media

Jay W. Dawson, Ronald Lacombe
U.S. Patent 11,095,085 B2
August 17, 2021

3D Printable Feedstock Inks for Signal Control or Computation

Maxwell Murialdo, Yuliya Kanarska, Andrew Pascall
U.S. Patent 11,101,255 B2
August 24, 2021

Awards

Lawrence Livermore materials scientist **Bill Pitz** was selected as a 2021 **SAE fellow** for his career contributions to chemical kinetic modeling of transportation fuels. Pitz was one of two national laboratory scientists selected as a 2021 fellow. Established in 1977, SAE fellow status is the highest grade of membership bestowed by **SAE International** to members from industry and academia.

The SAE fellow program honors long-term members who have made a significant impact on the mobility industry through leadership, research, publishing, innovation, and volunteering. This new class of fellows are recognized for outstanding engineering and scientific accomplishments that have resulted in meaningful advances in automotive, aerospace, and commercial vehicle technology.

The **Department of Energy's Office of Science** awarded two Livermore scientists with the 2021 **Early Career Research Program Award**. This year's award honored

83 scientists nationwide and marked the program's 12th year. The Early Career Research Program aims to bolster the nation's scientific workforce by providing support to exceptional researchers during crucial early years when many scientists do their most formative work.

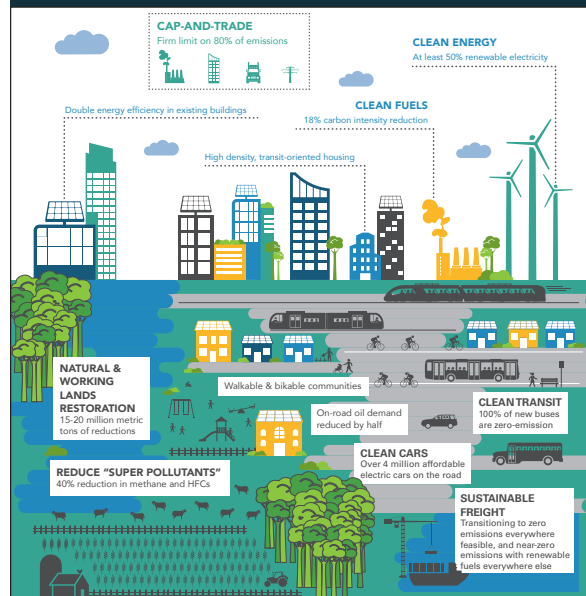
Xue Zheng, a scientist in the Atmospheric, Earth, and Energy Division in Livermore's Physical and Life Sciences Directorate, was recognized by the **Office of Biological and Environmental Research** for her work on aerosol-cloud processes. In her research, Zheng analyzes atmospheric observations and climate models to advance the understanding of cloud response to aerosols over ocean and land. **Andrea Schmidt**, a physicist in the National Security Engineering Division in Livermore's Engineering Directorate, was recognized by the Office of Fusion Energy Sciences for her work in neutron yield scaling with currents in dense-plasma focus discharges magnetically driven by Z-pinch plasmas.

Extremely Bright, Incredibly Fast

Since Ernest O. Lawrence's invention of the cyclotron, the evolution of more powerful particle accelerators and synchrotron radiation light sources have illuminated the inner workings of the atom and contributed to invaluable scientific advances. Today, multidisciplinary teams of Lawrence Livermore scientists and researchers have been leading a variety of experiments at various synchrotron light-source facilities around the world. Whether using shock or static compression, a diamond anvil cell, a gas gun, or a laser, these experiments are pushing materials to extreme states using some of the brightest x rays on the planet to observe how materials change in a fraction of a nanosecond and investigate equation of state, materials deformation, detonation science, and novel materials development that have yielded groundbreaking discoveries in support of the Laboratory's missions.

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The Path to a Carbon Neutral California



A report prepared by Lawrence Livermore National Laboratory outlines a strategy supporting the state's goal for net zero emissions by 2045.

Also in this upcoming issue...

- The first-ever shot with a high explosives sample at the National Ignition Facility expands understanding of explosive material characteristics.
- Advances in machine learning offer greater robustness, protecting computer model predictions from data changes and corruptions.
- A prototype microfluidic device developed at Livermore can rapidly analyze post-detonation debris following a nuclear event.

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