Science & Technology Review

March 1999

U.S. Department of Energy's
Lawrence Livermore
National Laboratory

High Tech Explodes at Site 300

Also in this issue:

- **Metallized Hydrogen's New Implications**
- **Surprising Behavior from Methane Hydrate**
- **Laser–Tissue Interaction Model**

About the Cover

The Laboratory's Experimental Test Site, more familiar as Site 300, uses the best and safest methods and materials to assist in experimental examinations of the nation's nuclear stockpile. An overview of these activities begins on p. 4.

Because Site 300 covers some 7,000 acres, we've juxtaposed three photos to show an overall idea of what it's like. In the background are buildings where high explosives and other non-nuclear components are put to the test by dropping, heating, vibrating, or shocking. Across the site is the tower where technician Ray Domingo guides placement of a component for a drop test. In between test areas, wildlife has free reign, and endangered species are protected.

About the Review

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

Please address any correspondence (including name and address changes) to *S&TR*, Mail Stop L-664, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, or telephone (925) 422-8961. Our electronic mail address is *str-mail@llnl.gov*.

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Prepared by **LLNL** under contract
No. W-7405-Eng-48

S&TR Staff

Scientific Editor
David Eimerl

Managing Editor
Sam Hunter

Publication Editor
Sue Stull

Writers
Ann Parker, Sue Stull, Katie Walter, and Gloria Wilt

Art Director and Designer
Kitty Tinsley

Internet Designer
Kitty Tinsley

Compositor
Louisa Cardoza

Proofreaders
Carolin Middleton and Al Miguel

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

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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-52000-99-3
Distribution Category UC-700
March 1999

Gel fights biological and chemical weapons

More effective and more environmentally acceptable than methods currently in use, Livermore's new oxidizing gel holds the promise of effectively fighting both biological and chemical weapons (BW and CW). The work is part of a DOE-sponsored project with Los Alamos and Sandia national laboratories.

Testing at Livermore was done using nontoxic simulants for biological and chemical agents such as anthrax, plague, variola, sulfur mustard, sarin, and VX. "Preliminary experiments with our peroxymonosulfate gel," says Ellen Raber, deputy department head of environmental protection at Livermore, "showed that it was 100 percent effective under laboratory conditions for all BW and CW simulants on all surfaces except for the VX simulant on carpet, where the gel was only 95 percent effective."

Now, the U.S. Army is testing the gel on actual chemical warfare agents. Before the gel is ready for use, additional tests will be done on live vaccine strains, and spraying systems will be evaluated. The team is also actively studying the level of cleanup needed for civilian settings.

Contact: Ellen Raber (925) 422-3985 (raber1@llnl.gov).

Livermore scientists help discover quasar

A team of researchers from six institutions, including Lawrence Livermore, has discovered a quasi-stellar object having one of the most luminous starbursts ever seen.

The team's findings were announced during the 193rd meeting of the American Astronomical Society in Austin, Texas. Mike Brotherton, a postdoctoral fellow with Livermore's Institute of Geophysics and Planetary Physics, headed the team composed of scientists from Australia, the U.K., and the U.S., including Wil van Breugel and Adam Stanford of Lawrence Livermore. During 1998, the researchers conducted a search for new quasars and found more than a hundred.

Quasars are quasi-stellar objects that are exceptionally bright and exist in the center of a galaxy, generally outshining the entire galaxy. Discovered in 1963, the enigmatic quasars emit prodigious amounts of energy from a very compact source. The most widely accepted theory is that a quasar is powered by a supermassive black hole in the core of a more-or-less normal galaxy. Starbursts are events that create firestorms of stars, normally through the collapse of a gas cloud.

"We believe that the amount of gas involved is as much as one-tenth the mass of the Milky Way," Brotherton said. This same collision may have provided the gases (mainly hydrogen and helium) to power the quasar.

Contact: Mike Brotherton (925) 423-8127 (mbrother@igpp.llnl.gov).

Glaze to head virtual EUVL lab

James Glaze has been chosen executive director of the Virtual National Laboratory (VNL), a consortium of researchers from three Department of Energy national laboratories. They are working with industry to develop extreme ultraviolet lithography (EUVL) into the next-generation technology for inscribing computer chips.

Glaze recently rejoined the staff at Lawrence Livermore and has assumed leadership of the project. The VNL combines researchers from Lawrence Livermore, Lawrence Berkeley, and Sandia national laboratories into a single unit dedicated to developing EUVL. Established in 1996, the VNL is working with Intel, Motorola, and Advanced Micro Devices to develop short-wavelength projection lithography for mass production of integrated computer circuits.

A silicon chip technology and technology policy expert, Glaze served as vice president of Technology Programs for the Semiconductor Industry Association. Previously, Glaze spent more than a decade at three semiconductor firms and had directed development of laser systems for fusion research at Livermore.

Contact: James Glaze (925) 422-5411 (glaze1@llnl.gov).

Virtual lab for heavy-ion fusion

A Heavy Ion Fusion–Virtual National Laboratory (HIF–VNL) is beginning collaborative research and small experiments that will validate accelerator design of a major accelerator project to support Livermore's National Ignition Facility (NIF). The construction decision will be made as NIF begins operation in 2003. A memorandum of agreement for combining research on heavy-ion fusion has been signed by Lawrence Livermore and Lawrence Berkeley national laboratories. Berkeley's Roger Bangerter and Livermore's Grant Logan will be director and deputy director, respectively.

The goal is to develop more synergistic research and make more rapid progress in the development of heavy ion drivers using both laboratories' staff and facilities. The virtual lab's experimental initiative, called the Integrated Research Experiment, will also address scientific and technological issues of the accelerator in an inertial-fusion-energy power plant as well as target and beam transport issues.

Contact: Grant Logan (925) 422-9816 (logan1@llnl.gov).

Site 300: Energy Experts Behind the Explosions

LAWRENCE Livermore is actively involved in developing many cutting-edge computational and experimental tools to help assure that the U.S. nuclear weapons stockpile remains safe and reliable. But our responsibilities don't stop there. Because the components of nuclear weapons are extremely complex, we can only achieve an in-depth understanding of the issues associated with these systems through a watchful and constant study of them. We must use our historical data, traditional scientific techniques, and world-class facilities just as much as new technologies to ensure that we have properly addressed existing issues and anticipated future ones.

Livermore originally created Site 300 to test high explosives that are used in nuclear weapons. These are the highly energetic materials that provide the energy to drive a nuclear weapon's fissionable material to criticality. In the beginning, we tested just the explosives for nuclear devices. Our test facilities have traditionally been dedicated to studying explosives performance and safety with outdoor tests that are remotely controlled. (Before the testing ban that began in 1992, nuclear weapons were tested underground at the Nevada Test Site some 80 miles north of Las Vegas.) Later, we began developing and testing new types of explosives, more reliable than other available materials. Eventually, we added explosives testing for advanced conventional weapons to our capabilities.

Today, with the increased need for data to validate computer models and for more diagnostic information about every explosion we conduct, Site 300's role has grown more complex as well. The article beginning on p. 4 describes the range of capabilities we use to support scientific, computational, and engineering activities at Livermore.

Some of our capabilities at Site 300 include formulating, machining, and testing explosives in both small and large quantities; studying the science of high-explosives performance; inspecting materials radiographically for defects such as cracks and voids; using ultrafast electro-optical imaging of projectiles; and performing impact testing with our 30-meter drop tower. Our recently upgraded Flash X-Ray (FXR) machine is the cornerstone diagnostic in the most versatile and complete explosives testing facility in the world. Soon, in the same area, construction will begin on the Contained Firing Facility, a 2,700-square-meter indoor explosives testing facility. The containment addition will include a reinforced firing chamber, a support staging area, and additional diagnostic space for testing up to 60 kilograms of explosives materials. Ever thinking about future environmental requirements and the neighbors of Site 300, we have designed the Contained Firing Facility to reduce environmental emissions such as hazardous waste, noise, and blast pressures.

Site manager Milt Grissom points out in the article that Site 300 is busier than ever with work from many areas of the Department of Energy. In addition to the continuing traditional work on high explosives, tests are providing data for the Laboratory's counterterrorism activities. And today the site is well positioned to conduct explosives testing that can benefit the aircraft, mining, oil exploration, and construction industries.

■ Michael Anastasio is Associate Director, Defense and Nuclear Technologies.

Site 300 Keeps High-Explosives Science on Target

Explosions and nondestructive tests at Site 300 assure that the nation's HE and other nonnuclear weapon components are safe and reliable.

Figure 1. Vehicles and personnel entering Site 300's firing area must pass the central control point, where Art Caya accounts for arrivals and departures.

YOU might hear a loud BOOM occasionally, but little else indicates what goes on there. Tucked away in the rugged, grassy hills between Livermore and California's Central Valley is Lawrence Livermore's Experimental Test Site. It has been known as Site 300 since the days when Livermore was part of Berkeley Radiation Laboratory: Berkeley was Site 1, Livermore was Site 2, and the testing range was Site 3. Times and names have changed, but the periodic BOOMS continue.

The explosions, known as shots, result from destructive tests of high explosives (HE) and other nonnuclear weapon components—100 to 200 of them a year in the last 10 years. Powerful x-ray machines, interferometers, high-speed cameras, and other diagnostic equipment record information about the experiment in the first nanoseconds after detonation. Site 300 also conducts nondestructive tests that may, for example, subject a prototype to vibration and extreme heat, conditions comparable to those it might encounter while being transported across a desert. Another big part of Site 300's work is fabricating and machining HE and assembling experiment devices prior to testing. All of these activities are potentially hazardous, yet Site 300 has a stellar safety record. In 44 years, no injuries involving high explosives have occurred.

Much of Site 300's effort supports Lawrence Livermore's main mission today of overseeing the nation's nuclear arsenal through the Department of Energy's science-based Stockpile Stewardship Program. As part of the program, the Accelerated Strategic Computing Initiative (ASCI) is bringing almost unimaginable power to Livermore's modeling capability to simulate weapons performance. And in a few years, the National Ignition Facility will be available for addressing the physics of thermonuclear fusion. Yet, even with these unprecedented capabilities at Livermore, tests at Site 300 are perhaps more important now than ever before.

HE testing, using nonnuclear materials, is almost the only available high-fidelity way of experimentally examining the operation of a nuclear weapon. The U.S. no longer conducts nuclear tests, and only a few subcritical (no nuclear yield) experiments are being conducted at the Nevada Test Site. The high-explosives tests are also important for improving our understanding of the effects that aging has on chemical high explosives in stockpile systems and of compatibility with other materials. Validation of models and simulations through actual experiments are essential for scientists to know whether their design is, figuratively speaking, on target.

Testing More Parameters

According to Randy Simpson, a chemist and HE expert at Livermore, "We understand the stars and supernovae better than we understand high explosives. When high explosives detonate, they can generate up to 500,000 atmospheres of pressure and may move at speeds of up to 10 kilometers per second. Reactions take place in less than a billionth of a second, releasing enormous amounts of energy. Our Site 300 experiments study how high explosives release their energy—for example, how they accelerate metals or what chemical reactions they cause."

The tests allow us to study the performance of HE materials, their reliability and safety, and ways to optimize the materials and manufacturing methods. Three avenues of testing ensure the HE portion of stockpile performance: core surveillance testing of operational weapon HE function, enhanced surveillance to test the effects of aging on HE, and testing of replacement and specialized HE components.

Protecting the Environment

Not bothered by the occasional noise, a healthy wildlife population runs over the hills and ravines of Site 300. Three endangered species—the San Joaquin kit fox, the red-legged frog, and the large-flowered fiddleneck plant—are afforded special protection. Site 300 is also a friendly spot for birds of prey, which use high-voltage power lines for perching because of the lack of trees. Laboratory staff have outfitted power poles with antielectrocution sleeves to protect the birds. Site 300's full-time wildlife biologist helped to invent the tiny MOLE, a remotely controlled robot (photo at right) that explores and observes certain sensitive species in their dens.

Past activities at Site 300 have contaminated some soil and groundwater, which are being treated in a variety of ways. For example, trichloroethylene (TCE), a toxic carcinogen and solvent, was used for many years in the environmental test area as a heat exchange fluid for thermal testing. An environmental restoration program is extracting groundwater and soil vapor from the subsurface to remove the contaminants.

Several "green" restoration technologies—which use less energy and have less impact on the environment than many conventional cleanup methods—are also being implemented at Site 300. "It makes sense to clean up the environment using techniques that are kind to the environment," notes environmental scientist John Ziagos, who is responsible for restoration work at Site 300. A geosyphon, which sucks water out of the ground by discharging elsewhere, is planned for a testing area. Electricity is needed only to get the pump started. Then gravity takes over and pulls water out for treatment. A system known as SWAT (solar-powered, water-activated-charcoal treatment) is being considered for remote parts of the site where no power lines run. Microbial methods and wind-powered treatment are also likely to be employed in the next year or so.

For as long as the U.S. has had a nuclear stockpile, personnel at Site 300 have been participating in core surveillance of the stockpile. Periodically, weapons have been taken apart and components put through their paces to ensure that everything is still operating as designed.

Now that weapons are being kept in the stockpile beyond their design lifetimes, a part of the Stockpile Stewardship Program known as enhanced surveillance uses experiments and modeling to predict what changes are likely to occur over time and their possible impact on safety or reliability. Enhanced surveillance is central to meeting the defense objectives of the U.S. and its allies in this era of no nuclear testing.

One series of enhanced surveillance tests at Site 300 compared the performance of new and aged explosives. According to Jon Maienschein, the Livermore chemical engineer who oversees the enhanced surveillance work with explosives, "The good news is that our high explosives are not degrading much, but that also makes predicting changes more difficult."

One difficulty in studying aged high explosives is that they are hard to obtain. The oldest are only about 25 years old, yet the enhanced surveillance program seeks to project changes 50 years from now. So scientists at Livermore's High Explosives Applications Facility (HEAF) are working to formulate substances that simulate high explosives of various ages. HEAF is permitted to manufacture up to 100 grams of high explosives, while larger amounts must be manufactured at Site 300. Maienschein anticipates that the simulated aging effort will reach the point sometime in the next year, when larger-scale HE manufacturing and additional testing can begin.

As parts and materials in weapons age, they must be replaced. Replacement is more complicated than it once was because most nuclear weapons manufacturing facilities have shut down, and environmental requirements have changed. As new manufacturing processes are devised and new nonnuclear parts are fabricated, many exlosives find their way to Site 300 for testing before they are installed in weapons.

For decades, Site 300 has also tested Livermore-designed conventional weapons, such as shaped charges, which have been deployed by the Department of Defense in specialized armaments. These conventional weapons contain high explosives whose behavior and effects on other weapon materials must be tested and compared to modeled predictions.

A Quick Tour

Site 300 is set on 7,000 acres of land about 15 miles east of Livermore. It is

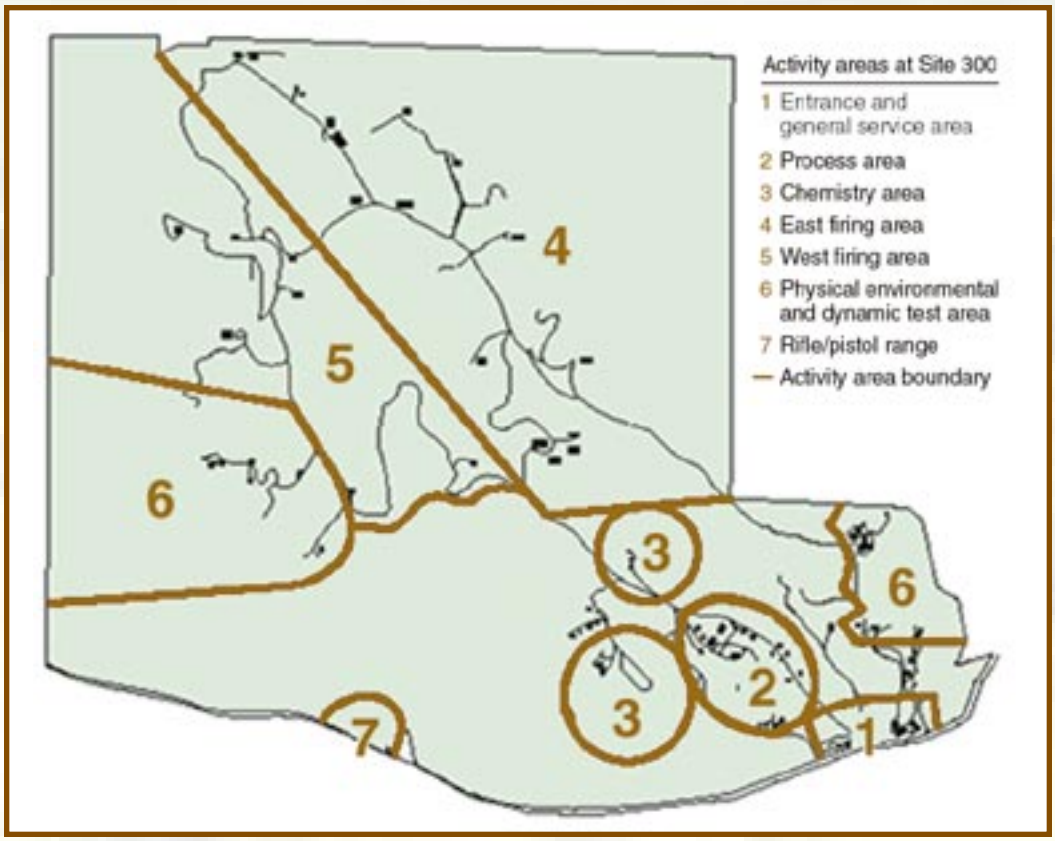


Figure 2. Activity area map of Site 300.

marked by both rolling hills and steep ravines with very few trees in sight aside from those planted around the parking lots and administrative buildings near the entrance. When it was established in 1955, Site 300 was a very remote area surrounded only by cattle ranches. It is still remote, but these days the city of Tracy is expanding toward the site from the east.

As shown in Figure 2, several administrative and service buildings are clustered near the entrance to the site where site manager Milt Grissom and others have their offices. The environmental test area is to the northeast. The area where high explosives are fabricated and test devices are assembled is to the north (areas 2 and 3 on the map). The firing bunkers, where high explosives and other weapon components are detonated on open firing tables, are still farther north, separated from each other and well away from the boundaries of the site. Scattered throughout the site are earth-covered magazines for storage of high explosives, waste collection and treatment areas, and numerous storage buildings.

Set on a knoll looking east and south is Site 300's weather station. It gathers weather information before each shot and helps Site 300 to be a good neighbor by not exceeding a self-imposed noise threshold. Two to three hours prior to a shot, a weather balloon is released with a sonde attached. The sonde collects temperature data during its ascent through the atmosphere and transmits the information back to the weather station. At the same time, radar tracks the balloon and collects wind velocity data. This information is used in a computer code to predict the maximum amount of high explosives that can be detonated without exceeding the Laboratory's noise limit of 126 decibels for populated areas. If the data indicate that a populated area will be "popped," the test is postponed until weather conditions are more favorable.

"All of our facilities are staffed by 48 highly skilled technicians, " notes

Countdown to a Shot

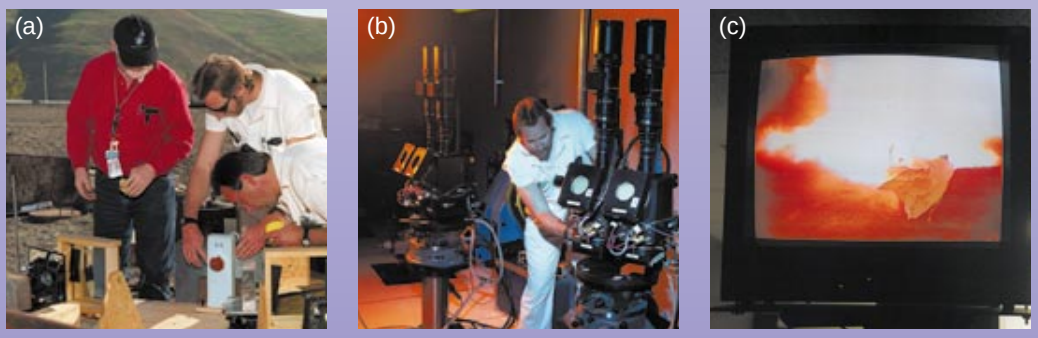
The explosion may be what you hear, but weeks and sometimes months of effort by many people go into making the shot perform as planned. A scientist at Livermore will have the original concept for an experiment. The scientist then needs engineers to turn the physics design into a manufacturable engineering design. Technicians in Livermore's engineering shops build most of the parts, except for the high explosives, which are manufactured at Site 300. Technicians at the high-explosives process area assemble the whole package, sometimes including a pin dome (Figure 6) and other devices needed for gathering information about the experiment.

The test assembly is moved to either Bunker 801 or 851, and all diagnostic equipment is set up. Electronic timing devices are set to synchronize all equipment for the experiment.

A weather balloon is sent up to assure that shot noise will not exceed 126 decibels in populated areas. The Stockton Airport is notified so that it can keep aircraft out of Site 300's air space. The bunker supervisor calls a muster, and every person who has signed in at the bunker must be accounted for. There is a final dry run, and last-minute adjustments are made. Someone goes to an observation point to assure that no unauthorized personnel enter the danger area by vehicle or aircraft. If there are, the shot is postponed.

After the console operator pushes the "FIRE" button, several things still must happen in the microseconds before and after detonation begins. The cameras are automatically synchronized, laser-pulsed flashlamps light up the shot for the cameras, the laser for the interferometer is pulsed, and the radiography system is pulsed.

Finally, weeks after work first started on the shot, the test assembly, so carefully constructed, is blown to smithereens while diagnostic equipment records the first moments after detonation. Then scientists back in Livermore evaluate the data and begin work on another test.



Setup activities for a shot (a) at the firing table and (b) in the high-speed camera room. (c) Video playback of a shot is just one of many diagnostics.

site manager Grissom. "The experiments we perform are expensive, so the techs have to get it right the first time. And they do, consistently." After years of employment, they have specialized knowledge about machining high explosives, operating environmental test equipment, or setting up the flash x ray for a hydrodynamic test. With no vocational or college major education in HE and testing, virtually all technicians have been trained on the job. Jack Lowry, supervisor of one of the firing bunkers, was a miner early in his career and learned about explosives then. Chuck Cook, who operates radiography equipment at the bunkers, was a hospital x-ray technician. They and others brought relevant experience with them when they started working on HE tests, but they still had much to learn about this unique field.

Fabricating Explosives

Research and development of high explosives for various applications take place at HEAF in Livermore (*S&TR*, June 1997, pp. 4–13). Notes A. J. Boegel, manager of Site 300's high-explosives process area, "The 100 grams of high explosives that HEAF can manufacture and 10 kilograms that HEAF can test are sufficient for laboratory-scale experimental purposes but not enough for full-scale testing."

Starting with HEAF's small recipe, technicians at Site 300 begin to scale up the formulation. Any cook knows that doubling or tripling a recipe is not always a simple linear process of doubling or tripling all ingredients. The end product may be too salty or there may be other problems. The same is true for HE formulations, but the results of errors are potentially much more serious than a too-salty cake. Scaling up takes place gradually, with samples tested frequently.

Site 300 personnel also manufacture the HE routinely used in tests and prepare new formulations for specific applications. In a recent project, a special formulation was developed at HEAF and manufactured at Site 300 for the Department of Defense. Site 300 also manufactured substances that have been used to train dogs to sniff out HE.

A pilot-scale plant at Site 300 is used to test a new way to synthesize TATB, an HE with such low sensitivity, that it is the safest high explosive available. But conventional manufacturing methods are expensive, and HEAF scientists have developed better methods.

Paste high explosives are used in shaped charges. They are extruded into the shaped-charge cavity, so they require no machining. Plasticized high explosives require a different process.

Figure 3. Readying high explosives for a test. (a) Mark Hoffman and Kirk Pederson mix HE, (b) Dean Adams and Monty Sappenfield remove an HE component from a presser, and (c) Aniceto Salmon machines a component to final tolerances.

First, they are manufactured into a powder, which is heated to soften the plastic binder. The heated mixture is then pressed into the shape needed for a particular experiment, x-rayed for cracks, machined, and inspected mechanically to test for tolerances (Figure 3). With both paste and plasticized high explosives, two units are often made: one is subjected to environmental tests to assure its safety before the other one is used in the planned shot.

All of this work—mixing, extruding, heating, pressing, and machining, whether for new or standard formulations—is done remotely. Thick concrete walls and earth berms separate the control rooms from these operations. Cameras and microphones trained on the work are the technician's eyes and ears, and redundant control systems provide additional safety. The work bays are buried in earth on one side with a blowout wall on the other side to release energy should an accident occur.

The final operation in this area—device assembly—cannot be done remotely. Some devices have more than 100 parts, and assembly can take two weeks to complete. The process must meet very tight tolerances if modeling codes and performance criteria are to be validated.

Shake, Rattle, and Roll

At the environmental test area, Ron Samoian directs safety characterization tests. Several facilities subject prototype high explosives, detonators, and other energetic materials as well as nonnuclear stockpile components to vibration, shock, impact, acceleration, twisting, and various combinations of heat and cold. Some tests simulate accidents, from dropping explosives to aircraft crashes and fuel fires. The test units can be subjected to vibration levels that encompass both ground and aircraft transportation over temperatures ranging from arctic to desert conditions. Some tests, such as a fall in the 30-meter drop tower (Figure 5a and b), are over in a few seconds. Other tests to study how materials age under various conditions have run for years.

All testing is done remotely with cameras, microphones, and electronic sensors reporting to a central control room. Testing bays are constructed like the ones in the high-explosives process area with a heavy earth berm behind a blowout wall and roof (Figure 4).

Vibration and shock testing can be done in any of three shakers. One of the electrodynamic shakers (Figure 5c) can reach 40,000 pounds of force with a 1-inch stroke. The hydraulic shaker goes to 60,000 pounds of force with a 6-inch stroke. All the shakers can be flipped 90 degrees so that testing can be done side to side as well as up and down. Frames for shock testing allow drops of 20 centimeters to 30 meters. Impulse testing is done using a gas-operated piston to accelerate a specimen into a specially designed target. Torsional testing is done at a table where samples are subjected to quick twisting (Figure 5).

All of these tests can be combined with thermal conditioning. High-explosive samples may be heated electrically to 73°C or cooled using liquid nitrogen to –73°C. A sample being dropped from the 30-meter drop tower must be thermally conditioned first. Thermal chambers fit over the shakers and smaller drop frames for simultaneous thermal conditioning.

Recent work has included testing of high-explosive components of the W87 nuclear weapon, which was designed at Livermore. When the weapon was first

Figure 4. The environmental test area at Site 300 includes a testing bay protected by an earth berm (at left).

developed, the high explosives in it were subjected to the full range of vibration, shock, and temperature testing, which established an "envelope" of safe responses. The testing that is done as the weapon and its components age determines how the collection of responses has changed and whether those changes affect weapon safety.

Fire Away!

The two main firing bunkers, 801 and 851, come under the management of Kent Haslam. Bunker 801 is now used primarily for tests related to nuclear weapons. Bunker 851 is generally used for testing conventional weapons such as shaped charges.

Back in 1955, the only diagnostic technique available for studying a shot was high-speed photography, and it was not possible to synchronize multiple cameras. More sophisticated versions of the same cameras are used today, along with radiography for recording the inside of thick metal parts and interferometry for measuring velocities of explosion-driven surfaces. Another often-used diagnostic is the pin dome (Figure 6). Its many fiber-optic wires electronically record the velocity and symmetry of an implosion. Today, a timing system synchronizes all of the diagnostic tools with the detonation.

Bunker 851 supervisor Jack Lowry notes, "There used to be lots of experiments with fewer diagnostics. Now each shot has lots of diagnostics. Computers make the difference, allowing us to gather huge amounts of information. And we at Site 300 and the scientists at Livermore are constantly trying to figure out ways to get more data."

High explosives produce pressures so high that solid materials, even when not melted, flow like fluids (Figure 7). Many of Site 300's shots are designed to study this hydrodynamic behavior

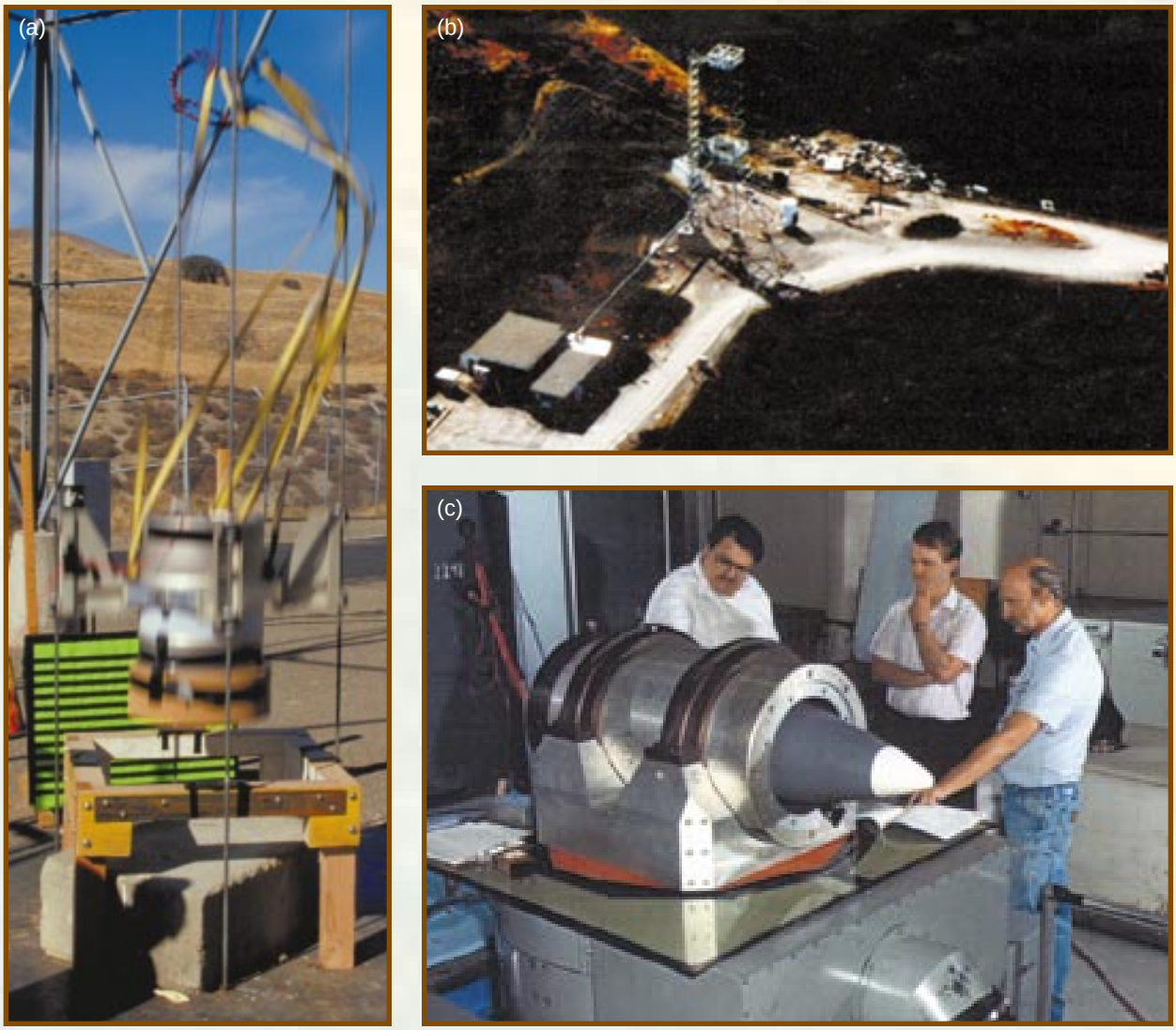


Figure 5. (a) The 30-meter drop tower in action, (b) an aerial view of the tower, and (c) (left to right) Bill Stigman, Jess Squires, and Bruce Kleg examine a re-entry vehicle after a test on the shaker.

either in conventional weapons or nuclear weapons. For studying the hydrodynamics of a nuclear weapon, a nonfissile material is wrapped in a high explosive with the same geometry as the core of a weapon. This mockup is detonated, resulting in an explosive compression that deforms the material, making it denser and causing it to flow. With "hydrotests," scientitsts seek to better understand this complicated behavior, whose physics are still not well understood.

The first hydrodynamics test facility at Site 300 was Bunker 801. Originally a Quonset hut, Bunker 801 now is a state-of-the-art testing facility housing the Flash X-Ray (FXR) machine, a linear induction accelerator specifically designed for diagnosing hydrotests by radiographing the interior of an imploding high-explosive device. Its x rays are so powerful that they can penetrate more than a foot of steel and record the motion of materials moving at ultrahigh speeds. Says Doug Bakker, supervisor of Bunker 801, "The typical shot using the FXR is a hydrotest for a mockup nuclear weapon assembly. Because of the high densities of the materials used in these assemblies, only the FXR can do the job."

Already the world's most sophisticated flash x-ray system, the FXR has recently been upgraded so that two x rays may be obtained during a single test. A gamma-ray camera system, designed by Livermore scientists and 70 times more sensitive than radiographic film, records the picture produced by the FXR's x rays (see *S&TR*, May 1997, pp. 15–17).

In April 1999, construction of the Contained Firing Facility (*S&TR*, March 1997, pp. 4–9) is scheduled to begin at Bunker 801 to provide a controlled environment for high-explosives testing (Figure 8). When construction is complete sometime in late 2001 or early 2002, Bunker 801 will also incorporate a multibeam Fabry–Perot interferometer to provide as many as 20 data collection points for measuring surface velocities during an experiment (*S&TR*, July 1996, pp. 12–19).

While Bunker 801 is out of commission during construction, most experiments will be moved to Bunker 851. Particularly large tests will be sent to the Nevada Test Site.

Diagnostic equipment at Bunker 851 is similar to that at 801, except that its radiographic equipment produces a lower dose of radiation than the FXR. Thus, Bunker 851's accelerator is effective in radiographing less dense materials. The bunker also houses portable x-ray equipment and a 15-beam Fabry–Perot interferometer, which is being upgraded to 20 beams.

The tests of aged high explosives for the enhanced surveillance program were run at Bunker 851. Another recent series of tests studied shaped charges for use in counterterrorism. Technicians recently ran a series of tests of shaped charges for an oil company, which uses them as perforators to open oil-bearing rock.

A Bright Future Ahead

"Site 300 is busier now than it's ever been in my nine years here," says site manager Milt Grissom. "Not only are we running experiments at our own bunkers,

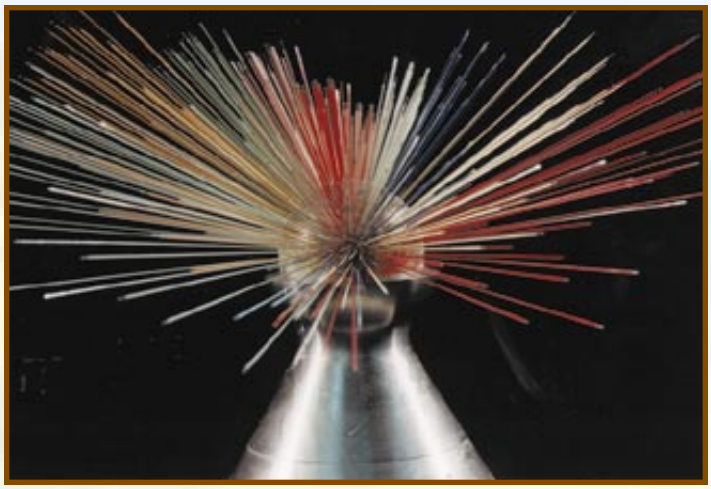


Figure 6. The fiber-optic "pins" on this pin dome receive velocity and symmetry information while a test device implodes.

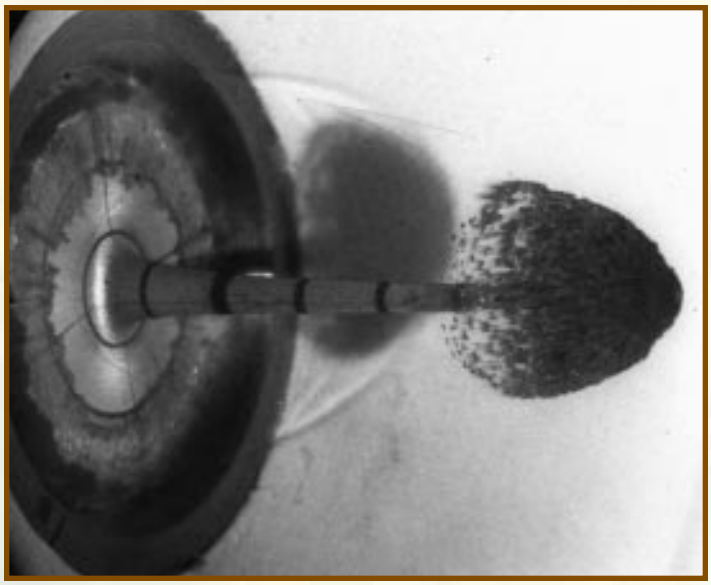


Figure 7. A shaped charge speeds to the right at 8 kilometers per second during a hydrodynamic test, which illustrates the fluid-like behavior of metals when they are subjected to extremely high pressures.

but our technicians are also working on experiments at the Nevada Test Site. They are manufacturing the high explosives and then going to Nevada to set up the experiments and run the diagnostics. On top of that, construction of the Contained Firing Facility will start soon, and we are getting more and more work.

"Our infrastructure has to support all of this activity," he continues. Construction will begin soon on a combination fire house, medical facility, and badge office near the entrance to the site. Administrative staff have outgrown available space and so will move into the old fire house.

Grissom goes on, "With over 200 people that work here representing so many areas of the Laboratory, my job ought to be tough. But it isn't at all. There's a great can-do attitude here." That attitude will stand Site 300 in good stead as it continues its busy schedule.

—Katie Walter

Key Words: enhanced surveillance, environmental restoration, Fabry-Perot interferometer, Flash X-Ray (FXR) machine, high explosives, High Explosives Application Facility (HEAF), hydrodynamic tests, MOLE, shaped charges, Site 300, stockpile stewardship.

For further information contact Site 300 site manager Milt Grissom (925) 423-1396 (grissom1@llnl.gov) or Jim Lane, deputy site manager, (925) 423-5217 (lane5@llnl.gov).

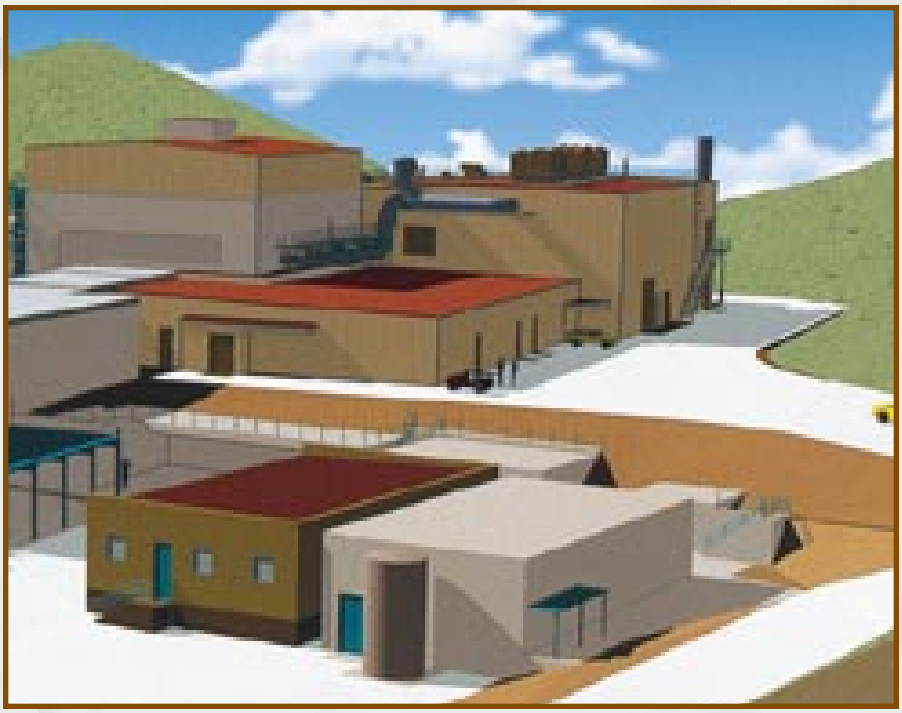


Figure 8. Bunker 801 as it will look when the Contained Firing Facility is complete.

About the Engineer

MILTON L. GRISSOM has been manager of Livermore's Experimental Test Site (Site 300) since 1990. During his 33-year career at the Laboratory, Grissom has held numerous technical and administrative leadership positions, including leading many projects within the Mechanical Engineering Department's Nuclear Explosives Engineering Division. He currently serves as a Laboratory Emergency Duty Officer (LEDO) and is chair for the Laboratory's Operational Security Program and Work Smart Standards committee.

Grissom holds a B.S. in mechanical engineering from the University of New Mexico and an M.S. in mechanical engineering from San Jose State University.

Putting More Pressure on Hydrogen

Flashes of light and deafening crashes punctuated Livermore's laser experiments to transform an isotope of hydrogen into a metal. The payoff: data for revising the hydrogen equation of state, fundamental not only to the Laboratory's national security projects but also to physical science itself.

THE laser experiments team knew they had to scramble. The dismantling of Nova, the world's largest laser, was on the agenda. Lawrence Livermore's even larger laser facility, the National Ignition Facility (NIF), needed Nova's space for support facilities as NIF construction was progressing. The two-beam laser target area necessary for the experiment was scheduled to be shut down imminently, and the Nova schedule was very full. But a place in line suddenly became available. Team members knew this was their opportunity to repeat some important but difficult work using new diagnostic techniques with the Nova facility. They were going to perform another round of experiments to laser-shock and compress deuterium, an isotope of hydrogen, and turn the element most familiar in a gaseous form into a metal.

For this experiment, Nova would be used to create conditions not very different from the atmospheres of giant planets and the outer envelopes of low-mass, largely hydrogen stars. The laser would subject hydrogen to extreme and hitherto unexplored pressure regimes. It would pulverize deuterium samples, allowing experimenters to collect, analyze, and verify thermodynamic and optical information about how hydrogen goes metallic.

The results would establish a substantially improved equation of state for the element hydrogen. They would also add to our understanding of large planets and stars, make it easier to design fusion targets for NIF's 192 laser beams, and prove important for

DOE's stockpile stewardship mission by providing new high-pressure deuterium data critical to safety and reliability assurances of the nation's nuclear weapons.

Simplicity Poses Difficulties

Scientists have been attempting to metallize hydrogen for some time. The desire to do so must have materialized as soon as Eugene Wigner (later a Nobel laureate for work in quantum mechanics) theorized in 1935 that under extreme pressure, hydrogen turns into a metal. Wigner's theory concerns the high-energy-density physics of hydrogen, an area of knowledge fundamental to solving problems in astrophysics, planetary physics, nuclear explosions, and inertial fusion. However, experimental tools to test theory were not available for some 30 years. Then, in 1994, Lawrence Livermore researchers saw the first evidence of metallization during shock compression experiments with a light-gas gun (*S&TR*, September 1996, pp. 12–18). In the meantime, theorists developed models of hydrogen at extreme pressure, density, and temperature, but the models were fraught with uncertainty and disagreement.

They still are. That is because hydrogen, with its one electron and one proton, is simple only in its atomic structure. At high pressures, it is among the most difficult elements to understand. At the extreme densities of very high pressure, its various particles—atoms, molecules, ions, electrons, even strings of molecules—are free to interact strongly and nonlinearly. Hydrogen bypasses the screening mechanisms in more complexly structured elements that work to regulate particle interactions and thereby make an element's behavior easier to predict. The basic problem for theorists: What mixture of particles should constitute the hydrogen model?

Different proposed particle mixtures and interparticle forces have led to different results from hydrogen metallization models. Therefore, scientists have yet to agree on a hypothesis of how highly pressurized hydrogen transforms from a diatomic insulator into a monatomic conducting metal. A major point of contention among theorists concerns the specific mechanism causing metallization: Does it happen when hydrogen molecules separate (the theory of dissociation)? Or when they ionize? And at what pressure and temperature?

Density and temperature effects on molecular separation and ionization must be considered and evaluated for their impact on hydrogen's equation of state. (An EOS is a mathematical representation of a material's physical state as defined by its pressure, density, and either temperature or energy. It is a necessary constituent of all calculations involving material properties.) Scientists also disagree on whether metallization occurs gradually or abruptly. Models have simulated the transformation both ways. In fact, the abrupt phase transition, a controversial theory postulated in 1989 by researchers Didier Saumon of Vanderbilt University and Gilles Chabrier from the Ecole Normal Superieure in Lyon, France, intensified the pace of research into the metallization phenomenon.

Scientists are eager to resolve this theoretical challenge so they can modify and refine the fundamentally important high-energy-density EOS for hydrogen. They realize the EOS is flawed; to improve it is to improve a necessary tool for answering important basic questions about high-energy-density matter.

Says Livermore physicist Robert Cauble in describing the goal he and his colleagues are seeking, "We're trying to fill in the box of hydrogen EOS theory. Right now, we know that the theory works in a couple of corners—we know something about plasma, condensed matter, metal, liquid metal, and insulators. If we could join those pieces together, maybe we could stretch the theory toward the other corners and produce one overriding hydrogen theory that spans all densities, temperatures, and pressures."

Experimentation to Guide Theory

Clearly, experimentation is necessary for clarifying hydrogen metallization theory. Experimentation was not possible until the 1970s, when the first tools for creating the requisite experimental conditions finally became available. At Livermore, scientists began using explosively driven systems to compress magnetic fields and, in turn, small hydrogen samples to megabar pressures. They performed hydrostatic experiments in which pistons were pressed on liquid samples inside a pressure vessel. They also used diamond anvil cells to squeeze liquid hydrogen samples. Almost 60 years after Wigner's theory, Lawrence Livermore scientists shocked deuterium, an isotope of hydrogen,* with a light-gas gun and saw evidence of metallization for the first time. The gas-gun data revealed the precise pressure at which metallization occurs at high temperature. They also demonstrated that, at high temperatures (about 4,000 kelvin), metallization occurred at pressures significantly lower than had been theorized—at 0.2 megabar instead of 3 megabars. (1 megabar is the pressure of 1 million atmospheres, 15 million pounds per square inch, or 100 pascals.)

The gas-gun data brought theory into a new realm of discovery and inspired other researchers at Livermore to extend experimentation to higher pressure regimes that are possible on the Nova laser. The laser could be used to shock liquid deuterium to a wide range of pressures above the metallic transition.

*Results apply to deuterium, hydrogen, and tritium; the experiment used deuterium for convenience.

The optical properties of the shocked state could be measured to verify that the metal–insulator boundary had been spanned and thermodynamic properties could be measured to determine the EOS.

However, the same techniques that are used in gas-gun shock experiments cannot be simply carried over to lasers. The spatial scale is about 50 times smaller, and the time scale is about 1,000 times shorter. Attempts to produce laser-driven shocks capable of yielding accurate high-pressure EOS data had been made since the mid-1970s but yielded no useful data. Unlike gas-gun shocks produced by a fast-moving but cold projectile, laser irradiation of matter produces a very hot plasma that can interfere with measurements. Before performing the hydrogen EOS experiments, the Livermore team had to overcome the challenges inherent in the technique. They did so using newly developed diagnostics and target designs.

The first set of laser shock experiments, reported in early 1997, yielded startling results.[1] When shocked to 1 megabar, the deuterium compressed to a much-higher-than-expected density. This fact raised new questions even as the viability of laser shock experiments was demonstrated, and the experimenters could not rest without attempting another round of experimentation. And so it was that a group of laser physicists found themselves working frantically to design or modify diagnostic equipment, rush fabrication, and get it all installed into the Nova chamber before the two-beam target area was dismantled. Over a long weekend, they prepared for this second round of laser shots, setting up and checking diagnostic and cryogenic target components, verifying shielding and alignment, and inspecting for leaks. They tested everything; they called in several shifts of technicians to work around the clock; then they prepared themselves and their families for the series of 16-hour days.

Tools for Shock Experiments

Although Livermore's light-gas-gun experiments marked the first time the shock compression method was used to metallize hydrogen, shock compression is common in high-energy-density physics experiments. Large amounts of energy are added suddenly to a material system, creating intense sound or pressure waves that become shock waves. Shock waves compress a material to greater pressure, changing it to a new state at higher density, temperature, and pressure.

For the laser experiments, the target of the shock waves consisted of liquid deuterium loaded inside a cylinder 0.45 millimeter tall and 1.5 millimeters in diameter that had been machined into a copper block (Figure 1). One end of the cell was capped with a metal (aluminum or beryllium) disk, or pusher, that absorbed the laser energy and transmitted the shock wave into the deuterium. At the opposite end of the cell, a 0.5-millimeter-thick sapphire window allowed optical data to be taken. On both sides of the cell, thin windows of beryllium foil covered holes that were used for transverse x-ray radiography.

The metal shock pusher was coated with a polystyrene layer that cushioned it from direct laser ablation and prevented overheating. Because the laser light would shine directly through the cold polystyrene, an extremely thin (10-nanometer-thick) aluminum film was added. (After the polystyrene heated up, it would become opaque to the laser.)

Two quantities were measured by x-ray radiography during the shock compression experiments. One was the speed of the shock in the deuterium. The other was the speed to which the shocked deuterium was accelerated; this is called the particle speed. The two

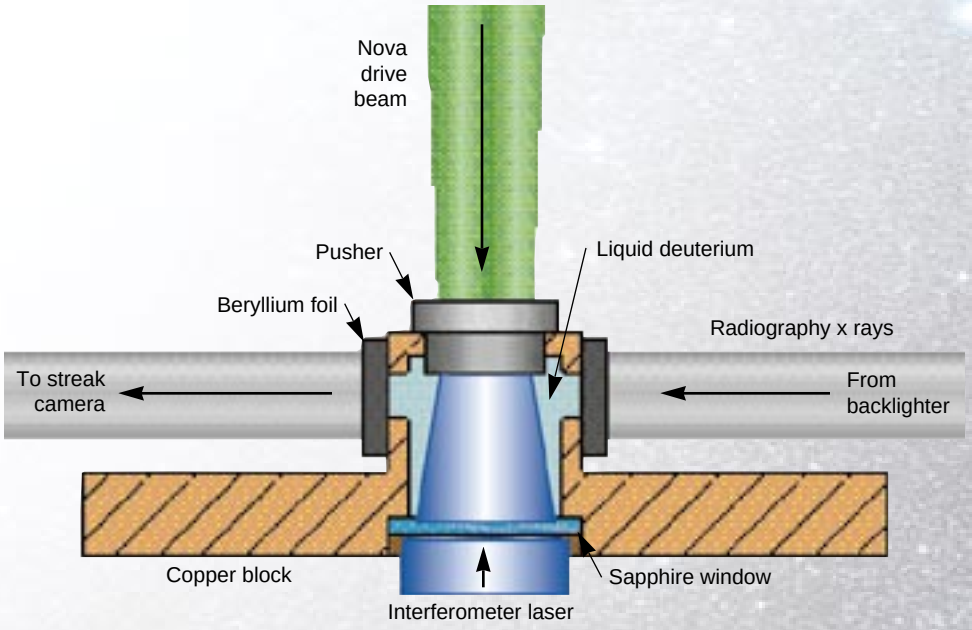


Figure 1. Schematic of the Nova laser shocking a target cell filled with liquid deuterium and machined into a copper block. One end of the cell is capped by an aluminum pusher, the other by a sapphire window used for rearview diagnostics. X-ray transmitting windows made of beryllium foil are located on each side of the cell.

quantities are used in so-called Hugoniot relations (calculations based on physical conservation laws) to determine the resulting compression and pressure of the shocked deuterium.

If a material with the same initial pressure, volume, and energy is subjected to a series of compression experiments of varying shock strengths, different pairs of initial and new compression states can be determined and plotted. The plots are the material's Hugoniot, a curve that relates the velocity of a single shock wave to the pressure, density, and total heat of the material before and after the shock wave passes. The Hugoniot is a relatively simple but well-defined curve that is unique for each material and as such is an invaluable tool for analyzing a material's EOS.

It Took Three Laser Beams

The experiments were conducted with three simultaneous laser beams: two from Nova (Figure 2) and the third from a tabletop laser. One Nova beam was used for shocking the deuterium.

Figure 2. Livermore experimenters check the setup for laser beams that will drive a shock in a tiny target cell so that transverse radiography can be performed to obtain shock-wave and reflectivity measurements.

The laser shot blasted the target's polystyrene layer, which heated up rapidly to drive a shock wave into the pusher and compress the deuterium. Aimed at the target cell, the laser's high energies produced a long and steady shock wave. The beam was smoothed by a phase plate to ensure a spatially planar and uniform shock front, critical for accurate measurements. If the shock had been delivered as a small, nonuniform laser spot, experimental data would have been difficult or impossible to interpret, and "edge effects" would interfere with the results as well.

The second Nova laser beam was used to create an x-ray source for transverse radiography by irradiating a nearby iron foil. X rays from the iron plasma illuminated the target cell from the side. The shocked deuterium absorbed and refracted the x-ray light differently because it had been changed by the propagating shock wave. The x rays transmitted through the cell were collected by a Kirkpatrick–Baez microscope, which improved data resolution, and were then focused onto a streak camera. In this way, the experimenters tracked the propagation of the shock front to find the shock speed. The pusher–deuterium interface, which moved at the particle speed, was tracked to determine that speed. Combining these speeds produced a single Hugoniot data point.

An example of a streaked radiograph of shock-compressed deuterium is shown in Figure 3. Because the pusher is opaque and the liquid deuterium is transparent, the interface between them is the boundary between the light and dark regions. When the laser-driven shock crossed the interface at 2 nanoseconds, the pusher surface accelerated to a steady speed, i.e., the particle speed. As the shock wave headed into the deuterium, a shock front (visible as a dark line because the backlight x rays

refract at density differences) moved ahead of the interface. The shock and particle speeds were determined from the film. The shock propagated steadily until a second, stronger shock, caused by shock reverberation in the pusher, entered the deuterium at 6 nanoseconds.

The third laser beam was used for optical interferometric measurements. In the earlier set of laser-shock experiments, this third beam was configured as a Michelson interferometer to monitor how much the target cell heated up before the arrival of the shock wave. This "preheat" had to be accounted for, or calculations of the shocked material's initial density would be inaccurate. The experiments would determine the compression (the ratio of shocked to unshocked deuterium densities), so knowledge of the initial, unshocked density was extremely important.

The Michelson interferometer beam was directed through the sapphire window at the bottom of the target cell. Its function was to monitor the movement of the pusher surface, indicative of expansion from radiative heating. The interferometer imaged this movement by splitting its beam into two arms: a reference arm and a sample arm that bounced off the pusher surface. When the two arms were recombined, their phase differences resulted in light fringes (bands caused by diffraction) that revealed, through measurements as small as a few tens of nanometers, what motion was detected in the pusher surface. The incorporation of a polystyrene coat on top of the pusher kept its bottom surface temperature below the detection limit of 400 kelvin.

The Michelson interferometer measurements had one additional use. Its reference beam verified the planarity and uniformity of the arriving shock wave. Experimenters saw that the shock front was uniform and planar to within 2.5 micrometers over a lateral region of 350 micrometers.

With concerns over preheat and shock-wave quality out of the way, it was unnecessary to repeat the Michelson interferometer measurements for the second set of laser experiments. Instead, the third beam was set up for velocity interferometry to determine the velocity and, importantly, reflectivity of the shock front. Because of its relationship to electrical conductivity, the reflectivity measurement established the occurrence of metallization.

Then There Were Measurements

The velocity interferometer used in these experiments was a particularly accurate instrument for measuring motion—in this case, the speed of the reflecting surface of a moving shock front. Unlike a conventional interferometer that first splits a laser beam into two arms, this interferometer shot the whole beam onto the experimental sample and split the beam after it exited the sample. Then one beam was passed through a piece of glass, called an etalon, which slowed it down. Because of this induced time delay in one arm, recombining the beams generated light fringes. The fringes changed when the shock front moved, doing so in proportion to shock speed.

Figure 4 shows a streak velocity interferogram. For times before $t = 0$, the fringes are reflections of the stationary pusher surface. For $t > 0$, the reflection is from the shock front in the deuterium. The amount of the fringe shift at $t = 0$ is proportional to the speed of the shock front.

The difference in reflected light intensity originating from the motionless pusher surface and that from the shock front moving in the deuterium reveals the reflectivity of the shock. The pressure at which a change in reflectivity occurs can be determined because particle and shock speeds can be measured. The measured reflectivity at low shock pressure (0.2 megabar) is only a few percent. Above 0.55 megabar, however, the measured reflectivity is about 60 percent—characteristic of a poorly reflecting metal. This measurement proves that the deuterium changed from an insulating state to a conducting one. The data also show that the transition occurs simultaneously with the earlier observed high compression. These effects are linked: the high compression is a result of the transition.

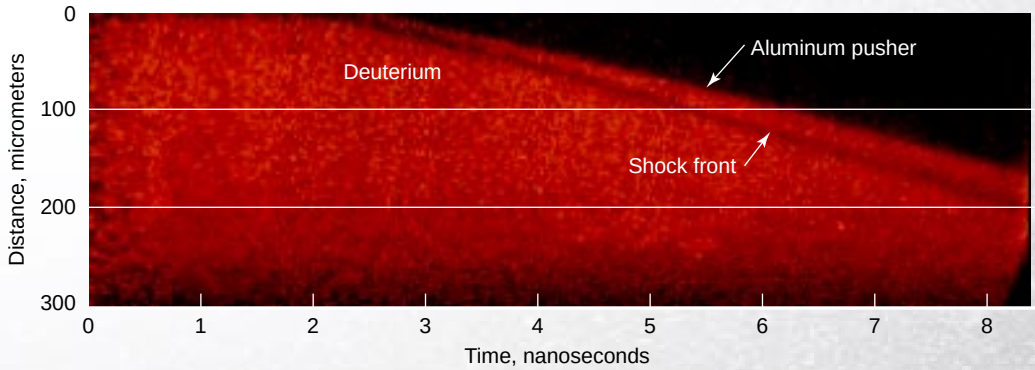


Figure 3. The image of the deuterium is moved across the film over time, producing a streak radiograph. In the figure, the pusher is above the deuterium, so the shock travels from top to bottom.

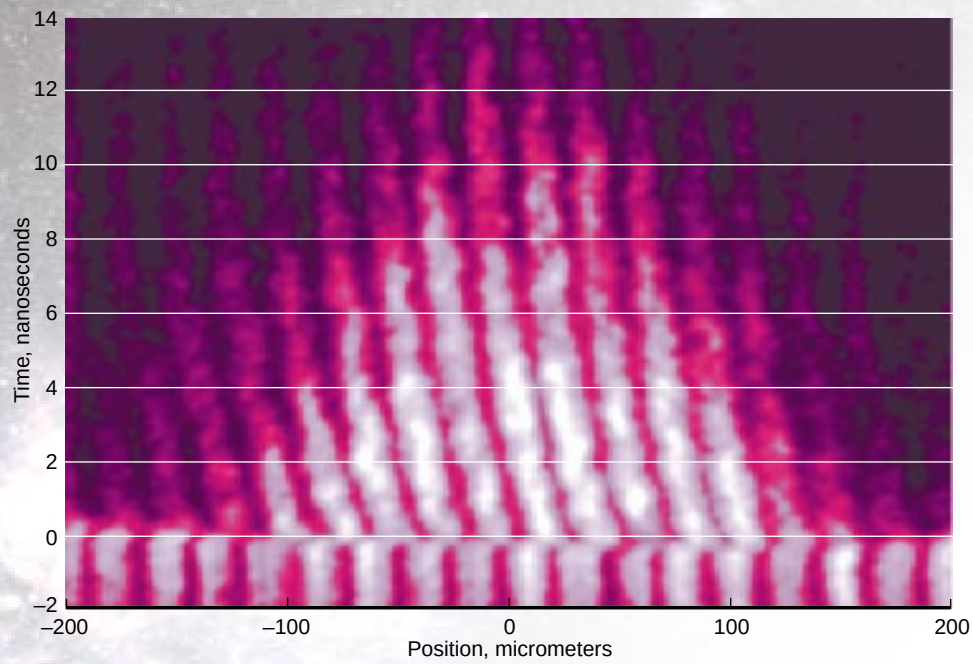


Figure 4. This velocity interferogram shows the deuterium in the Livermore Nova experiment had changed to a conducting state.

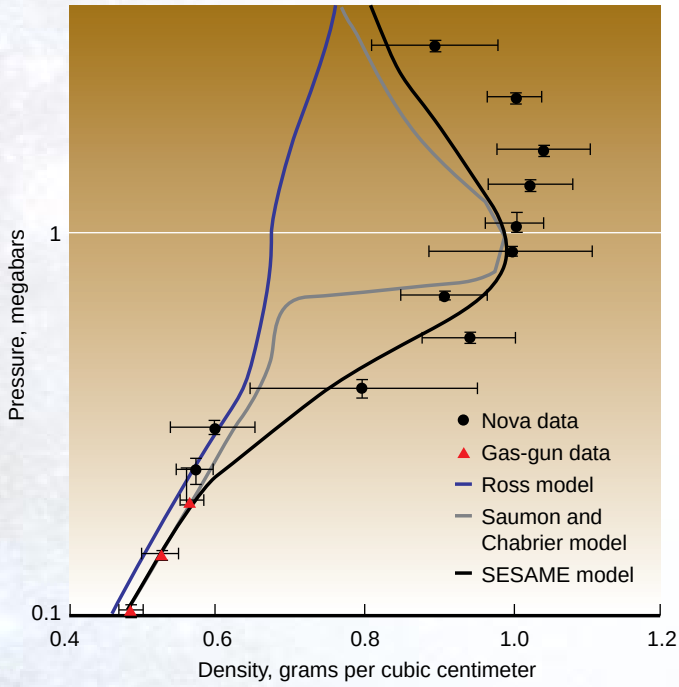


Figure 5. Livermore Nova data are significant because they show much higher compressibility than the SESAME EOS model, and they are similar to the gas-gun data and the Ross model of strong dissociation.

In addition to these measurements, the temperature of the shock was determined by recording the light emission of the shock front in several wavelength bands. An optical pyrometer viewed the shock through the sapphire window in the cell. Temperature is a fundamental component of the EOS, but it cannot be derived from the Hugoniot relations. It must be found separately. Because the form of the wavelength-dependent light intensity is a known function of temperature, fitting the emission data into that formula allowed the experimenters to find the value of temperature.

Implications for Hydrogen's EOS

The experimental team was tired but elated with their results. The data obtained from the latest round of effort would once again recharge their work on hydrogen theory and, furthermore, bring experimentation to another level. Their work had provided the first direct evidence on the Hugoniot to support the hypothesis that liquid deuterium transforms from a molecular fluid into a monatomic metallic fluid at lower pressures than postulated by earlier theoretical models.

Figure 5 shows the measured Hugoniot as pressure versus density. The figure compares Hugoniot curves for the laser data with a linear mixing model proposed by Livermore scientist Marvin Ross, an earlier model in the SESAME EOS library, the prediction of Saumon and Chabrier, and the Livermore light-gas-gun data. At the lowest compression, the laser data are in agreement with the gas-gun results, while at higher compressions, the data significantly deviate from the SESAME prediction. The data at 0.25 megabar are significant because they overlap the gas-gun data, providing confidence in current results. The current data show

an enhanced compressibility similar to that of the Ross linear mixing model in the region where strong molecular dissociation is predicted. Although the shocked density at 1 megabar is close to that of Saumon and Chabrier, the data do not show the abrupt transition predicted by their model. The conclusion is that molecular dissociation and ionization are significant factors in hydrogen isotopes compressed to megabar pressures. Reflectivity measurements, using the measured Hugoniot to find the pressure, are shown in Figure 6.

The current data provide an important benchmark for a revised EOS model of hydrogen and its isotopes in a regime relevant to high-energy-density physics applications. Additionally, the experiments demonstrate that laser-driven shock waves can effectively be used for EOS studies at pressures beyond those attainable by traditional techniques. The new hydrogen EOS will change the way planets such as Jupiter are modeled, especially the size of its metallic core. For fusion occurring on Earth, the higher compressibility of deuterium will make the goal of laboratory thermonuclear fusion easier to achieve than previously thought.

Prize-Winning Basic Science

The work in developing the techniques to perform laser-driven EOS experiments and in getting surprising data on an important material earned Robert Cauble, Peter Celliers, Gilbert Collins, and Luiz Da Silva—the principal members of the research team—the 1998 American Physical Society Award for Excellence in Plasma Physics Research. The "exquisite series of experiments" cited by the award were a fitting follow-up to the earlier Lawrence Livermore gas-gun shock compression experiments, which also pushed hydrogen EOS theory up another rung. The principal investigators for that work, William Nellis and Arthur Mitchell, received the 1997 American Physical Society Award for Shock Compression Science. It may be that Laboratory researchers, in furthering the fundamental science so important to Laboratory missions, are also setting themselves new standards for scientific execution.

— Gloria Wilt

Key Words: equation of state (EOS), gas gun, high-energy density, Hugoniot, metallized hydrogen, Nova laser.

Reference

1. L. B. Da Silva et al., *Physical Review Letters*, Vol. 78, No. 3 (January 1997), pp. 483–486.

For further information contact Robert C. Cauble (925) 422-4724 (cauble1@llnl.gov).

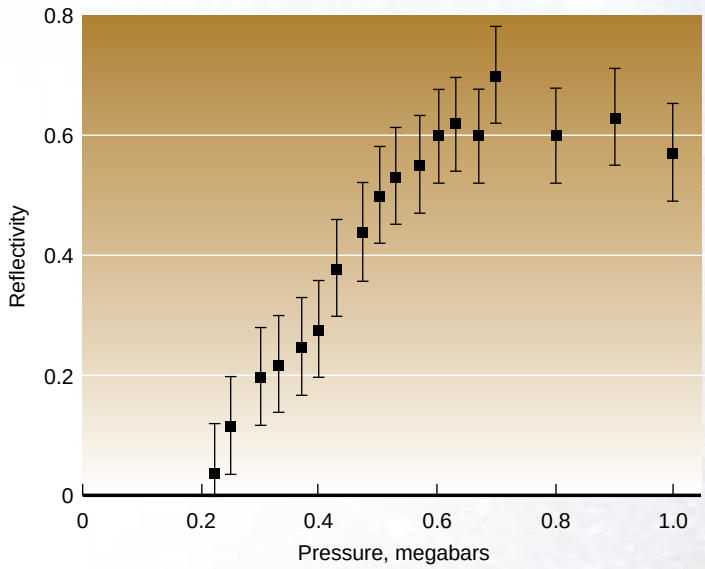


Figure 6. The steep curve between pressures of 0.4 and 0.6 megabar shows higher compressibility for deuterium than previously thought.

About the Scientist

ROBERT C. CAUBLE received his B.S. in physics in 1974 from the University of Arizona and his Ph.D. in nuclear engineering from the University of Michigan in 1980. In 1980, Cauble worked at the Naval Research Laboratory on theoretical predictions of the effects of high-density plasma on atomic transitions and particle transport. He came to Lawrence Livermore in 1985 to work on projects to produce atomic models for plasma simulations and to design and analyze experiments to use laboratory x-ray lasers as high-density-plasma probes and interferometers. More recently, he has worked on large-scale simulations and designs of experiments to elicit material properties, mainly equation-of-state data at extreme pressures using intense, laser-driven shocks.

Methane Hydrate:
A Surprising Compound

WHAT do you get when you combine water and swamp gas under low temperatures and high pressures? You get a frozen latticelike substance called methane hydrate, huge amounts of which underlie our oceans and polar permafrost. This crystalline combination of a natural gas and water (known technically as a clathrate) looks remarkably like ice but burns if it meets a lit match.

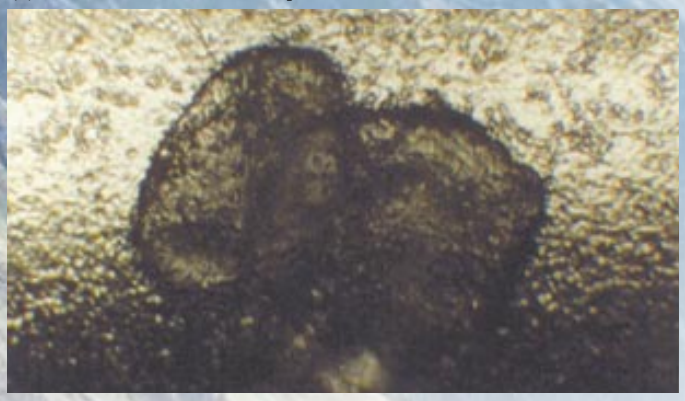
Methane hydrate was discovered only a few decades ago, and little research has been done on it until recently. By some estimates, the energy locked up in methane hydrate deposits is more than twice the global reserves of all conventional gas, oil, and coal deposits combined. But no one has yet figured out how to pull out the gas inexpensively, and no one knows how much is actually recoverable. Because methane is also a greenhouse gas, release of even a small percentage of total deposits could have a serious effect on Earth's atmosphere.

Research on methane hydrate has increased in the last few years, particularly in countries such as Japan that have few native energy resources. As scientists around the world learn more about this material, new concerns surface. For example, ocean-based oil-drilling operations sometimes encounter methane hydrate deposits. As a drill spins through the hydrate, the process can cause it to dissociate. The freed gas may explode, causing the drilling crew to lose control of the well. Another concern is that unstable hydrate layers could give way beneath oil platforms or, on a larger scale, even cause tsunamis.

Lawrence Livermore's William Durham, a geophysicist, began studying methane hydrate several years ago with Laura Stern and Stephen Kirby of the U.S. Geological Survey in Menlo Park, California. With initial funding from NASA, they looked at the ices on the frigid moons of Saturn and other planets in the outer reaches of our solar system. One of these ices is methane hydrate.

Their work on the physical properties of this plentiful but poorly understood material has put the team in the forefront of methane hydrate research in the U.S. While they continue to study icy moons, Laboratory Directed Research and Development funding allows them to focus on applications that their research might have closer to home. In the process, they have run across a few surprises.

(a) Pressure = 27.6 MPa; temperature = 275 K.



(b) Pressure = 4 MPa; temperature = 275 K.

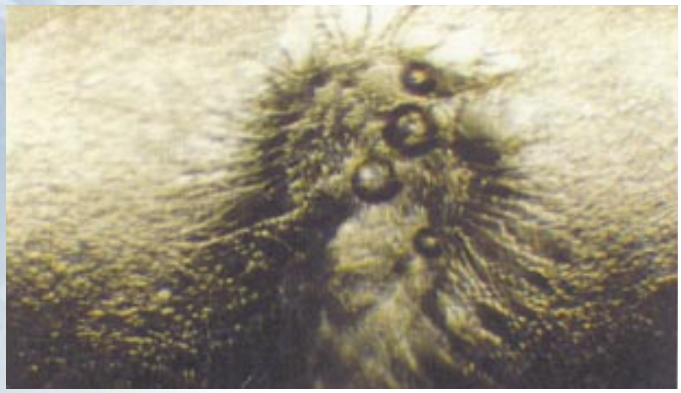


Figure 1. Partially reacted grains of methane hydrate that still contain cores of solid water ice and the same grains after the ice has begun to melt. In (a), the reaction proceeds rapidly as the hydrate mantle thickens and consumes the ice core. In (b), the rate of hydrate formation slows to almost zero. Melting of the superheated ice cores, apparently suppressed in (a) by rapid hydrate formation, is allowed to proceed. The grains become misshapen as liquid pools inside, causing distortion and partial collapse of the outer hydrate mantle within 10 minutes. Liquid water is radially expelled along fissures and crystallized as fine crystalline hydrate to surround the original grains.

Ice That Doesn't Melt

For their research, Durham, Stern, and Kirby needed good-quality samples of methane hydrate. But samples of the real thing are tough to acquire, requiring expensive drilling and elaborate schemes for core recovery and preservation. Previously developed methods for synthesizing the stuff in the laboratory generally resulted in an impure material still containing some water that had not reacted with the methane.

The Livermore–USGS team attempted an entirely new procedure. They mixed sieved granular water ice and cold, pressurized methane gas in a constant-volume reaction vessel and slowly heated it. Warming started at a temperature of 250 kelvin (K) (–10°F) with a pressure of about 25 megapascals (MPa).* The reaction between methane and ice started near the normal melting point of ice at this pressure (271 K, or 29°F) and continued until virtually all of the water ice had reacted with methane, forming methane hydrate.

The team studied the resulting material by x-ray diffraction and found pure methane hydrate with no more than trace amounts of water. This simple method produced precisely what they needed: low-porosity, cohesive samples with a uniformly fine grain size and random crystallographic grain orientation.

Says Durham, "In a way, we got lucky. We used the same technique we use for producing uniform water ice samples from 'seed' ice. We tried adding pressurized methane gas and heating it. And it worked."

It worked, but some unexpected things happened along the way. The ice did not liquefy as it should have when its melting temperature was reached and surpassed. In fact, methane hydrate was formed over a period of 7 or 8 hours, with the temperatures inside the reaction vessel reaching 290 K (50°F) before the last of the ice was consumed. Repeated experiments produced the same result: ice that did not melt (Figure 1).

A control experiment replaced the methane with neon, which does not form the cagelike latticework of gas and water molecules that is a gas hydrate. Under otherwise identical experimental conditions, the ice melted as it should. Other experiments replaced the methane with both gaseous and liquid carbon dioxide, which does form a hydrate. Here the superheating phenomenon reappeared, indicating that it is not unique to methane hydrate.

Durham and his team believe the superheating phenomenon is related to active hydrate formation. The reaction at the free ice surface somehow suppresses the formation of a runaway melt. Figure 1 shows that when the reaction ceases, melting happens immediately. The American Chemical Society was impressed enough with these rather bizarre results to give the team a cash prize and award in late 1997.

Another Surprise

Once the team had large, pure samples they could work with, they began studying the material's physical properties and the way it forms and dissociates. This is research at its most basic. But its applications are clear when one considers that dissociation of seabed methane hydrate deposits could cost the lives of workers on an oil drilling platform.

Methane hydrate's stability curve (Figure 2) has been established for some time. If conditions fall outside that curve, the material will dissociate into its components, methane and water. Durham, Stern, and Kirby looked at how the dissociation occurs under a variety of temperature and pressure conditions outside the curve.

After the samples were created, the pressure was reduced to 0.1 MPa, the pressure at sea level. They did this in two ways: by slow cooling and depressurization and by rapid depressurization at a range of temperatures.

The compound decomposed to ice and gas as expected in all experiments except those that involved rapid depressurization at temperatures from 240 to 270 K (Figure 3). In these experiments, the team found yet another surprise. Even after the pressure drop, the methane hydrate was "preserved" as a compound for as long as 25 hours before it decomposed.

This behavior may have implications for future exploitation of the material. Preserving the mixed hydrates may be possible at an easily accessible temperature, just a few degrees below ice's melting temperature.

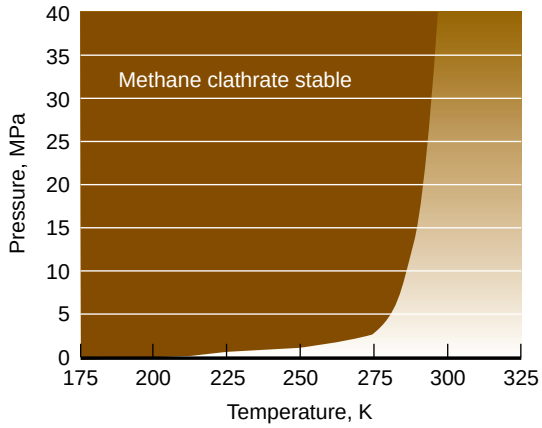


Figure 2. The stability curve shows that methane hydrate is stable at 0.1 MPa if temperatures are low enough and that it is stable far above the melting point of water ice if pressures are high enough.

* 0 K is absolute zero. At 0.1 MPa (1 atmosphere), water freezes at 273 K and boils at 373 K.

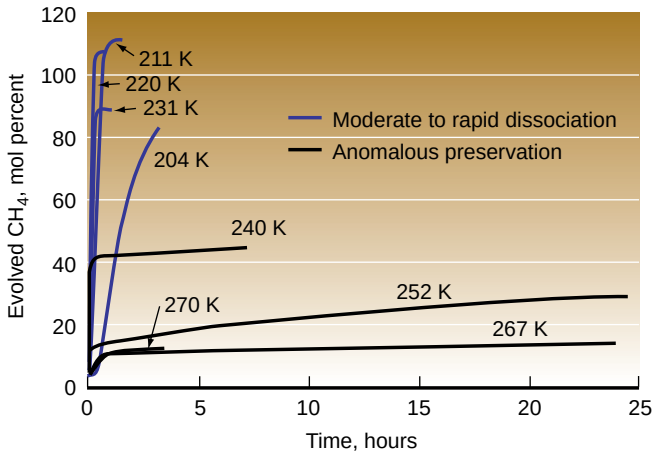


Figure 3. At lower temperatures (the blue lines), methane hydrate dissociates rapidly after rapid depressurization. At warmer temperatures (the red lines), dissociation is complete only after periods as long as 25 hours.

Figure 4. Used to compare the strengths of water ice and methane hydrate, a sample containing both was subjected to axial stress from a piston inside a cryogenic container about 25 millimeters in diameter. Inside this vessel, the weaker water ice (toward left of photo) deforms, causing a bulge, while the stronger methane hydrate under the same stress does not bulge.

In another series of experiments, the team is looking at the strength of gas hydrate samples in various temperature and pressure scenarios. Results of these experiments may indicate the possible effects that stresses from gravity, tectonic activity, or human disturbance might have on gas hydrate deposits.

Thus far, the team has found that water ice and methane hydrate have about the same strength at very low temperatures of 180 K and below. But the hydrate is much stronger than ice at temperatures of 240 K and above. The most recent data indicate that methane hydrate is several times stronger than ice (Figure 4). Although methane hydrate is not as strong as rock, the data may be good news for the stability of the deposits.

More Work Ahead

Plenty of work remains to be done. The team plans to measure the molecular diffusion of gases through methane hydrate and to study special compounds that might suppress the formation of hydrates in cold pipelines. They also will do experiments to measure methane hydrate's thermal properties. Says Durham, "We already know that it is a very poor conductor of heat. If you hold a piece of it in your hand, it doesn't feel like ice at all. It almost feels like styrofoam."

A new heat exchanger installed in December at Livermore's ice physics laboratory allows Durham to heat samples from 180 to 260 K in about an hour, a process that used to take 24 hours. Durham notes, "Now we can do experiments much more quickly and thus can run a lot more experiments. Methane hydrate is a material with plenty of surprises, so there is no telling what we might discover next."

—Katie Walter

Key Words: clathrate, energy sources, gas hydrates, methane hydrate, global climate, superheating.

For further information contact
William B. Durham (925) 422-7046 (durham1@llnl.gov).

LATIS Modeling Laser Effects on Tissue

LASER beams—used for swashbuckling effect in the movie *Star Wars* nearly a quarter century ago—are now proving an effective weapon in the war against medical conditions such as stroke and arthritis, as well as in surgical procedures. A critical ally in this battle is LATIS (an acronym for LAser-TISsue), a computer code developed at Lawrence Livermore. It is a two-dimensional, time-dependent code that simulates the interaction of laser light with living tissue. LATIS is based on experience gained during 25 years of modeling high-intensity laser–matter interactions for inertial confinement fusion.

Medical researchers from the Department of Energy's national laboratories, as well as from universities and industry, have been turning to LATIS and its new, three-dimensional counterpart, LATIS3D, for help in the design and use of new laser medical tools. LATIS was originally developed by Livermore physicists Richard London, George Zimmerman, David Bailey, and Mike Glinsky (now at Shell Co.). The codes are particularly useful in analyzing novel laser systems used for photothermal, photochemical, and photomechanical applications.

For these medical applications, LATIS explores laser-light propagation, thermal heat transport, material changes such as thermal coagulation and photochemistry, and hydrodynamic motion. "LATIS was originally funded as part of a Laboratory Directed Research and Development project looking at ways to diagnose and treat stroke," London explains. "In developing the code, we leveraged experience, expertise, and technologies already available at the Laboratory in areas such as computational modeling, laser technologies, and precision engineering of laser–matter interaction and radiation hydrodynamics. The results are having an effect on healthcare technologies and economics by making it easier—and less expensive—to develop some of these laser tools."

In the past three years, LATIS codes have simulated a laser system that will break up blood clots in stroke patients and experiments using a tissue "welding" system based on laser light. Current work includes a new technique for easing arthritis.

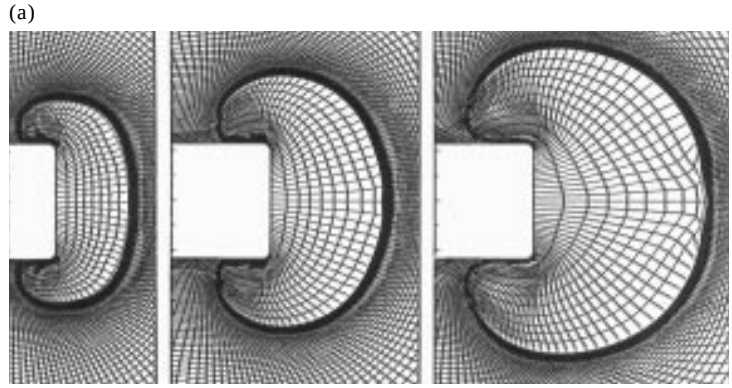
Attacking Strokes at the Source

Strokes, like heart attacks, usually result from decreased blood flow interrupting the supply of oxygen and nutrients to tissue. Most frequently, the flow is decreased because of a blockage in blood vessels.

In 1995, Livermore's stroke-initiative team began developing optical therapies for breaking up clots in the blood vessels of the brain as well as the laser–tissue interaction modeling that was the beginning of LATIS (for more information see *S&TR*, June 1997, pp. 14–21). The clot-busting system delivers low-energy laser pulses through a fiber-optic microcatheter positioned close to the cerebral clot. The optical light is converted to acoustic stress waves that break up the clot and restore blood flow in the cerebral arteries.

"With LATIS, we simulated the interaction of the laser beam with fluids (blood, saline solution), the blood clot, and tissue near the end of the fiber. We then compared the results with experiments," London said (Figure 1). "We modeled the generation of acoustic waves near the interaction and the

(a)



(b)

Figure 1. Sophisticated two-dimensional computer simulations made with LATIS by Peter Amendt predicted experimental behavior for a device that breaks up stroke-inducing blood clots using laser energy converted into acoustic energy. (a) Two-dimensional simulation of bubble dynamics, showing a "special zoning scheme" that is also potentially useful for laser fusion modeling. (b) Close-up of a bubble generated in experiments.

acoustic energy on the blood clot. The results provided direction to researchers on the optimal parameters for laser wavelength, pulse length, and optical fiber diameter. The modeling also helped reduce the number of experiments needed."

LATIS incorporated a number of variables—the size and composition of the clot, strength of the blood-vessel tissue, and buildup and transport of heat during laser clot-busting. The code then numerically simulated the hydrodynamics of the laser-created energy and predicted the energy needed to break up the clots without damaging other tissue.

This clot-busting instrument, now being advanced by Endovasix Inc., is entering clinical tests and should be commercially available within a couple of years.

Modeling Temperatures for Tissue Welding

In another effort spearheaded by Livermore's Medical Photonics Laboratory, researchers, led by Duncan Maitland, designed a system that uses laser light to join tissue, much like sutures. The laser energy activates tissue bonds between surgical surfaces, fusing them together. If there's too much heat, however, the tissue is damaged, and poor healing results. If there's not enough heat, the bonds don't form.

In this case, LATIS helped researchers analyze data from tissue experiments and then design the system. LATIS modeled the heating effects and the heat transport of the laser energy absorbed by the tissue. The researchers made interesting discoveries in this modeling effort. For instance, for a pulse of many seconds to a few minutes, they found that the evaporation of water from the surface of the tissue cools the tissues, much like sweating. Before this, no one had determined quantitatively how important cooling was to the process. They also simulated the temperature profile of the underlying tissue, something that wasn't possible to measure experimentally. The findings had a significant impact on the system's design.

LATIS modeled the in-depth temperature profile for two temperature-control techniques: one, by dripping water on the tissue surface, the other by using a feedback system incorporating an infrared thermometer, developed at the Laboratory, that

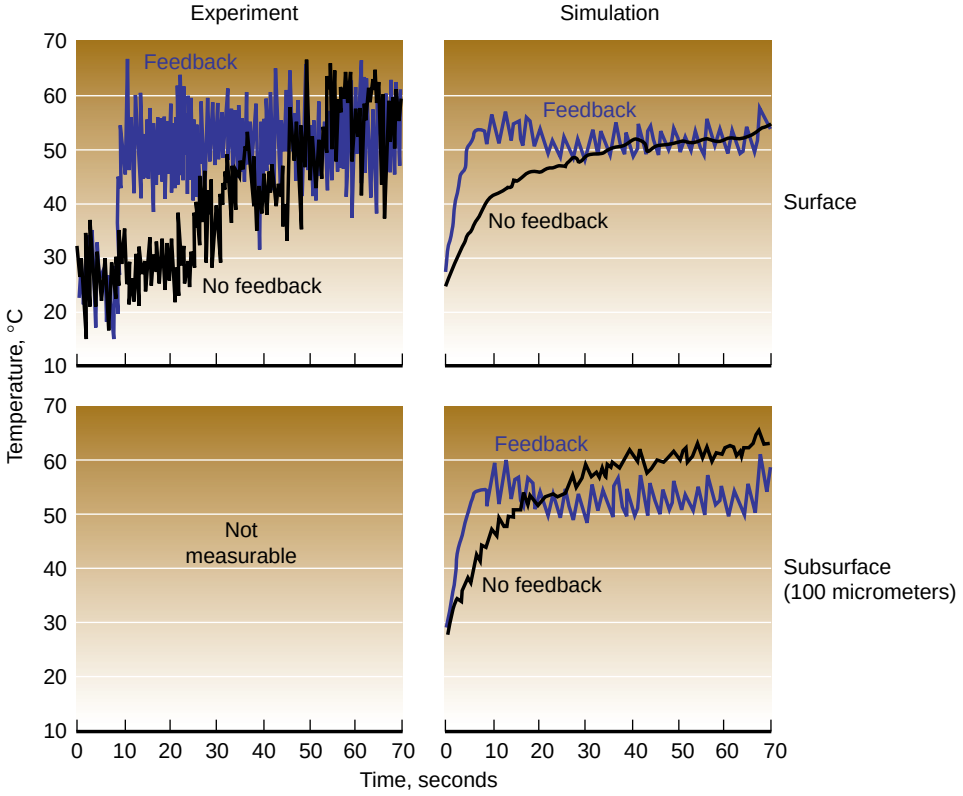


Figure 2. Numerical simulations performed with LATIS by David Eder suggested that the improved results of the tissue-welding technique are related to better control of the temperatures below the surface of the tissue. Such control was provided by a temperature sensor/feedback system developed at Lawrence Livermore's Medical Photonics Laboratory.

controls the amount of laser energy delivered to the tissue surface (see *S&TR*, October 1998, pp. 14–15). Both methods cool the surface of the tissue, but the question was which method better controls the temperature below the surface.

"The modeling predicted that temperatures below the surface would stay more uniform with the feedback system," said London (Figure 2). "The experimental results showed that the welds using the feedback technique were superior in several ways. The only way the techniques differed was in their in-depth temperature profiles."

The resulting tissue-welding system is showing particular promise in heart surgery on newborns, and the Laboratory is collaborating with the University of California's San Francisco Medical Center and Conversion Energy Enterprises on experiments to eventually bring this system to market.

Easing Arthritis

Another medical application for advances of the LATIS code is photodynamic therapy, using light-activated drugs to treat medical conditions including cancer and arthritis.

As part of the Center for Excellence for Laser Applications in Medicine, formed in 1998 by the Laboratory and the University of California at Davis's Medical Center, researchers are developing a treatment for arthritis based on photodynamic techniques. This project correlates with a Laboratory Directed Research and Development project to develop a successor to LATIS—a three-dimensional interactive code called LATIS3D. It is being used to make an accurate calculation of the distribution of laser light in a joint.

"We set up a model of the geometry of a knee joint, which is a very complicated three-dimensional (3D) structure," said London. "Developing a numerical description of the joint required making a three-dimensional numerical mesh, or grid. We are using magnetic-resonance images—MRIs—of knee joints as a basis for our 3D model. We will then define the properties of each tissue in each mesh."

With the model in place, the team uses Monte Carlo probability methods to determine light distribution in the various tissues. "We calculate where the light goes. Combining that with estimates from our collaborators of where the drug is concentrated, we can then calculate how the tissue is affected," said London.

These modeling efforts will help in designing the photodynamic therapy instrument, determining the laser energies needed, and positioning the light source.

For this application, LATIS3D could also be used to develop physician treatment plans. A physician can transfer a patient's MRI data into the model and come up with a plan that includes where to place the fiber, how long to make the exposures, how much energy is needed, and so on.

Powerful Modeling Tool Meets the Medical Future

Developing new instruments and procedures for use in laser medicine typically involves extensive experimental and clinical studies. As London noted, computational modeling codes such as LATIS and LATIS3D can help medical researchers define experimental parameters more narrowly and gain deeper understanding of specific laser medical processes. LATIS will also have a future role in designing patient-specific treatment plans and in training physicians.

"In these ways," said London, "modeling can lead to more rapid development of new medical systems, to the genesis of new ideas, and to more individually tailored treatment plans. All, of course, to the ultimate benefit of patients."

—Ann Parker

Key Words: arthritis, laser surgery, laser–tissue interaction modeling, LATIS code, LATIS3D code, stroke, tissue welding.

For further information contact Rich London (925) 423-2021 (london2@llnl.gov), or see the Livermore Medical Technology Program's Web site at http://lasers.llnl.gov/lasers/mtp/modeling.html.

Patents and Awards

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

Patents

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Paul G. Carey Patrick M. Smith Thomas W. Sigmon Randy C. Aceves	**Method for Formation of Thin Film Transistors on Plastic Substrates** U.S. Patent 5,817,550 October 6, 1998	A process for forming thin-film transistors (TFTs) on plastic substrates to replace standard techniques, using sufficiently lower processing temperatures so that inexpensive plastic substrates may be used in place of standard glass, quartz, and silicon wafer-based substrates. The process relies on techniques for depositing semiconductors, dielectrics, and metals at low temperatures; crystallizing and doping semiconductor layers in the TFT with a pulsed energy source; and creating top-gate self-aligned as well as back-gate TFT structures. The process has use in large-area, low-cost electronics, such as flat-panel displays and portable electronics.
Abraham P. Lee Peter A. Krulevitch M. Allen Northrup Jimmy C. Trevino	**Microvalve** U.S. Patent 5,819,749 October 13, 1998	Micromachined thin-film cantilever actuators to individually control the deflection of the cantilevers, valve members, and rudders for steering same through blood vessels or positioning same within a blood vessel. Actuators include tactile sensor arrays mounted on a catheter or guide wire tip for navigation and tissue identification, shape-memory alloy film-based catheter/guide wire steering mechanisms, and rudder-based steering devices that allow the selective actuation of rudders that use the flowing blood itself to help direct the catheter through the blood vessel.
Michael J. Moran	**Transverse-Structure Electrostatic Charged Particle Beam Lens** U.S. Patent 5,821,543 October 13, 1998	Electrostatic particle-beam lenses using a concentric coplanar array of independently biased rings. Traditional electrostatic lenses often consist of axial series of biased rings, apertures, or tubes. The science of lens design has devoted much attention to finding axial arrangements that compensate for the substantial optical aberrations of the individual elements. Thus, a multi-element, charged-particle lens can have optical behavior that is far superior to that of the individual elements. This design is convenient for numerical and theoretical analysis.
Michael Glinsky Richard London George Zimmerman Steven Jacques	**Intraluminal Tissue Welding for Anastomosis** U.S. Patent 5,827,265 October 27, 1998	A method and device for performing intraluminal tissue welding for anastomosis of a hollow organ. A retractable catheter assembly is delivered through the hollow organ and consists of a catheter connected to an optical fiber, an inflatable balloon, and a biocompatible patch mounted on the balloon. The disconnected ends of the hollow organ are brought together on the catheter assembly, and, upon inflation of the balloon, the free ends are held together on the balloon to form a continuous channel while the patch is deployed against the inner wall of the hollow organ. The ends are joined, or "welded," using laser radiation transmitted through the optical fiber to the patch. The laser radiation delivered has a pulse profile to minimize tissue damage.

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Bill Neuman John Honig Lloyd Hackel C. Brent Dane Shamasundar Dixit	**Phase Plate Technology for Laser Marking of Magnetic Discs** U.S. Patent 5,828,491 October 27, 1998	A design for a phase plate that enables distribution of spots in arbitrarily shaped patterns with very high uniformity and a continuously or near-continuously varying phase pattern. A continuous phase pattern eliminates large phase jumps typically expected in a grating that provides arbitrary shapes. The design can be easily adapted to minimize manufacturing errors and maintain high efficiencies. This grating is significantly more efficient than previously described Dammann gratings and is easier to manufacture and replicate than a multilevel phase grating.
Barry L. Freitas	**High Density, Optically Corrected, Micro-Channel Cooled, V-Groove Monolithic Laser Diode Array** U.S. Patent 5,828,683 October 27, 1998	An optically corrected, microchannel-cooled, high-density laser diode array able to achieve stacking pitches to 33 bars/cm by mounting laser diodes into V-shaped grooves. The design delivers over 4 kW/cm^2 of directional pulsed laser power. The laser is usable in solid-state systems that require efficient, directional, narrow-bandwidth, high-optical-power-density pump sources.
Thomas E. McEwan	**Micropower RF Material Proximity Sensor** U.S. Patent 5,832,772 November 10, 1998	A level or proximity detector for materials capable of sensing through plastic container walls or encapsulating materials of the sensor. An antenna has a characteristic impedance that depends on the materials in proximity to the antenna. An RF oscillator, which includes the antenna and is based on a single transistor in a Colpitt's configuration, produces an oscillating signal. A detector coupled to the oscillator signals changes in the oscillating signal caused by changes in the materials close to the antenna. The antenna detects the fill level within the container as the material reaches the level of the antenna.
Vincent Malba	**Process for 3D Chip Stacking** U.S. Patent 5,834,162 November 10, 1998	A process for fabricating electrical interconnects that extend from a top surface of an integrated circuit chip to a sidewall of the chip using laser pantography to pattern three-dimensional interconnects of an L-connect or L-shaped type. The process includes holding individual chips for batch processing, depositing a dielectric passivation layer on the top and sidewalls of the chips, opening vias in the dielectric, forming the interconnects by laser pantography, and removing the chips from the holding means. The process enables low-cost manufacturing of chips and increased performance, reduced size, and increased function per unit volume.
John P. Warhus Jeffrey E. Mast	**Ultra Wideband Ground Penetrating Radar Imaging of Heterogeneous Solids** U.S. Patent 5,835,054 November 10, 1998	A noninvasive imaging system for analyzing engineered structures comprising pairs of ultrawideband radar transmitters and receivers in a linear array that are connected to a timing mechanism that allows a radar echo sample to be taken at transmission. Transmitters and receivers are coupled to a position-determining system for each group of samples measured. Return signal amplitudes represent relative reflectivity of objects within the volume, and the delay in receiving each signal echo represents the depth of the object in the volume and the propagation speeds of intervening material layers.

(continued on page 28)

(continued from page 27)

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
Eric L. Altschuler Farid U. Dowla	**Encephalolexianalyzer** U.S. Patent 5,840,040 November 24, 1998	The encephalolexianalyzer uses digital signal processing techniques on electroencephalograph (EEG) brain waves to determine whether someone is thinking about moving, actually moving, or at rest and not thinking of moving. The mu waves measured by a pair of electrodes are signal processed to determine the power spectrum. At rest, the peak value of the power spectrum in the 8- to 13-Hz range is high; during movement or thought of movement, the peak value is low. This measured change in signal power spectrum is used to produce a control signal. The encephalolexianalyzer, used to communicate either directly or via a cursor, will benefit people with disabilities and be invaluable for studying the brain.
Stephan P. Velsko	**Frequency Agile Optical Parametric Oscillator** U.S. Patent 5,841,570 November 24, 1998	The frequency-agile optical parametric oscillator converts a fixed wavelength pump laser beam to arbitrary wavelengths within a specified range with pulse agility, at a rate limited only by the repetition rate of the pump laser. Uses of this invention include laser radar (LIDAR) active remote sensing of effluents/pollutants, environmental monitoring, antisensor lasers, and spectroscopy.

Awards

Recognized for bringing "unusual distinction to the engineering profession," **James Candy** and **Robert Deri** have been elected as **Fellows of the Institute of Electrical and Electronics Engineers.** Candy, director of the Laboratory's Center for Advanced Signal and Image Sciences, was cited for "contributions to model-based ocean acoustical processing," used for detecting and localizing submarines. IEEE cited Deri's "contributions to photonic devices and integrations on compound semiconductors" for developing small microchips that can be used to transmit and receive light in fiber-optic systems. Deri, associate division leader in electronic engineering technology, was cowinner of two R&D 100 awards.

Laboratory physicists **Neil Holmes** and **Dmitri Ryutov** were recently elected **Fellows of the American Physical Society**. Holmes was cited for "innovative experimental studies to elucidate and understand the response of condensed matter to dynamic high pressure." Holmes's career at the Laboratory has included research for laser-driven shockwaves and light-gas guns, leader of the Physics Directorate's equation-of-state program and dynamic experiments, and associate division leader. Areas of Ryutov's research include plasma and space physics, advanced dynamics, and astrophysics. He came to Livermore in 1994 from the Budker Institute of Nuclear Physics in Novosibirsk, Russia. His citation reads: "For contributions to the diverse areas of fusion plasma and astrophysical research, in a career characterized by exceptional analytical skills and innovative ideas."

The **LDRD Working Group**, led by deputy director of the Laboratory Directed Research and Development Program **Rokaya Al-Ayat**, received the DOE/Albuquerque Operations top honor—the **Platinum Team Quality Award**—as part of the team effort for "outstanding management and oversight of three LDRD Programs at three Defense Programs Laboratories." The team includes **Nathan Lucas**, associate director of the DOE/OAK Weapons Research Division, and Livermore's **Cathy Sayre**, **Pat Taylor**, **Nancy Campos**, and **Pamela Harris**.

Site 300 Keeps High-Explosives Science on Target

Much of Livermore's Experimental Test Site, known as Site 300, supports the DOE's science-based Stockpile Stewardship Program. Explosions, called shots, result from destructive tests of high explosives and other nonnuclear weapon components—100 to 200 of them a year for the last 10 years. Powerful x-ray machines, interferometers, high-speed cameras, and other diagnostic equipment record shot information in the first nanoseconds after detonation. The tests are important for improving understanding how aging affects chemical high explosives in stockpiled weapon systems and of compatibility of explosives with other materials.

Nondestructive tests at Site 300 include subjecting prototype explosives to vibration and extreme heat, possible conditions encountered during transport. Other work includes fabricating, machining, and assembling test devices prior to testing.

The article also describes the process of a test at Site 300 and the measures taken to protect the environment in the course of testing and experiments at the site.

Contact:
Site 300 site manager Milt Grissom (925) 423-1396 (grissom1@llnl.gov) or deputy site manager Jim Lane (925) 423-5217 (lane5@llnl.gov).

Putting More Pressure on Hydrogen

A thorough understanding of hydrogen, the most common and most abundant element in the universe, is an important part of understanding basic matter. Until recently, there was no way to subject hydrogen to extremely high pressure—such as that found on giant, hydrogen-bearing planets.

In conjunction with the new techniques, diagnostics, and instrumentation developed at Livermore, laser scientists ran experiments to shock hydrogen at extreme pressures using the Nova laser, causing hydrogen to metallize. The phenomenon was accurately recorded by the suite of experimental instrumentation and then plotted and analyzed.

The surprising experimental data showed hydrogen to compress more than expected and metallize at lower pressures and at a more gradual rate than previously theorized. There is good confidence in the results: the data points at lower shock pressures overlap those of an earlier Livermore hydrogen shock experiment performed with a light-gas gun and agree with a hydrogen model posited by another Livermore scientist. Hydrogen theorists now are working to revise models to fit the data and use them to better define high-density hydrogen equations of state, long considered uncertain.

Contact:
Robert C. Cauble (925-422-4724) cauble1@llnl.gov.

U.S. Government Printing Office: 1999/683-051-60055

Coming Next Month

Building a Structural Biology Capability at Livermore

A progress report of the Biology and Biotechnology Research Program's efforts to contribute to the field of molecular medicine by understanding the mechanistic basis of disease.

Also in April

- *Duplicating the plasmas of stars in the laboratory.*
- *Successfully testing seismic monitoring of clandestine nuclear explosions.*
- *Tracking MTBE effects on groundwater.*

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