Lawrence Livermore National Laboratory

Science and Technology Review

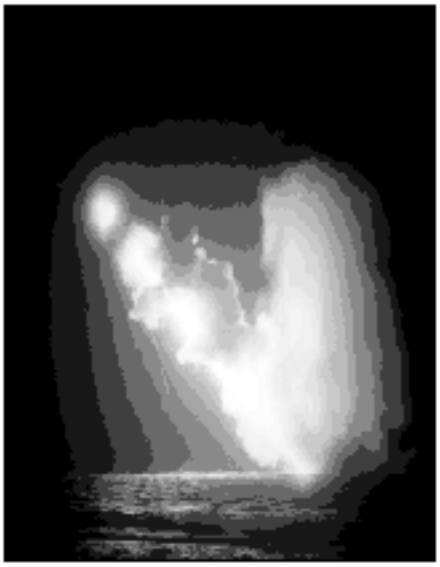
Stockpile Stewardship Program

UCRL-LR-129781

A collection of articles from Science & Technology

About the Cover

A photograph of the second of three non-nuclear W87/Mk12 flight test units in the Kwajalein Missile Range, showing the high-explosive endpoint performance. The camera taking this photograph was triggered by signals from the test unit, which activate a radio transmission to the camera control via special diagnostics systems on ocean surface rafts.



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Science and Technology in the LLNL

THE primary mission of the Lawrence Livermore National Laboratory (LLNL) is to ensure that the nation's nuclear weapons remain safe, secure, and reliable and to prevent the spread and use of nuclear weapons worldwide. The mission of maintaining the U. S. stockpile in the absence of nuclear testing is carried out by the Defense and Nuclear Technologies (DNT) and its Stockpile Program. This special collection of articles, previously published in the Science & Technology Review, highlights science and technology within the Stockpile Program that contribute to the fundamental understanding of the stockpile. While this collection cannot cover a complete spectrum of our stewardship activities without introducing classified materials, this body of work represents the scientific underpinnings necessary to ensure the safety, security, and reliability of the nation's nuclear stockpile.

Background

The breakup of the Soviet Union brought an end to the bilateral tensions that dominated U.S. national security policy for decades. However, economic disparities, cultural and ethnic differences, regional tensions, and uncertainties about the future can give rise to international tensions and conflict. Global interests will keep the U.S. actively engaged in world events. Thus, the nation must both prepare for anticipated security threats and expect surprises.

Nuclear deterrence and nonproliferation are important elements of U.S. national security policy. The future course for the nation's nuclear weapons program was set in 1995, when President Clinton announced that the U.S. would pursue a comprehensive nuclear test ban. In making that decision, he reaffirmed the importance of maintaining a safe and reliable U.S. nuclear stockpile. Subsequently, the President directed necessary programmatic activities to ensure stockpile safety and reliability in the absence of nuclear testing. The Department of Energy's Stockpile Stewardship Program (SSP) was developed in response to this directive, and in 1996 the President signed the Comprehensive Test Ban Treaty to end all nuclear testing.

Developing a science-based predictive capability to replace the previous nuclear-test demonstration- based program is the defining responsibility of LLNL's Defense and Nuclear Technologies Program.

LLNL Stockpile Stewardship Program

The willingness of the U.S. to sign the Comprehensive Test Ban Treaty hinged, in large part, on the confidence of the Administration and Congress in the national laboratories' ability to help maintain the U.S. nuclear deterrent through the Stockpile Stewardship Program.

Significant milestones already have been achieved. On December 19, 1996, the Secretary of Energy signed the Record of Decision for the Stockpile Stewardship and Management Programmatic Environmental Impact Statement. This document defines the overall architecture of the program. In addition, an SSP implementation plan has been developed by DOE's Office of Defense Programs, working closely with the laboratories and production plants. This plan—already in its first revision—describes program requirements in detail. The first annual certification of the U.S. stockpile under the Stockpile Stewardship Program was completed on February 7, 1997.

Defense and Nuclear Technologies Program at LLNL is involved in a number of complex-wide SSP initiatives and activities. Highlights of some of these stewardship activities are described below.

Demonstration-Based Assessment and Certification without Nuclear Testing

The nuclear stockpile program has always been demonstration-based. However, with nuclear testing no longer the primary demonstration tool, we must develop sufficient predictive capability to generate confidence in the safety and performance details of aging stockpile weapons. This requires establishing laboratory and simulation demonstration capabilities that together can replace, to the extent possible, nuclear testing.

The task is daunting. Not only does demonstration-based stockpile stewardship require significant advances in research and simulation facilities but it also poses the tremendous challenge of understanding heretofore unimportant details. That is, it requires the ability to quantitatively predict a large number of details whose

Stockpile Stewardship Program

integrated performance was once adequately assessed by nuclear tests. These details tend to be three-dimensional in nature and are often nonlinearly cross-coupled (meaning small changes in one detail can cause enormous changes in another). In the past, stockpile weapons were assessed using computational models developed in conjunction with nuclear test data plus data from aboveground experiments using surrogate materials. Now, and in the future, we must rely on a web of interrelated calculations, validated by non-nuclear experiments and by benchmarking against past nuclear tests, to provide confidence in the stockpile. There are risks inherent in this approach; history has shown that very small changes in a nuclear weapon can sometimes lead to failure of the entire weapon.

Our goal is to provide nuclear weapon experts who possess the integrity and technical knowledge necessary to assess the existing stockpile. Moreover, these experts must have at their disposal the advanced experimental and computational tools necessary to do the task.

The Nova Laser and the National Ignition Facility

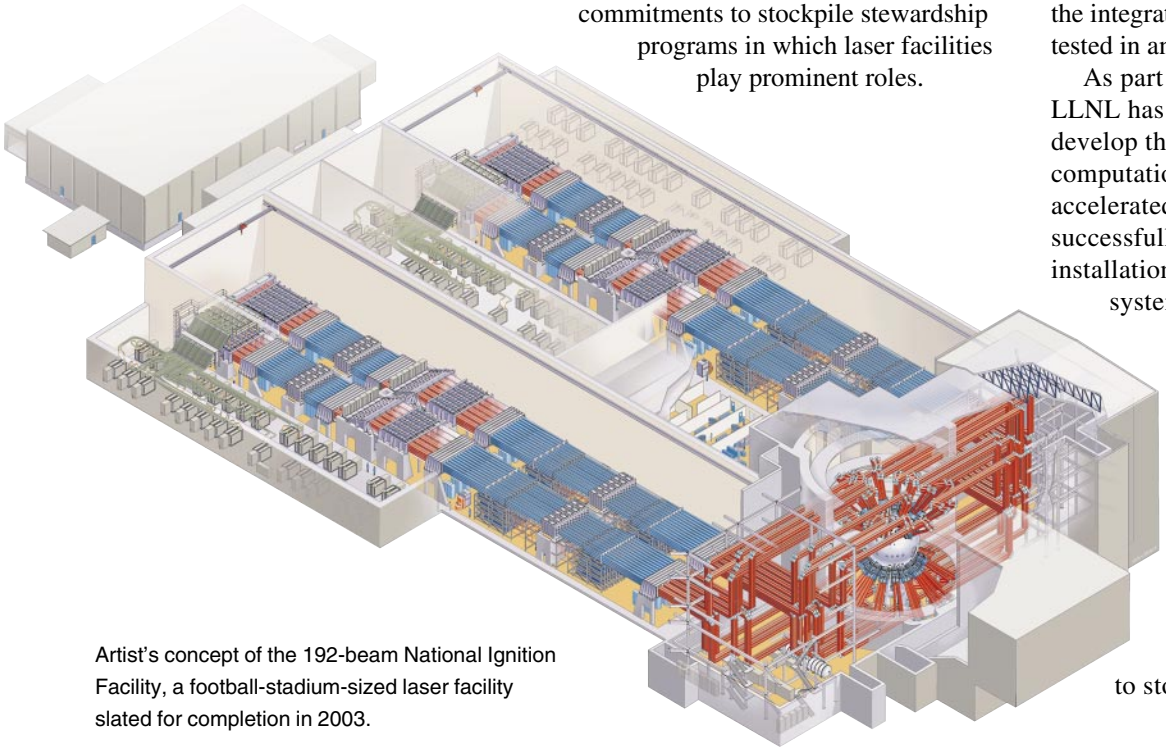
In coming years, the National Ignition Facility (NIF) will be an experimental cornerstone of SSP, providing an important research tool for studying the physics of nuclear weapon primaries and secondaries. It is the only currently planned U.S. facility that will be available for conducting experiments to examine fusion burn and for studying weapon-related processes at nuclear-weapons-relevant energy density. The ignition experiments on NIF will provide an analogous process for exercising some of the tools by

DOE's Stockpile Stewardship Program will assure that we can depend on experiments and simulations to predict, detect, evaluate, and correct problems affecting nuclear weapons—all without nuclear testing. Critical to meeting this challenge will be the development of higher-resolution computer models of the performance of nuclear weapons and the conditions that affect weapon safety. This example shows the molecular-level sequence of a shock wave from a piston driving into a piece of metal, including the effects on a nanometer-size void or defect (the empty circle). Developing molecular dynamics simulations using elements of the DOE's Accelerated Strategic Computing Initiative (ASCI) is made possible through partnering of massively parallel processing, software development, and data storage among the nation's three nuclear weapons laboratories.

which nuclear weapons will be evaluated under SSP. In concert with a number of other facilities that can field different and complementary nuclear-weapon-relevant experiments, NIF will provide information necessary to maintain the nuclear stockpile as a viable defense asset. Available to all members of the U.S. weapons complex as well as to many academic and industrial partners, NIF will serve as a national facility sited at LLNL.

Construction has begun on NIF, which is scheduled for completion by the end of 2003. LLNL led the design team, composed of engineers and scientists from LLNL, Los Alamos National Laboratory, Sandia National Laboratories, and the University of Rochester. While NIF's primary role will be in support of stockpile stewardship, it will also serve as a national facility for basic research in high-energy-density physics. When ignition is demonstrated, NIF will play a major role in fusion energy research. The facility will be available for limited experiments by the end of 2001, when the first bundle of laser beams will be activated. In the immediate future, weapon physics experiments will continue on Nova, the Laboratory's precursor to NIF. Although far less powerful than NIF, the ten-beam Nova laser is a potent research tool with more than a decade of operation to demonstrate its value in support of stockpile stewardship.

We are partnering on NIF with U.S. allies, particularly the French CEA Division Applications Militaire. With Congressional approval, France conducts joint research with the U.S. on NIF for inertially confined fusion (ICF). Also with Congressional approval, the British AWE Ministry of Defense conducts research with the U.S. on certain aspects of stockpile stewardship and ICF. Both countries have strong commitments to stockpile stewardship programs in which laser facilities play prominent roles.



Artist's concept of the 192-beam National Ignition Facility, a football-stadium-sized laser facility slated for completion in 2003.

Advanced High-Performance Computing

The Accelerated Strategic Computing Initiative (ASCI) is primarily a tri-laboratory DOE program whose goal is to dramatically advance our ability to simulate computationally the performance of an aging stockpile and conditions affecting weapon safety. Although it will take more than a decade to achieve ASCI's long-term goals—a ten-thousand-fold increase in computer speed and data storage capacity—each year, the initiative is structured to deliver major new capabilities to support stockpile stewardship.

Central to ASCI is the accelerated development over the next decade of highly parallel, "terascale" computers in partnership with the U.S. computer industry. A terascale computer performs a trillion operations per second, which, at modest operating efficiency, is a thousand-fold improvement over current capability. Computers of this size and speed are necessary to simulate the integrated details that were once tested in an underground explosion.

As part of the ASCI initiative, LLNL has partnered with IBM to develop these highly advanced computational capabilities. The accelerated pace of ASCI was successfully demonstrated by the rapid installation of an IBM initial delivery system at Livermore and its almost immediate application to real problems related to weapon technologies. The 512-node IBM SP2 (the largest machine currently available from IBM) was delivered 30 days ahead of schedule, was up and running three days later, and was applied to stockpile-related problems

two weeks after that. The speed with which boxes of components were transformed into a working supercomputer was a direct result of the dedication and close collaboration of Livermore and IBM personnel.

ASCI's computers of the future will face the challenge of providing accurate and detailed simulated predictions of the complex processes involved in nuclear weapon explosions as well as of the detailed materials changes in weapons due to aging and refurbishment. The success of SSP will depend on the credibility of the weapons laboratories' simulations, as measured by their ability to accurately predict complex laboratory experiments at facilities such as NIF at LLNL or DARHT at Los Alamos.

Enhanced Surveillance

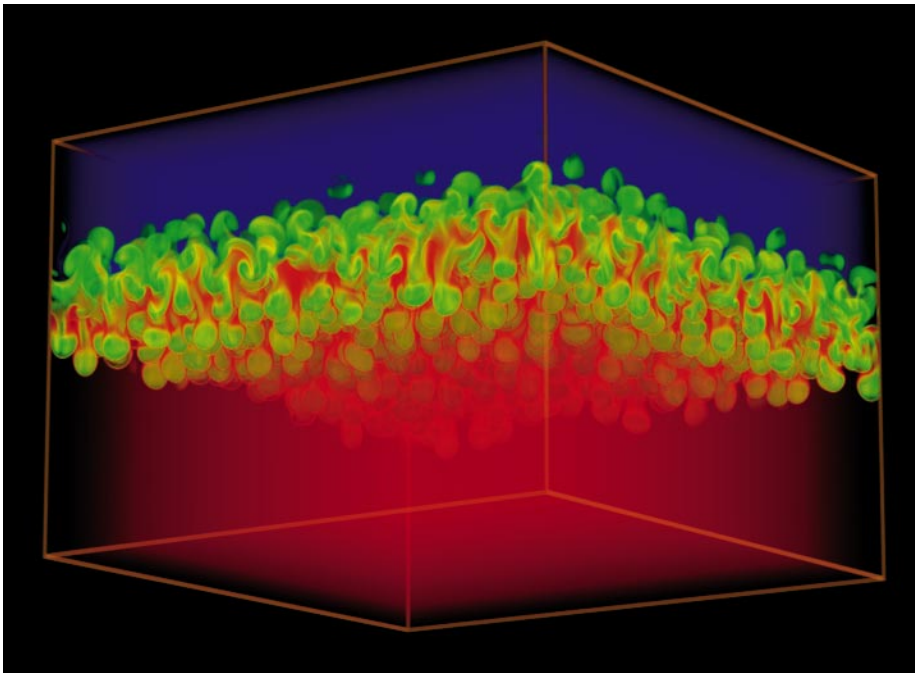
Aging is a critical issue. It affects the physical characteristics of all materials, producing premature materials failure in airplanes, cars—and nuclear weapons. With a better understanding of aging, our stockpile surveillance can become more predictive, making possible systematic refurbishment and preventive maintenance activities that can correct problems that threaten weapon safety or reliability.

With fewer weapons and fewer types of weapons in the stockpile, together with reduced capabilities and capacity in the production complex, we must become more proficient at detecting and predicting potential problems early on to provide enough time for thorough evaluation and action before problems affect stockpile safety or reliability. To this end, we will improve our databases on the characteristics and behavior of stockpiled weapons so that we can identify anomalies in aging weapons. We will improve the sensors and techniques used to inspect stockpiled weapons. And, we will develop a better understanding of how aging alters the physical characteristics of weapon materials and how these changes affect weapon reliability and safety.

High Explosives and the Contained Firing Facility

The Laboratory's High Explosives Applications Facility (HEAF) provides ultra-modern capabilities for high explosives research. Coupled with this research is the need for separate facilities to study the dynamic implosion of simulated weapons using high explosives. These dynamic simulations are known as explosive hydrodynamics tests.

In the absence of nuclear testing, explosive hydrodynamics tests will be our principal experimental means of assessing the integral performance of primaries in stockpile nuclear weapons. The flash x-ray radiographic accelerator (FXR) at LLNL's Site 300 is currently the only modern, fully capable hydrodynamics testing facility in the DOE complex. Originally designed for open-air testing, the facility must be upgraded to comply with impending more stringent environmental regulations. The resulting Contained



One of the great scientific challenges of SSP is the detailed, three-dimensional, computer simulation of fluid plasma instabilities that impact the performance of weapons. These instabilities, inherent in all nuclear weapons, used to be parameterized by nuclear tests, but now must be predicted by computer. Shown here is a simulation of a compressible Rayleigh-Taylor instability with turbulent mixing. This simulation was made possible by the 128-node ASCI Blue Pacific ID System recently installed at LLNL.

Firing Facility (CFF) will provide environmental containment and waste handling for all hazardous and radioactive materials at the FXR facility, as well as additional space for an expanded suite of diagnostic instruments. Testing will be conducted in a large containment chamber, which will include an automatic washdown system for rapid experiment turnaround.

During the FY98-00 shutdown for CFF construction, a major upgrade of the FXR accelerator also will be completed, providing increased radiographic dose and resolution and a double-pulsing mode to support dynamic radiography. The additional space will be used to house multibeam-velocimeter and laser-illuminated image converter camera diagnostics. It will also include ample room for future diagnostic additions to support SSP. When complete, the CFF will be a principal source of the high-fidelity measurements of primary performance that will be needed to preserve confidence in the integrity of stockpile weapons.

Materials Research and Development

Almost all national security programs depend on the successful development, control, and characterization of materials. LLNL's materials research and development activities are a common thread closely integrating these efforts.

Stockpile stewardship will depend on the continued proper and safe application of high explosives, organics, and special nuclear materials used in weapons components. We will use experiments and models to understand the complex mechanisms that govern aging in these materials. Since predicting kinetics is crucial to avoiding surprise requirements for large-scale refurbishment and remanufacture of weapons components, we will develop multi-length, scale-modeling techniques within ASCI to understand materials processes at the atomic and molecular level, and then scale up the results to understand the effects of these processes on parameters that affect weapon performance.

The National Ignition Facility and its SSP applications will depend on material capabilities for creating laser glasses, crystals, target components, and advanced diagnostics. The facility will incorporate a large number of optical components that must operate reliably for long lifetimes in a very stressing environment. Challenges range from the processing and conditioning of glass and optical coatings, to the solution-growth of extremely large high-quality single crystals, to the fabrication of complex SSP targets.

LLNL materials-research activities in advanced defense technologies will focus on energetic materials, including high explosives and rocket and gun propellants. Our efforts will be directed toward developing the world's most powerful materials, creating the most precise explosive forms using injection-mold technology, and developing the most energetic explosives for reduced-volume munitions. Technologies will be developed to chemically convert Department of Defense surplus energetic materials for environmental remediation via chemical and bacterial processes and for waste destruction using the molten-salt-oxidation process.

Researchers prepare a detonation experiment inside a nearly five-meter-diameter, stainless steel containment vessel at LLNL's High Explosives Applications Facility.

Tritium Production

No tritium has been produced for the U.S. weapons stockpile since 1988. At present, DOE is meeting stockpile needs by recycling tritium from dismantled weapons. Since tritium decays at a rate of 5.5% per year, the

total tritium inventory available without further production will decline to a level where, in the year 2007 or so, the inventory will be insufficient to maintain even a START II stockpile. Livermore is actively involved in the new Accelerator Production of Tritium (APT) program, which will use a high-energy, high-current proton accelerator to produce tritium. The DOE's national security laboratories are responsible for designing the APT facility, with Los Alamos as lead lab. LLNL is making important contributions in such technical areas as beam handling and computer modeling.

Advanced Manufacturing

The DOE national security laboratories must work more closely with the production plants to maintain the enduring U.S. stockpile through a combination of as-needed repairs, refurbishments, and replacements. Workforce skills, formerly developed and maintained through new-weapon development, also must be maintained through this repair-refurbish-replace process.

DOE's Advanced Design and Production Technology (ADaPT) program is a complex-wide effort to meet these challenges. The program integrates the skills and facilities of LLNL, the other national security laboratories, and the production plants to develop the innovative new processes and practices that will be needed to achieve a requirements-based, cost-effective production complex. To this end, ADaPT has defined four areas for strategic future investment: (1) enterprise integration, through a secure, complex-wide, high-speed digital network; (2) integrated product and process design ("concurrent engineering"); (3) process-development programs to produce new, environmentally benign production processes; and (4) contingency planning for various scenarios, such as major rebuilds. Livermore is actively involved in each of these endeavors.

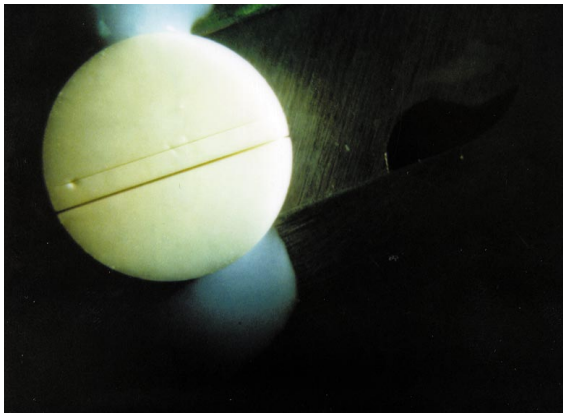
Future Scientific Challenges

DOE and its national security laboratories are focusing their best talents on defining the key SSP scientific challenges. These challenges include vastly increased computational capabilities, a much deeper understanding of materials processes (from the atomic to the macroscopic level), major improvements in our ability to model complex nonlinear dynamic processes, and experimental facilities that can produce plasma density and pressure regimes well beyond any available in the world today.

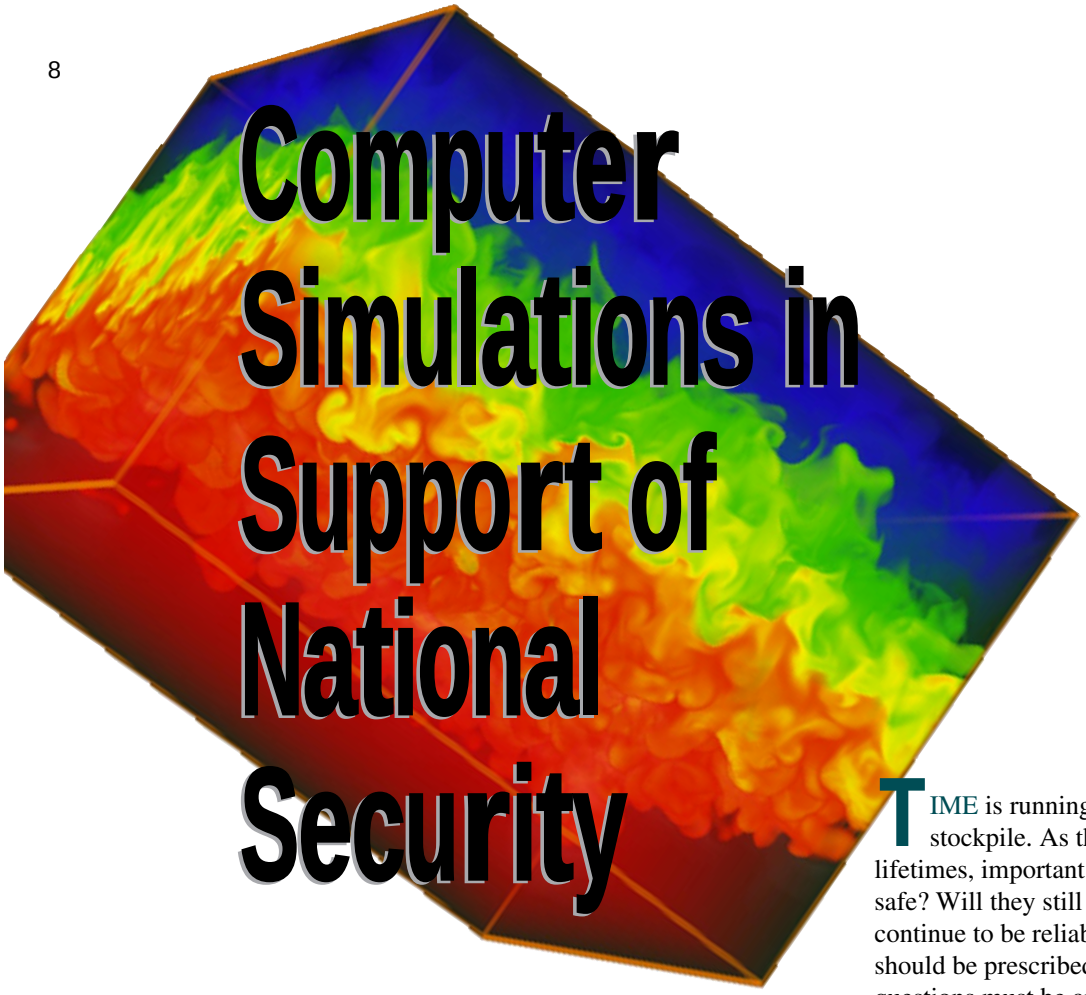
The scientific infrastructure that will support SSP, now and in the future, depends on a myriad of small experimental facilities whose data provide single pieces of the large jigsaw puzzle. We must work to ensure that these capabilities in physics, chemistry, and other basic sciences, as well as their theoretical counterparts, remain a robust and productive mainstay of stockpile stewardship.

As with all high-quality technical programs, the scientific underpinnings of SSP undoubtedly will evolve in directions that are unforeseen today. This is an evolving challenge. As we continue to further understand SSP problems, critical needs for new facilities and capabilities most surely will present themselves. For example, the Advanced Hydrodynamics Facility, which would provide sequences of multiple views of explosive hydrodynamics tests, is emerging as an essential component that we will need in the future to ensure the reliability of a more aged stockpile.

At the same time, we recognize that the nuclear weapons program must continue to be fiscally responsible. Our developing needs will have to be carefully prioritized to identify and support only the most critically needed facilities and projects. We will rely on quality peer review in the technical and resource communities to achieve this end.



For SSP, Livermore has developed a safe, new, short-pulse laser-cutting technique for high explosives. Photo shows high explosive being cut using the new process. Note the lack of burning, deflagration, or detonation often associated with conventional laser cutting.



Computer Simulations in Support of National Security

The Accelerated Strategic Computing Initiative is making significant progress toward meeting its major challenge: dramatically increasing the nation's computing power as a necessary contribution to the assurance by scientists of the safety and reliability of our nuclear deterrent in the absence of testing.

TIME is running out on the U.S. nuclear weapons stockpile. As the weapons age beyond their design lifetimes, important questions arise: Are the weapons still safe? Will they still perform reliably? How long will they continue to be reliable? What maintenance and retrofitting should be prescribed to extend their working life? These questions must be answered with confidence as long as nuclear deterrence remains an essential part of U.S. national security policy.

With the U.S. commitment to the Comprehensive Test Ban Treaty, the viability of the U.S. nuclear arsenal can no longer be determined through underground nuclear testing. Thus, new approaches are being taken to maintain and preserve the U.S. nuclear deterrent through DOE's Stockpile Stewardship Program.

One key component of the multifaceted Stockpile Stewardship Program is the Accelerated Strategic Computing Initiative (ASCI), an effort to push computational power far beyond present capabilities so scientists can simulate the aging of U.S. nuclear weapons and predict their performance. To calculate in precise detail all the complex events of a thermonuclear explosion requires computational power that does not yet exist, nor would it exist any time soon without the ASCI push, even at computer development speeds predicted by Moore's Law (that computer power doubles about every two years). ASCI's goal is to put such a high-fidelity simulation capability in place in the near future. To do that, the American computer industry must dramatically speed up the pace of computational development. Currently, computing's top

speed is 1.8 teraflops, that is, 1.8 trillion floating-point (arithmetic) operations per second. This speed must increase to at least 100 teraflops by 2004, growth that must be coordinated with a host of accomplishments in code development and networking.

Why is this accelerated schedule necessary? Not only are weapons aging, so are the nuclear weapons experts with experience in designing and testing them. The Stockpile Stewardship Program must have this high-fidelity, three-dimensional simulation capability in place before that expertise is gone. "It's a tremendously ambitious goal, especially under such a short schedule," says Randy Christensen, ASCI's deputy program leader at Lawrence Livermore National Laboratory. Christensen describes the work as something akin to "trying to get a computer code to run in a few days a simulation that would have taken so long with current capability that it would not have been attempted."

Orchestrating Integration

ASCI is reaching for computational powers in the hundreds of teraflops, but the ASCI challenge demands more than hardware. Meeting it will require careful integration of the major elements of a national effort: platform development, applications development, problem-solving environment, and strategic alliances—coordinated work conducted at three national laboratories in partnership with the commercial supercomputer industry and the nation's great universities (Figure 1).

To ensure this balanced development, ASCI planning began with a "one program–three laboratories" approach. Project leaders at each laboratory, guided by the DOE's Office of the Assistant Secretary for Defense Programs, are implementing this collaboration and extending it to ASCI's industrial and academic partners. The overriding challenge for the ASCI scope of work is to synchronize the various technological developments with each other. For example, sufficient platform power must be delivered in time to run new advanced codes, and networking capabilities must enable the various parts of the system to behave as if they were one. The success of ASCI depends on this integration as much as it depends on the success of ASCI's individual elements.

Developing the Platform

ASCI's computer hardware is being developed by a consortium of three national laboratories and a select group of industrial partners in a prime example of government–industry cooperation. The national laboratories—Lawrence Livermore, Los Alamos, and Sandia—are each teamed with a major commercial computer manufacturer—IBM, Silicon Graphics–Cray, and Intel, respectively—to design and build parallel, supercomputing platforms capable of teraflops speeds.

The development of infrastructure technologies seeks to tap all available resources to make these computer platforms perform the kind of high-fidelity simulation that stockpile stewardship requires. ASCI has a PathForward component, a program that invites computer companies to collaborate in developing required technologies. For instance, the program's first PathForward contracts, announced on February 3, 1998, awarded more than $50 million over four years to four major U.S. computer companies to develop and engineer high-bandwidth and low-latency technologies for the interconnection of 10,000 commodity processors that are needed to build the 30-teraflops computer. (See box, p. 10.) As a result of this effort, subsequent collaborations involving other agencies, academia, and industry are expected.

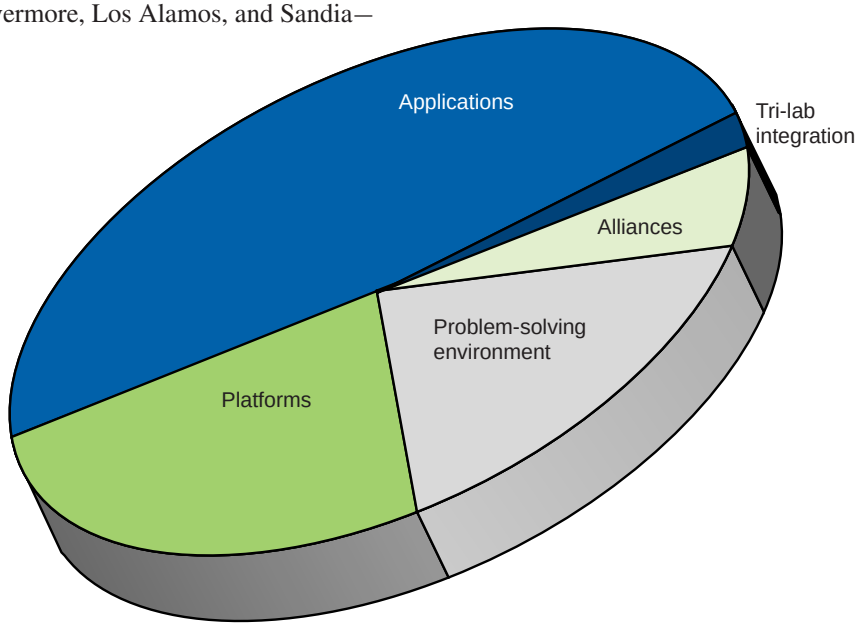


Figure 1. Meeting the challenge of ASCI requires careful integration of the major elements of the program across three national laboratories and ASCI's industrial and academic partners.

Developing Applications

ASCI is an applications-driven program. Unprecedented computer power with a first-rate computing environment is required to do ASCI's stockpile stewardship job, which is to run new computer codes programmed with all of the accumulated scientific knowledge necessary to simulate the long-term viability of our weapons systems. The new generation of advanced simulation codes being developed in the ASCI program must cover a wide range of events and describe many complex physical phenomena. They must address the weapon systems' normal performance from high-explosive initiation through final nuclear yield and the effects of changes introduced by remanufacturing (perhaps using different materials and fabrication methods) or defects brought on by aging. In addition, they must simulate weapon behavior in a wide variety of abnormal conditions to examine weapon safety issues in any conceivable accident scenario. If this weren't difficult enough, the new codes must provide a level of fidelity to the actual behavior of weapons that is much higher than their predecessors provided.

The major challenges facing the developers of these advanced simulation codes are to base them on rigorous, first-principles physics and eliminate many of the numerical approximations and simplified physics that limit the fidelity of current codes; make them run efficiently on emerging high-performance computer architectures; validate their usefulness by means of nonnuclear experiments and archival nuclear test data; and do all of these in time to meet stockpile needs.

Meeting these challenges requires the coordinated efforts of over a hundred physicists, engineers, and computer scientists organized into many teams. Some teams create the advanced weapon simulation codes, writing and integrating hundreds of smaller programs that treat individual aspects of weapon behavior into a single, powerful simulation engine that can model an entire weapon. Other teams are devoted to developing the advanced numerical algorithms that will allow these codes to run quickly on machines consisting of thousands of individual processors—a feat never before achieved with programs this complex. Still others are developing much improved models for the physics of nuclear weapon operation or for the behavior of weapon materials under the extreme conditions of a nuclear explosion. Both the scale (the largest teams have about 20 people) and the degree of integration demanded by this complex effort have required a much greater level of planning and coordination than was needed in the past.

One example of the advanced simulation capabilities being developed in the ASCI program is its material modeling program. Enormously powerful ASCI computers are being used to carry out very accurate, first-principles calculations of material behavior at the atomic and molecular level. This information is then used to create accurate and detailed models of material behavior at larger and larger length scales until we have a model that can

PathForward Contracts Awarded February 1998

Industrial Partner	PathForward Project
Digital Equipment Corporation (DEC) Maynard, Massachusetts	Develop and demonstrate a processor interconnect capable of tying together 256 Digital UNIX-based AlphaServer symmetric multiprocessing (SMP) nodes.
International Business Machines (IBM) Poughkeepsie, New York	Develop future high-speed, low-latency, scalable switching technology to support systems that scale to 100 teraflops.
Silicon Graphics–Cray Research (SGI/Cray) Chippewa Falls, Wisconsin	Develop and evaluate advanced signaling and interconnect techniques. The technology will be used in future routers, switches, communication lines, channels, and interconnects.
Sun Microsystems (SUN) Chelmsford, Massachusetts	Perform hardware and software viability assessments by constructing interconnect fabric and verifying scalability and correctness of the interconnect monitoring facilities, resource management, and message-passing interface (MPI) capabilities.

be used directly in the weapon simulation codes (Figure 2). This computational approach to material modeling has already produced a much better understanding of the phase changes in actinides (the chemical family of plutonium and uranium). The new approach is expected to be applied to many weapons materials, ranging from plutonium to high explosives. When fully developed, it will become a powerful tool for understanding and predicting the behavior of any material (for example, alloys used in airplane construction, steel in bridges), not just those used in nuclear weapons.

Developing the Infrastructure

In addition to platform and applications development, ASCI is also developing a powerful computer infrastructure. A high-performance problem-solving environment must be available to support and manage the

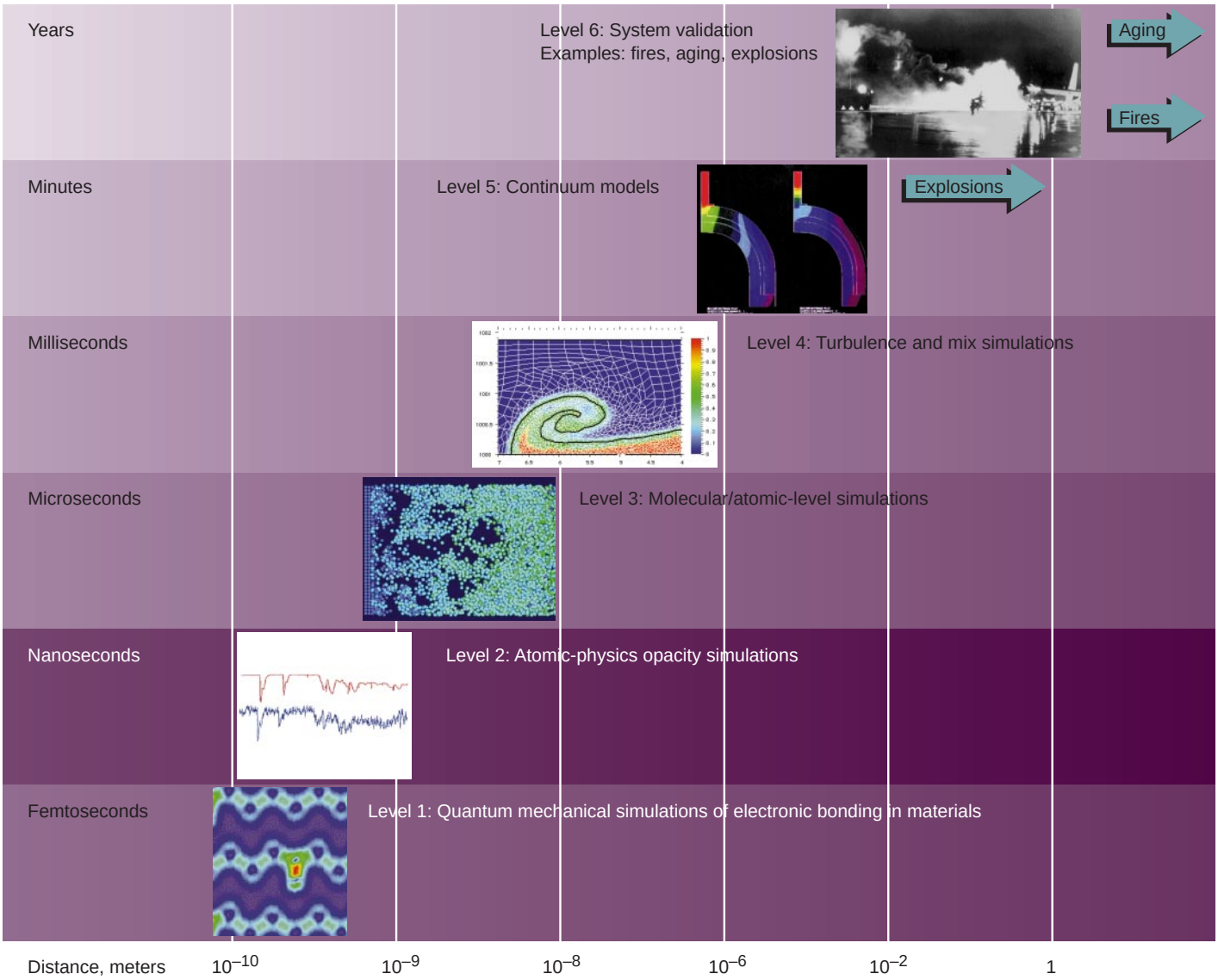
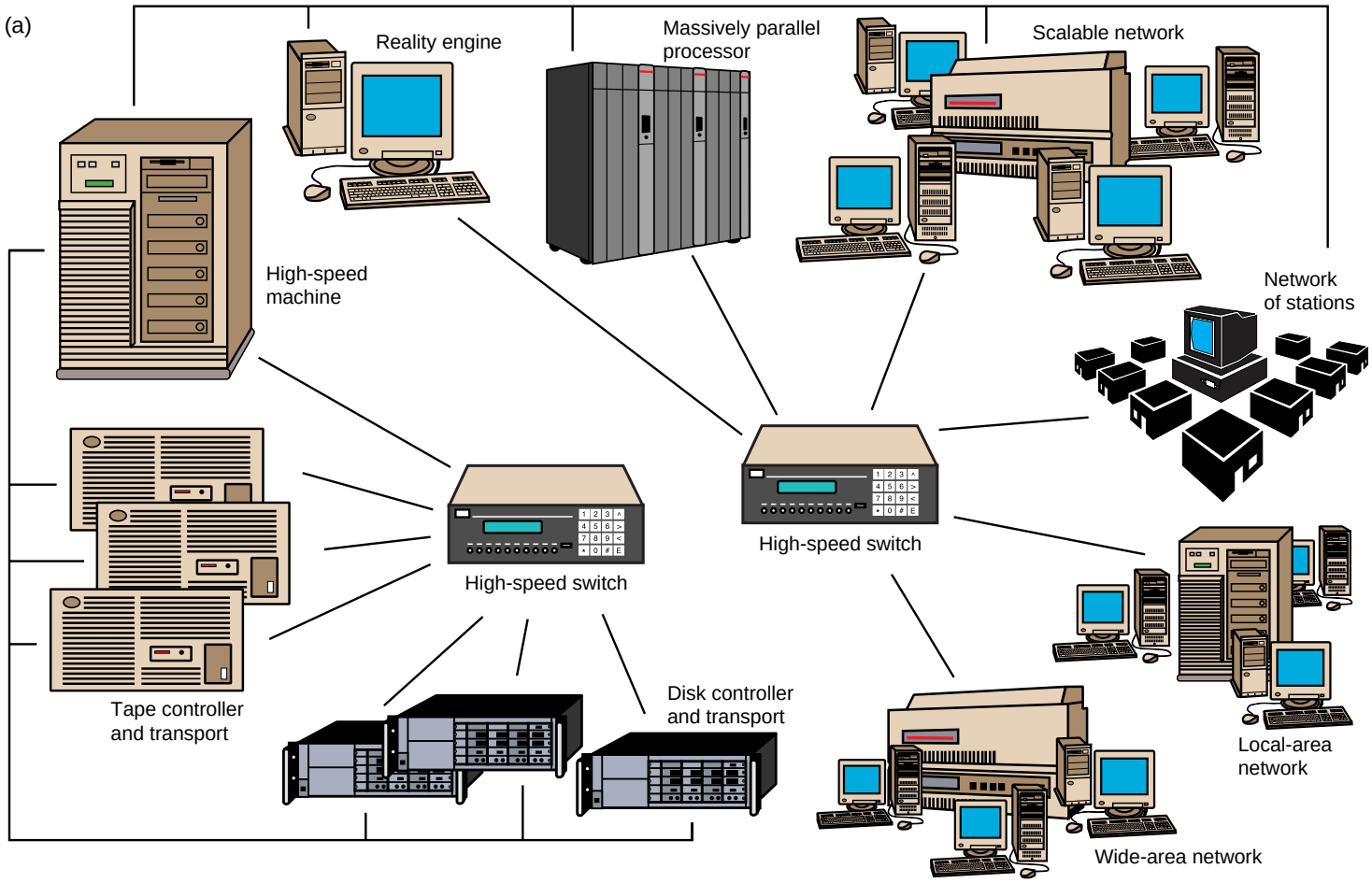


Figure 2. ASCI is providing DOE's Stockpile Stewardship Program with a hierarchy of models and modeling methods to enable predictive capability for all processes relevant to weapon performance.



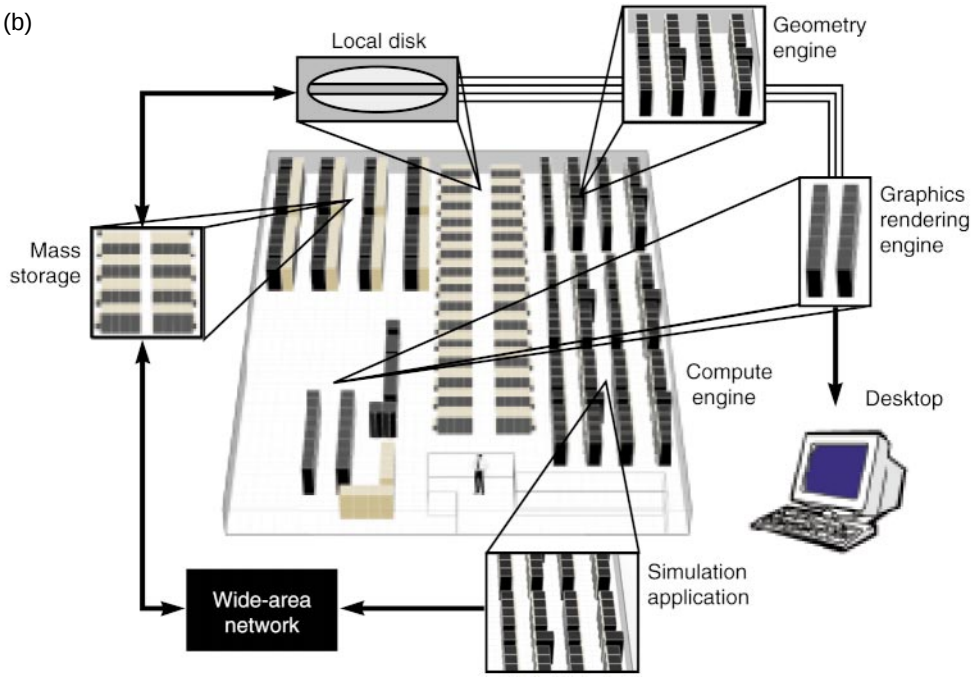


Figure 3. (a) A high-performance problem-solving environment manages the workflow and communications among all ASCI computers. (b) The result is ASCI's ability to bring three-dimensional images resulting from calculations to scientists on their desktops regardless of the physical location of the processors doing the work. This distance-computing option features remote caching of simulation data.

workflow and the communications between all the ASCI machines. At any time, over 700 classified and unclassified code developers and testers may be accessing ASCI computers, either from within the national laboratories or via the Internet. A scalable network architecture, in which individual computers are connected by very high-speed switches into one system, makes this high-demand access possible. With such a configuration, the network is, in effect, the computer (Figure 3).

Allowing large numbers of computers to communicate over a network as if they were a single system requires sophisticated new tools to perform scientific data management, resource allocation, parallel input and output, ultrahigh-speed and high-capacity intelligent storage, and visualization. These capabilities must be layered into the computer architecture, between user and hardware, so that the two can interact effectively and transparently. The applications integrate the computing environment and allow users, for example, to access a file at any of the three national laboratory sites as if it were a local file or to share a local file with collaborators at any ASCI site.

At Livermore, ASCI staff are performing numerous projects to develop this integrated computing environment. One team is working on a science-data management tool that organizes, retrieves, and shares data. An important objective of this tool is to reduce the amount of data needed for browsing terascale data sets. Another team is developing data storage that will offer a vast storage repository for keeping data available and safe 24 hours a day. The repository will store petabytes (quadrillions of bytes) of information, equivalent to one hundred times the contents of the Library of Congress. The storage device will also rapidly deliver information to users, at a rate of billions of bytes per second. Another ASCI team is writing scalable input and output software to move data from computer to computer and reduce congestion between computers and storage. The changes resulting from its improvements will be tantamount to moving busloads of data, as compared to carloads—a sort of mass transit for data.

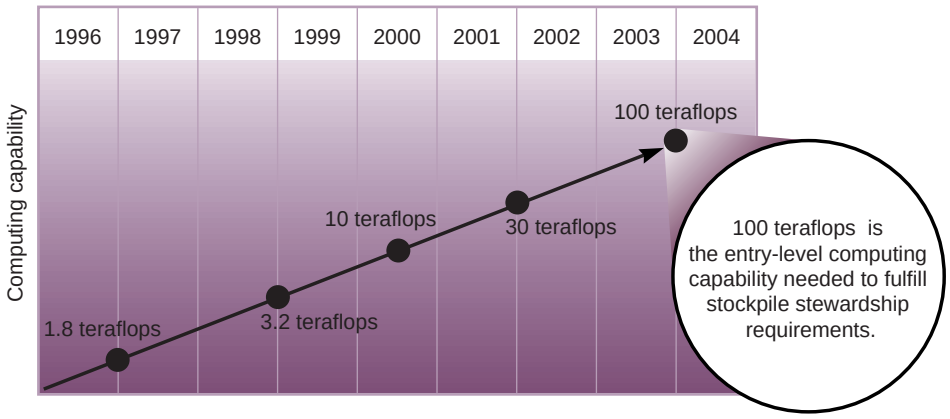


Figure 4. The ASCI goal is to achieve the 100-teraflops (trillion-floating-point-operations-per-second) threshold by 2004.

Weapons scientists will be confronted with analyzing and understanding overwhelmingly large amounts of data derived from three-dimensional numerical models. To help them, ASCI is developing advanced tools and techniques for computer visualization, wherein stored data sets are read into a computer, processed into smaller data sets, and then rendered into images. The development of visualization tools for use across three national laboratories will require close collaboration with regard to programming language, organization, and data-formatting standards. The Livermore team is focusing on how to reduce data sets for visualization—because they surely will become larger and larger—through the use of such techniques as resampling, multiresolution representation, feature extraction, pattern recognition, subsetting, and probing.

While the fast, powerful machines and complex computer codes garner most of the headlines, this problem-solving-environment effort is fundamental to fulfilling the ASCI challenge. As we come to understand that "the network is the computer," the significance of this element of the ASCI program comes sharply into focus.

In Pursuit of 100 Teraflops

The 100-teraflops milestone, the entry-level computing capability needed to fulfill stockpile stewardship requirements, is ASCI's goal for 2004 (Figure 4). Fulfilling it will require enough computational power to run calculations distributed over 10,000 processors, which is just enough to conduct three-dimensional weapons simulations at a level of complexity that matches the current understanding of weapons physics. While this computing capacity is not the final goal, it is already 100,000 times more than the computing power used

(a)

(b)

Figure 5. (a) The IBM Blue Pacific computer arrived at Livermore on September 20, 1996, just two months after the IBM/Livermore partnership was announced by the White House and about six weeks after the contract was signed. (b) The initial-delivery system has already begun significant calculations in important areas of stockpile stewardship such as three-dimensional modeling of material properties, turbulence, and weapon effects. Upgrades will bring system power to 3.28 teraflops (trillion floating-point operations per second) by 1999, with an option to upgrade to 10 teraflops in fiscal year 2000.

by weapons scientists today, represented by Livermore's J-90 Cray computer. At 100 teraflops, all of the calculations used to develop the U.S. nuclear stockpile from the beginning could be completed in less than two minutes.

ASCI's approach to the 100-teraflops goal has been to use off-the-shelf, mass-market components in innovative ways. It aggregates the processors developed for use in desktop computers and workstations to scaleup computing power. It is this approach that makes ASCI development cost-effective; and leveraging of commercially available components will encourage technology development in the commercial sector. The mass-market approach will take advanced modeling and simulations into the computational mainstream for universal PC use.

Improvements to ASCI power will occur over five generations of high-performance computers. To ensure success, multiple-platform development approaches are being attempted. This strategy will reduce risk, allow faster progress, and result in greater breadth of computing capability. For example, the Sandia/Intel Red machine, which was put on line in August 1995, has achieved 1.8-teraflops speed (currently the world's fastest) and is now being used for both code development and simulation. The Lawrence Livermore/IBM Blue Pacific and the Los Alamos/Silicon Graphics–Cray Blue Mountain systems, which resulted from technical bids awarded in late 1996, are already running calculations.

Blue Pacific was delivered to Lawrence Livermore on September 20, 1996, with a thousand times more power than Livermore's existing Cray YMP supercomputer (Figure 5a). The Lawrence Livermore/IBM team installed and powered up the system and had it running calculations within two weeks. Already, it is conducting

some of the most detailed code simulations to date.

The Blue Pacific initial-delivery system, which arrived in 340 refrigerator-sized crates, takes up a significant portion of Livermore's computing machine room space, operates at 136 gigaflops, and has 67 gigabytes of memory and 2.5 terabytes of storage (Figure 5b). Initially, each of its 512 nodes contained one processor. During March 1998, these nodes were replaced with four-way symmetrical multiprocessors, quadrupling the number of processors. A further improvement will endow it with thousands of significantly improved processor nodes for the ASCI production model. These reduced-instruction-set computing microprocessors operate at a peak of 800 megaflops and, in this configuration, will bring the system to a total of 3.28 teraflops.

In that three-teraflops configuration, the Blue Pacific's "Sustained Stewardship Teraflops" system alone would more than fill up all the space in Livermore's current machine room. For that reason, construction crews are now building and wiring new space to accommodate it. In new, larger quarters, workers have been installing electric power, replacing air handlers and coolers, and hooking up new fans as part of necessary building upgrades. The numbers are impressive: 12,000 square feet of building extension, 5.65 megawatts of power, 11 tons of air conditioning, 16 air handlers that replace the air four times per minute, and controllers that keep the temperature between 52° and 72°F at all times. This machine is scheduled to be installed in March or April of 1999 (Figure 6).

Involving Academia

Although work on weapons physics is classified, work on the methods and techniques for predictive materials models encompasses unclassified research activities. ASCI thus can pursue a strategy of scientific exchange with academic institutions that will more rapidly establish the viability of large-scale computational simulation and advance simulation technology. This strategy is embodied in the Academic Strategic Alliances Program. The program invites the nation's best scientists and engineers to help develop the computational tools needed to apply numerical simulation to real-world problems. In this way, a broader scientific expertise is at work making the case for simulation; simulation algorithms are tested over a broad range of problems; and the independently produced simulations provide a peer review that helps validate stockpile stewardship simulations (see box below).

Computers Changed It All

In the short span of time since computers came into general use, the nature of problem-solving has changed, by first becoming reliant on computers, and then becoming constrained by the limits of computer power. ASCI will develop technologies that will make computational capability no longer the limiting factor in solving huge problems. Just as important, ASCI will change the fundamental way scientists and engineers solve problems, moving toward full integration of numerical simulation with scientific understanding garnered over decades of experimentation.

In the stockpile stewardship arena, the ASCI effort will support high-confidence assessments and stockpile certification through higher fidelity simulations. Throughout American science and industry, new products and technologies can be developed at reduced risk and cost. Advanced simulation technologies will allow scientists and engineers to do such things as study the workings of

The Academic Strategic Alliances Program

In July 1997, the Academic Strategic Alliances Program awarded Level I funds to five universities to perform scientific modeling to establish and validate modeling and simulation as viable scientific methodologies.

- Stanford University will develop simulation technology for power generation and for designing gas turbine engines that are used in aircraft, locomotives, and boats. This technology is applicable to simulating high-explosive detonation and ignition.
- At their computational facility for simulating the dynamic response of materials, the California Institute of Technology will investigate the effect of shock waves induced by high explosives on various materials in different phases.
- The University of Chicago will simulate and analyze astrophysical thermonuclear flashes.
- The University of Utah at Salt Lake will provide a set of tools to simulate accidental fires and explosions.
- The University of Illinois at Urbana/Champaign will focus on detailed, whole-system simulation of solid-propellant rockets. This effort will increase the understanding of shock physics and the quantum chemistry of energetic materials, as well as the effects of aging and other deterioration.

These Level I projects are part of a 10-year program, in which projects can be renewed after five years. Also under the Alliances program, smaller research projects are being funded at universities across the country as Level II and III collaborations.

Figure 6. Rendering of the 3.28-teraflops IBM Blue Pacific "Sustained Stewardship Teraflops" system in its new home being constructed at Lawrence Livermore. The machine is scheduled for installation in early 1999.

disease molecules, so they can design drugs that combat the disease; observe the effects of car crashes without an actual crash; and model global weather to determine how human activities might be affecting it. The uses are limitless, and their benefits would more than justify this investment in high-end computing, even beyond the benefits of ASCI's principal national-security objective.

—Gloria Wilt

Key Words: Academic Strategic Alliances Program, Accelerated Strategic Computing Initiative (ASCI), computer infrastructure, computer platform, parallel computing, PathForward, problem-solving environment, Stockpile Stewardship Program, simulation, teraflops, weapons codes.

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About the Scientist

RANDY CHRISTENSEN is Deputy Program Leader of the Department of Energy's Accelerated Strategic Computing Initiative (ASCI). He has broad management responsibilities within the ASCI program as well as specific responsibility for applications development. He holds a B.S. in physics from Utah State University and an M.S. and Ph.D. in physics from the University of Illinois. Following a postdoctoral fellowship at the Joint Institute for Laboratory Astrophysics (1978–1981), he joined Lawrence Livermore National Laboratory as a code physicist in the Defense and Nuclear Technologies Directorate. He held a number of leadership positions in that directorate before becoming Deputy Associate Director of the Computation Directorate in 1992, where his responsibilities included management of the Livermore Computing Center.

Enhanced Surveillance of Aging Weapons

WITHIN the Department of Energy, the word "surveillance" has a meaning closely akin to the word from which it derives—"vigilance." For years, the DOE has had an ongoing surveillance program to verify the safety and reliability of U.S. nuclear weapons. Surveillance has always dealt with the possible effects that aging may have on weapon materials and components. The study of aging effects is even more important now that nuclear testing has ceased, no new weapons are being developed, and the existing arsenal is growing older. Current plans call for many of the weapon systems in the arsenal to be in the stockpile well beyond their design lifetimes, and scientists must be able to predict the behavior of these systems as they age.

DOE's enhanced surveillance program is just one facet of science-based stockpile stewardship.[1] Since the program began in 1995, it has been managed by DOE's Office of Defense Programs. But the work is actually being done by the seven DOE facilities that designed and fabricated the weapons in the first place—Livermore, Los Alamos, and Sandia national laboratories as well as the Y-12, Kansas City, Pantex, and Savannah River plants.

The objective of the enhanced surveillance program is to develop diagnostic tools and predictive models that will make it possible to analyze and predict the effects that aging may have on weapon materials, components, and systems. With this information, program participants will be able to determine if and when these possible effects will impact weapon reliability, safety, or performance and thus will be able to anticipate needs for weapon refurbishment. Because the DOE weapons complex has been reduced in numbers of plants and personnel, the lead time necessary to manufacture critical components must be as long as is practical. Enhanced surveillance is crucial to providing the longest lead time the DOE complex can afford to provide.

Specifically, the program's goals are to predict component and material failure mechanisms; predict the service lives of materials, components, and overall systems; determine the feasibility of monitoring critical components in place, in real time, nondestructively; and develop diagnostics for failure mechanisms when time to failure cannot be adequately predicted.

Surveillance of Thermonuclear Weapons

The seven participating facilities are working on 110 tasks in three focus areas: primaries, secondaries, and nonnuclear components. Livermore has only minor involvement with project work related to nonnuclear components, which is Sandia's specialty. However, the Laboratory is heavily involved in the first two areas because its specialty has always been the development of primaries and secondaries, where the fission and fusion processes occur in a thermonuclear weapon. For the work at Livermore, Jeffrey Kass and John Kolb are leading a multidisciplinary team that includes physicists, engineers, materials specialists, and technicians from several directorates.

For weapon primaries, the Livermore team is evaluating changes that occur over time to the pit's special nuclear materials and to various types of high explosives. For example, plutonium irradiates itself and, given enough time, may change shape ever so slightly. Other tasks involve developing sensors, imaging devices, and diagnostic techniques for nondestructive evaluation of a primary. The team is also developing methods for studying the dynamic properties of primaries through small-scale testing.

Similar work is under way for weapon secondaries, characterizing materials in detail and developing material aging models to predict material life. Livermore staff are also developing diagnostic technologies to verify material and system predictability.

The Livermore project contributes to the work of the Surveillance Information Group, which includes representatives from all the DOE laboratories and plants. The

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Surveillance Information Group has conducted pilot projects in support of the DOE-wide Nuclear Weapons Information Group,[2] whose mission is to develop a secure, Web-based, electronic archive of old and new classified documents and other information on weapons design, production, and testing.

Nondestructive Evaluation

Livermore is leading a task to develop a technique called microextraction for nondestructive evaluation of the weapon primary. Microextraction is one of several technologies under development that will be used to determine how aging and the environment may affect the stability of a weapon's components.

Initial work with microextraction analyzed the primary's headspace gases. Studies show that primaries outgas at significant levels. To study these outgasses, Laboratory scientists exposed a microfiber coated with a solid-phase adsorbent to the weapon headspace gas to collect any chemical species. They then analyzed the microextraction fiber using gas chromatography and mass spectrometry. They have also developed methods to move the fiber as close to the weapon's purge valve as possible to permit essentially direct sampling of the weapon headspace and obtain more accurate data (Figure 1).

The Livermore team then characterized the material standards associated with various weapon systems. It found that many of the compounds absorbed in some high explosives may be traced to the use of other materials. For example, significant levels of toluene arise from its use as a solvent in the synthesis of the high explosive TATB. Data analysis thus far demonstrates that the outgassing and absorption processes observed on the core samples would not have significant effects on other materials in the near term because the outgassed species are nonreactive. The next step, which is still under way, is to complete an initial survey of systems and associated materials developed at Livermore.

Livermore is also leading an effort to implement microextraction to assess the aging of organics in closed environments. Valuable baseline information on new and aged weapons components has been obtained at DOE's Savannah River and Kansas City plants, with Livermore providing guidance on the effort.

Another task that Livermore is leading addresses modeling of material aging in the nuclear explosive package (NEP) of thermonuclear weapons. The NEP is a closed environment that contains exceptionally pristine and dry materials. It is enclosed in a can that prevents the interaction of the materials in the NEP with the outer atmosphere.

Livermore's goal is to develop a comprehensive computer model of the chemistry of this closed environment. Models are being developed of the interaction between the materials and between the materials and the gases left in the NEP during assembly. The time it will take for significant interaction to occur is important for the question of when these components will need to be refurbished or remanufactured.

The team is developing models for the reaction of gases with materials and for the diffusion of gases through the NEP. The reaction of gases with metals is a complicated process. Frequently, a layer of oxide on the metal causes the reaction to occur nonuniformly. As shown in Figure 2, a two-dimensional model demonstrates the pitting that may occur during this reaction.

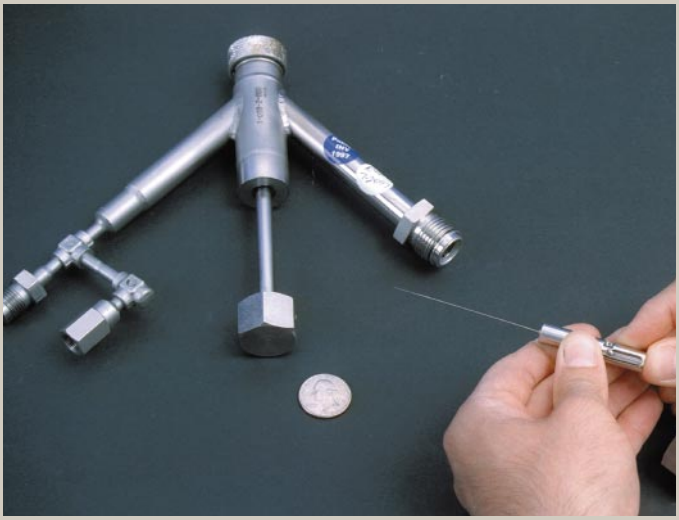

Figure 1. The relative size of the vacuum-tight microextractor assembly (left) and the coated microextraction fiber (right) compared to a quarter. The fiber is less than 400 micrometers in diameter.

These reaction models must be incorporated into a larger model of the transport and reaction of gases in the system. The Livermore team has begun to do just that using TOPAZ, one of the computer codes developed at the Laboratory for calculating the mechanical properties of materials. The team has demonstrated that TOPAZ, which was designed to model thermal diffusion, can be adapted to calculate gas transport through the NEP system when the grid for TOPAZ is carefully developed. Detailed models of the transport paths in the NEP have already been produced.

Continuing work for this task includes creating advanced gas–solid reaction models and, more important, modifying the computer code to include these models.

A Look Ahead

Work on the enhanced surveillance program continues. By about 2002 or 2003, DOE hopes to have in place the models and diagnostic tools it needs to determine when weapon components need replacement and ultimately to predict a weapon's safety, reliability, and lifespan. This knowledge will be significant for effective management of our nuclear arsenal.

—Katie Walter

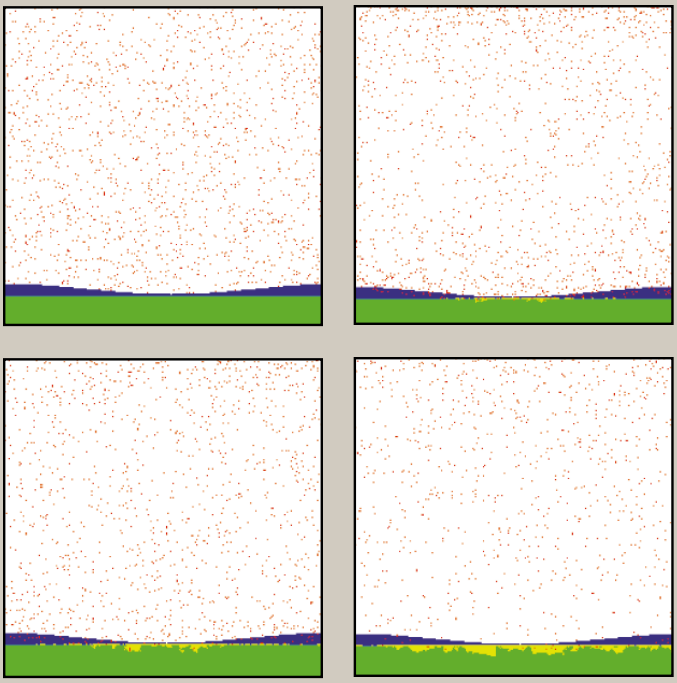

Figure 2. A two-dimensional model of the hydriding of a material surface inside a mock thermonuclear weapon's nuclear explosive package in the presence of a layer of oxide. Red particles represent hydrogen, the purple overlayer is metal oxide, green is pure metal, and yellow is the hydrided metal. The sequence is from left to right and top to bottom.

Key Words: diagnostics, enhanced stockpile surveillance, high explosives, nondestructive evaluation, nuclear explosive package (NEP), Nuclear Weapons Information Group, stockpile stewardship.

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1. For more information on science-based stockpile stewardship, see "Keeping the Nuclear Stockpile Safe, Secure, and Reliable," *Science & Technology Review*, Lawrence Livermore National Laboratory, Livermore, California, UCRL-52000-96-8 (August 1996), pp. 6–15.
2. See "Preserving Nuclear Weapons Information,"*Science & Technology Review*, Lawrence Livermore National Laboratory, Livermore, California, UCRL-52000-97-5 (May 1997), pp. 18–19.

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A New Precision Cutting Tool: The Femtosecond Laser

CHIRPED-pulse amplification strikes again. Using it in a high-peak-power mode, Laboratory scientists produced first the 100-terawatt laser and then the petawatt laser, opening up new opportunities for applying laser–matter interactions. Now a Livermore team has won an R&D 100 Award for applying chirped-pulse amplification in a high-average-power mode for cutting and machining materials. The system was developed for disassembling nuclear weapons components, but it has many other uses as well.

The team, led by Brent Stuart, illustrates Livermore's collaborative nature by combining research and development expertise from Laser Programs and Defense and Nuclear Technologies Directorates.

From Demilitarization to Dentistry

By ionizing the material being cut—removing it atom by atom—the cutting technique allows precise machining of everything from steel to tooth enamel to very soft materials like heart tissue. Each pulse of this machining system is extremely short, lasting just 50 to 1,000 femtoseconds (or quadrillionths of a second). These ultrashort pulses are too brief to transfer heat or shock to the material being cut, which means that cutting, drilling, and machining occur with virtually no damage to surrounding material. Furthermore, this revolutionary laser can cut with extreme precision, making hairline cuts in thick materials along a computer-generated path.

In dentistry applications, the thermal nature of the conventional laser ablation process can heat and crack a tooth and produce a random-shaped hole within a large area of collateral damage. In contrast, at the same ablation rate, Livermore's new laser precisely removes the material and leaves the surrounding areas in their original state (see a and b of the figure, p. 21).

The ultrashort-pulse laser represents a major advancement in cutting technology. Conventional lasers, diamond saws, and water jets are used commercially for a variety of cutting and machining applications. But each one has drawbacks. None of them can achieve the precision of the femtosecond laser machine tool (0.1 millimeters), and most of them damage surrounding material to varying degrees. Because of these shortcomings, no commercial cutting system can be used on the range of materials or applications of Livermore's new tool.

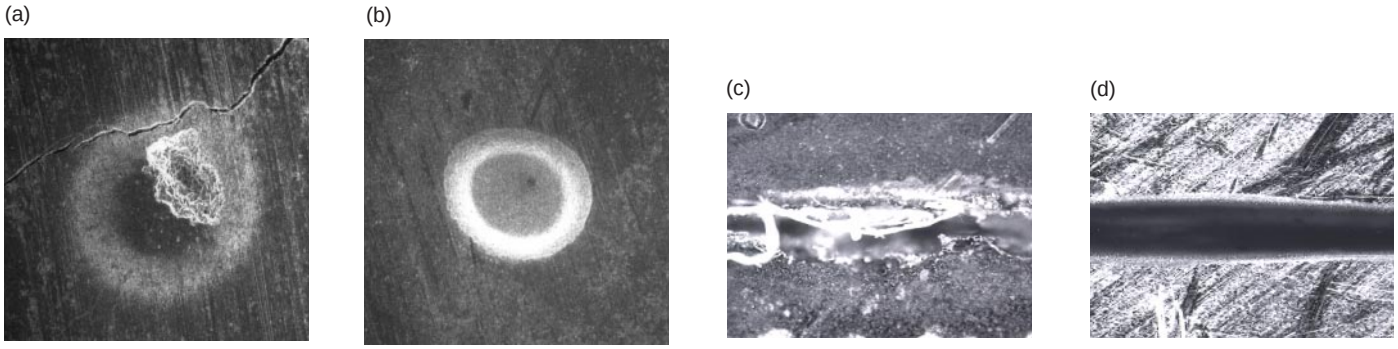
Industrial lasers, which melt and boil material to remove it, are often used in precision cutting. The heat and shock cause considerable damage to the area surrounding the cut that can range from changes in the grain structure to cracking. The damage may extend from a few micrometers to several millimeters from the cut, depending on the properties of the material, the laser pulse duration, and whether a cooling method is used. Very tiny structures only a few tens of micrometers in size, such as biological tissue or semiconductor devices, are extremely fragile. Even the slightest thermal stress or shock creates intolerable collateral damage.

These conventional cutting methods also leave slag around the cut. When material is vaporized, some of it is deposited on the walls or upper surface of the cut. This residue reduces the quality of the cut and the efficiency of the cutting system.

With each short pulse of the Laboratory's new laser cutter, material is heated to temperatures far beyond the boiling point, producing an ionized plasma, while leaving surrounding material cool. The pulse deposits its energy so quickly that it does not interact at all with the plume of vaporized material, which would distort and bend the incoming beam and produce a rough-edged cut. The plasma plume leaves the surface very rapidly, ensuring that it is well beyond the cut edges before the arrival of the next laser pulse. And because only a very thin layer of material is removed during each pulse of the laser, the cut surface is very smooth and does not require subsequent cleanup (see c and d of the figure, p. 21).

Removal of minimal amounts of material makes this new cutting system useful for processing extremely valuable or hazardous materials. If the cutting is done in a vacuum, better than 95% of the removed material can be recovered.

Another Livermore team is building a high-powered femtosecond machining system for the Department of Energy's Y-12 Plant at Oak Ridge, Tennessee, one of this country's primary manufacturers of nuclear weapon components. A second unit at Livermore will be used as engineering support to the Y-12 unit. The high precision of this cutter will maximize the plant's ability to reuse high-value components and minimize the amount of waste generated during the cutting process.



For cutting teeth, (a) a conventional laser cutter causes heating and cracking a result of large thermal stresses, while (b) the femtosecond cutter produces a clean hole with no collateral damage. In stainless steel, (c) a conventional infrared laser (wavelength of 1,053 nanometers) operating at a pulse duration of more than 1 nanosecond produced a jagged cut and much slag, but (d) Livermore's new cutter, with a pulse duration of 350 femtoseconds and the same wavelength, produced a clean cut with no slag.

Livermore is studying the use of the Femtosecond Laser to machine high explosives for experiments at its High Explosives Applications Facility. Because so little energy or mechanical shock is transferred to the part being machined, the team has demonstrated that materials such as high explosives or parts containing high explosives can be cut without danger of detonation. The team is also working on the design of a system for demilitarizing chemical weapons.

Other potential applications abound. Using the laser as a surgical tool for soft tissue has already been discussed in *Science & Technology Review* (October 1995, pp. 28–31). A semiconductor device producer is exploring the use of the unit for cutting high-value semiconductor wafers. Other major U.S. manufacturers are looking into incorporating femtosecond machining systems into their production lines. In manufacturing, new materials are constantly appearing, and the features on all kinds of devices are becoming smaller and smaller. The femtosecond machining system may be the most effective way to respond to both challenges with its high precision on all materials regardless of composition.

—Katie Walter

The team that developed the Femtosecond Laser includes (front) Paul Armstrong; (middle, left to right) Alexander Rubenchik, Hoang Nguyen, Steve Herman, and Brent Stuart; (back) Michael Feit, Booth Myers, Michael Perry, Joseph Sefcik, and Howard Powell (Paul Banks is not pictured).

Key Words: chirped-pulse amplification, demilitarization, femtosecond laser, laser surgery, R&D 100 Award.

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Commentary by E. Michael Campbell and Michael Anastasio

Superlasers as a Tool of Stockpile Stewardship

DRAMATIC changes in U.S. nuclear weapons policy have followed the end of the Cold War, among them halts to the development of new types of weapons and to weapon testing. The current stockpile must remain safe, secure, and reliable into the indefinite future as it undergoes changes caused by aging or remanufacturing and replacement of aging components. This challenge has led to the development by DOE of the Stockpile Stewardship and Management Program. Henceforth, confidence in America's nuclear arsenal will depend more than ever on our fundamental understanding of weapon science and technology. That understanding must now be pursued without recourse to system-level tests of integrated performance—the detonation of full-scale nuclear devices.

Scientists have turned to several tools, including advanced hydrotesting, subcritical experiments, advanced computer simulation and modeling, and what have come to be called superlasers, to address some of the remaining scientific issues. Nuclear detonations produce enormous total energy; no laboratory tool can deliver more than a small fraction of nuclear yield. But nuclear detonations also produce very high levels of energy per unit volume, that is, high energy density. High-power lasers can approach such high energy densities, even if only momentarily in very small spaces. Extremely powerful lasers can, in short, create microscopic versions of some important aspects of nuclear detonations, something available through no other experimental technique. They also can permit the production and study of fusion ignition in the laboratory.

As a result of superlasers and other laboratory tools, the study of high-energy-density physics can be moved from the Nevada Test Site to the laboratory, at least in part. Doing so can offer some real advantages. High-power lasers can support more frequent experiments than full-scale weapon testing could. They also offer more precise control of experimental conditions and greater access for detailed measurements; that is, the variables can, to some extent, be separated. These capabilities contribute significantly to the feasibility of stockpile stewardship and management.

The development of high-power lasers has enhanced the ability to pursue basic research on nuclear detonation. Since 1985, weapon scientists from various laboratories have used the Nova laser system to conduct more than 12,000 experiments. Even as Nova research continues, preparations are under way for its successor; the National Ignition Facility will become a cornerstone of DOE's Stockpile Stewardship and Management Program.

Although ten times more powerful and forty times more energetic than Nova, NIF will still produce total energies only a tiny fraction of those in full-scale nuclear detonations—total energy in the laser beams will be equivalent to a half pound of TNT, or one billionth of the energy of a nuclear weapon. Yet NIF will be able to approach much more closely than Nova the range of high energy-densities (and therefore temperatures) produced by nuclear weapons and necessary to achieve fusion ignition. With NIF, many of the fundamental processes of thermonuclear detonation become, for the first time, fully accessible to laboratory study and analysis. As a bonus, NIF will provide a unique means of testing nuclear weapon effects and a powerful new tool for basic science applications of high-energy-density physics (e.g., astrophysics, plasma physics, and fusion energy).

The next generation of superlasers, such as NIF in the United States and the French Laser MegaJoule (LMJ), will provide still more detailed understanding of the processes of nuclear detonation. It will enable scientists to gain a much improved understanding of the basic physics of nuclear weapons, greatly enhance their ability to predict weapon performance, and provide a sounder basis for assuring the safety and reliability of the nuclear stockpile.

■ E. Michael Campbell is Associate Director, Laser Programs.

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

Nova Laser Experiments and Stockpile Stewardship

Livermore's Nova laser is proving to be a powerful laboratory tool in support of DOE's Stockpile Stewardship and Management Program.

THERMONUCLEAR weapons are extremely complex devices, both in design and operation. When a nuclear weapon detonates, it initiates a chain of physical processes ranging from chemical explosion to thermonuclear burning, not all of which scientists understand in every detail. Although sophisticated computer programs model these processes, such models unavoidably require many approximations.

Until a few years ago, scientists could rely on nuclear tests to provide regular integral tests of a weapon's performance. Only by actually testing weapons did they obtain the experimental data against which to measure their physical models and computer codes. This approach worked extremely well, as long as scientists did not stray too far beyond the body of direct evidence. The match between data and calculation steadily improved, leading to increasingly good prediction of overall weapon performance, even though some phenomena remained less than completely understood. Under these circumstances, the laboratories could, with great confidence, certify the safety and reliability of the nuclear stockpile.

Circumstances have now changed. The unavailability of nuclear testing requires new approaches to assuring the safety and reliability of our nation's nuclear stockpile. Notably, there is greater reliance on computer codes, the accuracy of which must be evaluated against historical underground testing data and data provided by laboratory experiments.

In a variety of experimental facilities, scientists are addressing different aspects of nuclear explosions. In the laboratory, the highest energy-density conditions (that is, the highest levels of energy per unit volume) are obtained mainly through laser research on inertial confinement nuclear fusion. Over the years, Lawrence Livermore has designed a series of increasingly powerful lasers, culminating in the National Ignition Facility, now under construction.[1] NIF will be a neodymium–glass laser system with 192 beams. It will be capable of delivering as much as 3 to 4 million joules of laser energy in millimeter-scale or greater volumes in less than 10 billionths of a second in a variety of wavelengths, pulse lengths, and pulse shapes. At peak power, NIF will generate up to 750 trillion watts of laser light.

Although far less powerful than NIF, Lawrence Livermore's Nova laser is a very potent machine with over a decade's operation to demonstrate its enormous value.[2] It is a neodymium–glass laser with ten beams. Typically operating at a wavelength of 0.35 micrometers and 40,000 joules in 2.5-nanosecond pulses, Nova produces 16 trillion watts of laser light.

Nuclear detonations produce very high energy-density. High-power lasers like Nova can approach such high energy-densities, even if only momentarily in very small spaces. Extremely powerful lasers can, in short, create microscopic versions of some important aspects of nuclear detonations, something available through no other experimental technique.

Using Nova, scientists have been able to explore at least the lower reaches of the high-energy-density regime in which the physics of nuclear weapons poses the most unsolved problems.[3] Figure 1 depicts the Nova laser facility

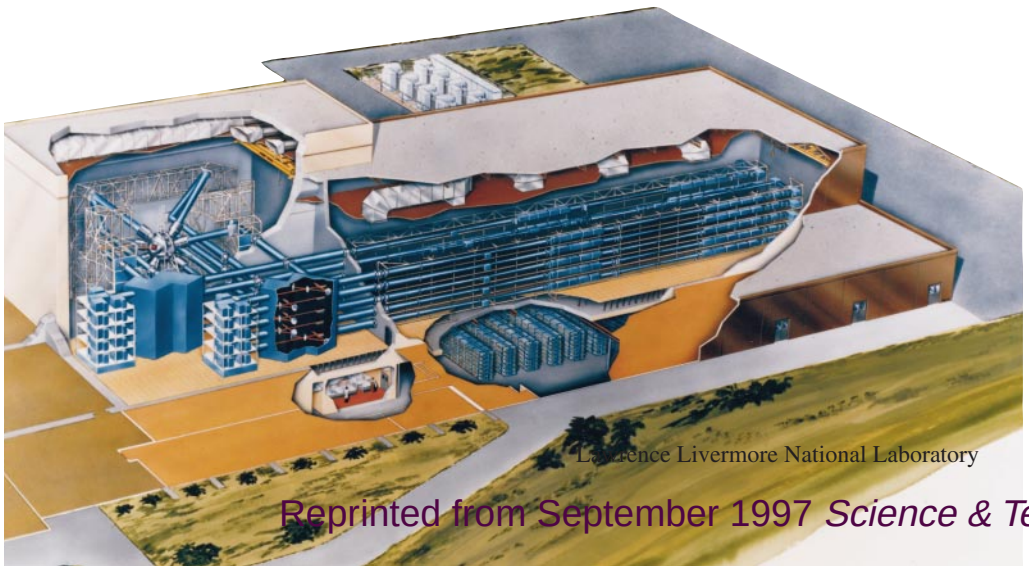

Figure 1. Cutaway view of Nova laser facility when it opened in 1985. The space frame (right) supports the ten-laser amplifier chains. A system of high-reflectivity mirrors ensures that the ten laser beams arrive simultaneously at the target, centered in the spherical chamber (left).

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in a cutaway view. Major optical components of a single Nova beamline are shown schematically in Figure 2.

Nova can produce the high energy-densities demanded by weapon physics experiments in two ways. Conceptually, the simplest is the method known as direct drive. All the laser beams focus directly onto the target, or physics package, in the target chamber. The absorbed energy delivers a strong shock to the target, compressing and heating it.

Although direct drive produces high energy-densities, this method has definite drawbacks. Simulating direct-drive experiments requires calculating the complex interaction of laser light with matter, an interaction not typically modeled in computer codes used for weapon design. Perhaps more significant are the high standards of laser uniformity and target fabrication required; even minor flaws of homogeneity or surface roughness may negate a direct-drive experiment. To avoid these problems, scientists have usually preferred to rely on an alternative method.

Instead of directly striking the target, the laser beams enter the open ends of a hohlraum, a hollow gold cylinder a few millimeters long (Figure 3). When the laser light strikes the inner walls of the hohlraum, they absorb the laser energy, which is transformed into an intense flux of x rays that heats the hohlraum and any sample it contains. Because the laser-generated x rays (rather than the laser energy itself) drive the experiment, this alternative mode of operation is known as indirect drive.

One advantage of the indirect-drive technique derives from the measurability and uniformity of the x-ray flux. The interaction of the uniform x-ray flux with matter also can be accurately modeled. Another advantage of indirect drive is the relative uniformity with which soft x rays heat a physics sample in a hohlraum. Figure 3 shows two views of a typical Nova hohlraum; Figure 4 is a rendering of the target chamber housing the tiny hohlraum.

Although significant progress has also been made for direct-drive experiments, Nova is not configured to exploit this concept. NIF is designed to handle both indirect- and direct-drive experiments.

Essentially, physics experiments on Nova address two basic phenomena: hydrodynamics and radiation. Hydrodynamics is the physics of the motion of fluid materials. Strongly influencing hydrodynamic phenomena is a property of matter termed equation of state—the relationship between a material's pressure, temperature, and volume.

Radiation studies center on the emission, transmission, and absorption of energy in hot dense plasmas. Experiments determine the x-ray opacity of various materials and how it varies with temperature and density. They also

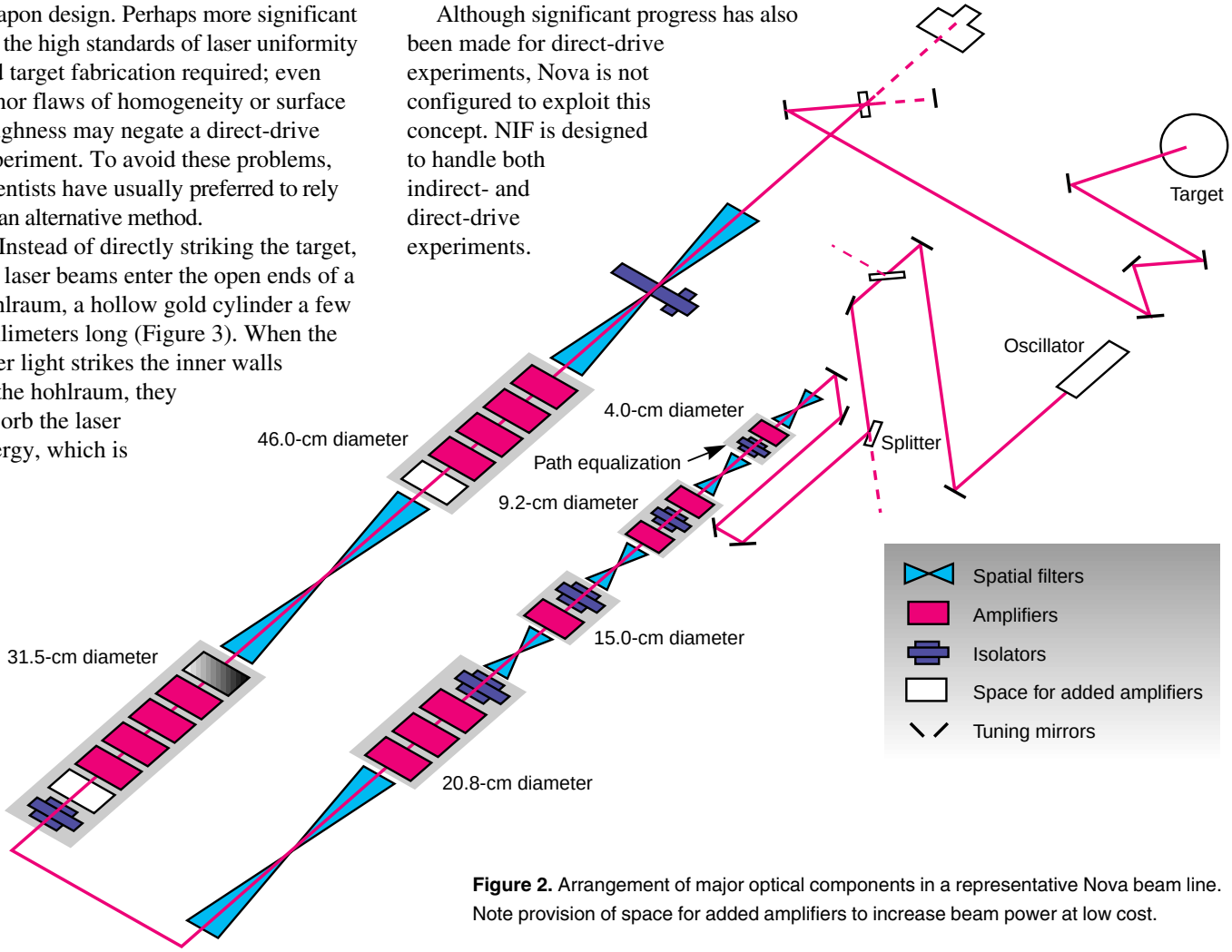

Figure 2. Arrangement of major optical components in a representative Nova beam line. Note provision of space for added amplifiers to increase beam power at low cost.

address radiative heat transfer as well as the interaction of radiation fields with matter, including the absorption and re-emission of radiation.

Shocking Matter

The basic science of nuclear detonations begins with learning how matter behaves at high energy-densities. To describe these conditions in a particular material, scientists rely on an equation of state, which mathematically expresses the thermodynamic relationship between the energy content of a mass of material, its volume, and its temperature. High-energy-density equations of state are fundamental in describing such phenomena as hydrodynamics and radiation transport; their fundamental importance also makes them crucial in understanding the operation of nuclear weapons.

Suddenly adding large amounts of energy to a material system creates intense sound or pressure waves, which become shock waves. Shock compression is a widely used method for experimentally determining equations of state at high pressures. An experiment begins with determining the initial pressure, volume, and energy of the material. Compressed by a single shock wave to greater pressure, the material's volume changes to a new state at higher density, temperature, and pressure.

By varying the shock strength in a series of experiments from the same starting conditions, scientists can obtain a set of pressure–volume pairs. They can then plot these pairs to produce the material's Hugoniot—that is, the mathematical curve relating the velocity of a single shock wave to the pressure, density, and total heat of the transmitting material before and after the shock wave passes. Because of its relative simplicity, the Hugoniot is the primary avenue for investigating a material's equation of state experimentally.

Each material possesses its own unique equation of state. No single valid model exists for the entire range of variables, which may cover many orders of magnitude in nuclear weapons operations. Thus, the equation of state for a particular material derives from models of limited scope for particular regimes of pressure, density, and temperature. These models are usually collected in a table of equation-of-state values that can be used in code calculations.

For nuclear detonations, the equation of state extends through two distinct regimes. In the early phase of implosion, before any significant nuclear yield, temperatures are relatively low and such factors as strength of material and chemical reaction are most significant. Scientists study this relatively low-energy-density regime through

(a) (b)

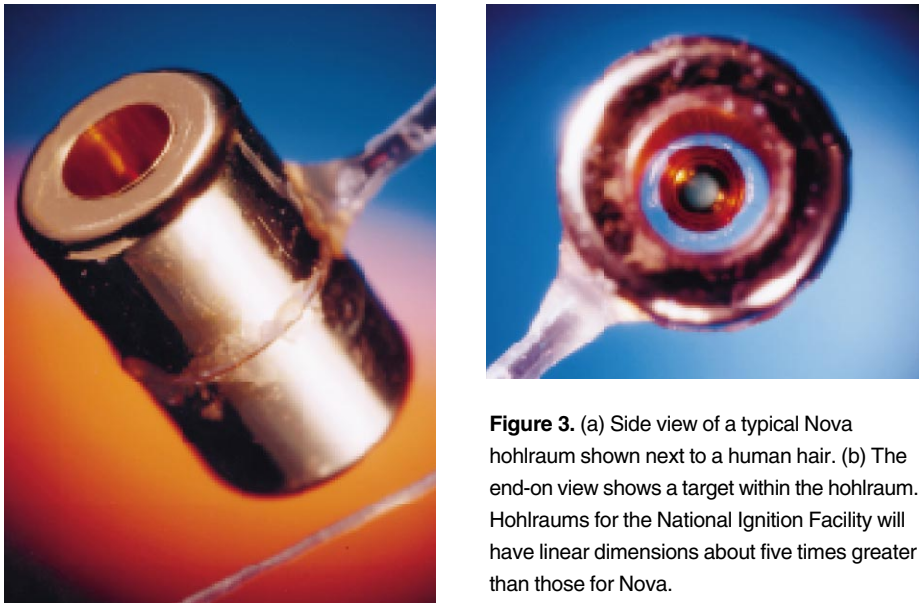

Figure 3. (a) Side view of a typical Nova hohlraum shown next to a human hair. (b) The end-on view shows a target within the hohlraum. Hohlraums for the National Ignition Facility will have linear dimensions about five times greater than those for Nova.

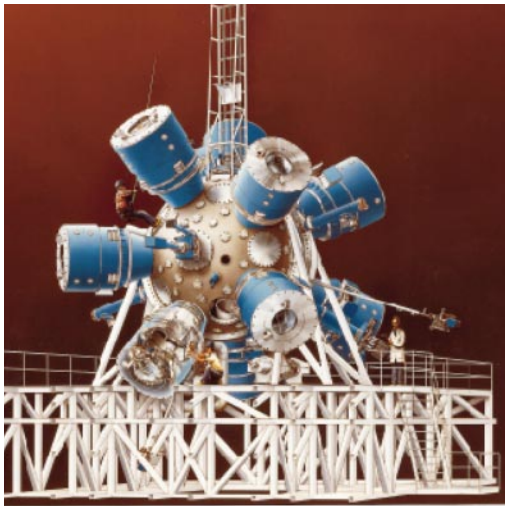

Figure 4. Artist's rendering of the outside of the Nova target chamber, where the ten laser beams converge to heat and shock a tiny hohlraum. Note the two human figures at work on the platform. The entire structure is three stories high, and the spherical target chamber is 4.5 meters (15 feet) in diameter.

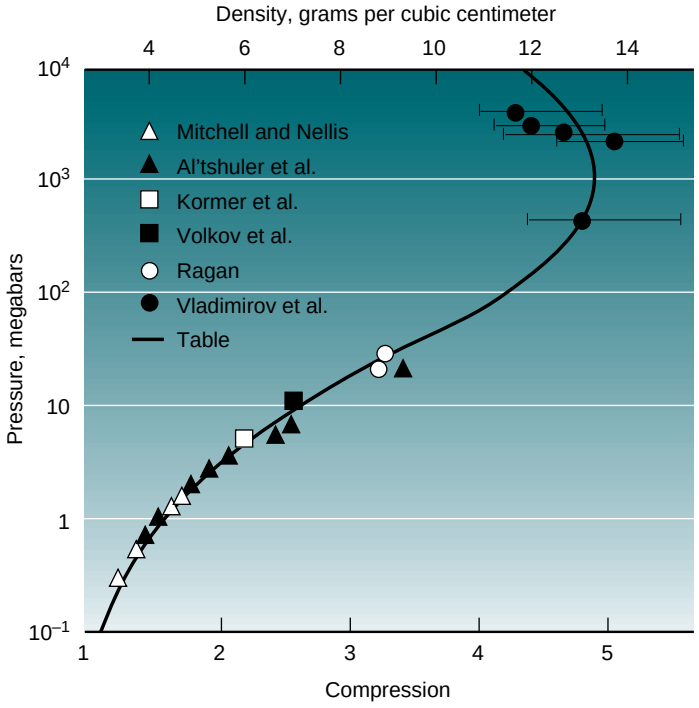

Figure 5. Comparison of experimental and theoretical shock Hugoniots of aluminum. The data points at the upper, highest pressure portion of the graph come from experiments conducted in Soviet nuclear weapons tests and reported in the open literature.

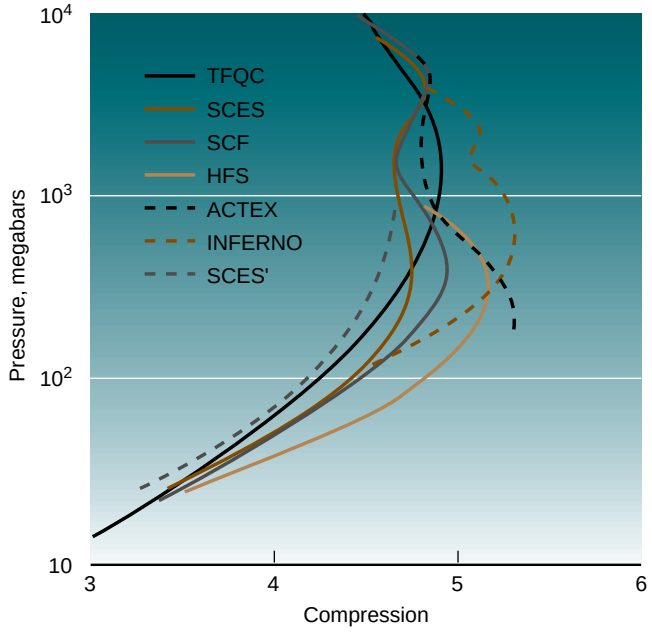

Figure 6. Calculations of the principal Hugoniot of aluminum using a variety of theoretical methods, plotted for high pressure and compression, where the various models exhibit differences: Thomas–Fermi model with quantum corrections (TFQC), semi-classical equation of state (SCES), self-consistent field (SCF), Hartree–Fock–Slater (HFS), ionization equilibrium plasma (ACTEX), INFERNO, and another version of the semi-classical equation of state (SCES').

experiments using high explosives or gas guns (essentially converted cannons), which in high-density materials can generate pressures up to a few megabars—that is, up to a few million times normal atmospheric pressure. Such data determine the lower end of the curve in Figure 5, which shows the Hugoniot of aluminum.

Vastly higher pressures, hundreds of megabars, characterize high-energy-density regimes, where scientists formerly acquired data only through nuclear tests. Data points at the upper end of the curve in Figure 5 come, with large uncertainties, from openly published work based on the Soviet underground nuclear test program. Because of insufficient experimental data, scientists must interpolate the intermediate portion of the curve and extrapolate to pressures beyond the data.

At multi-megabar pressures, neighboring atoms are packed so tightly as to disrupt each other's outermost electron shells. The resulting ionization caused by pressure absorbs large amounts of energy and makes the material more compressible. Various theories predict different curves, as Figure 6 illustrates for aluminum. Potentially, powerful lasers can provide experimental data to fill in the curve, not only for aluminum but for many other materials.

For each point on the Hugoniot, scientists must measure two quantities. One is usually the speed of the shock in the material. Another can be the speed to which the shocked material has been accelerated, the so-called particle speed. To measure shock-wave and particle speeds, scientists use a technique called x-ray backlighting. A shock can be driven into a material with a laser. A beam of x rays generated by a second laser with well-known and closely controlled characteristics illuminates the target from the side. Material changes caused by the shock wave absorb the x-ray backlight differently as it passes through the target. Captured on film, these differences provide the data required to compute points on the Hugoniot.

Nova Laser Experiments

To measure the principal Hugoniot, the target material at standard temperature and pressure is struck with single shocks of different strength. Measuring the thermodynamic states created when single shock waves pass through the target material gives scientists a set of data points that lie on the principal Hugoniot, which they can then plot. Figure 7 illustrates a recent Nova experiment to measure thermodynamic states. The target had two parts: a flat, very thin plastic "piston" and a wafer of the compound under study. Laser-generated x rays launched a strong shock, several tens of megabars, into the piston, sending a shock wave through the wafer.

Another measurement technique, impedance matching or shock breakout, relies on comparing shock velocities in a reference material of known characteristics (often aluminum) with those in a test sample. Laser-generated x rays or a laser-accelerated flyer plate shocks the target, which comprises precisely measured thicknesses (called steps) of the test sample alongside reference material.

Diagnostic instruments record the time it takes the shock wave to break through the opposite faces of the steps, thereby determining the shock speed in both materials. Comparing the test sample with the known standard yields information on the equation of state of the sample.

Uncertainties in important details can complicate interpretation of the results of equation-of-state experiments. Was an absolutely planar shock delivered to the target? Could electrons or radiation from the hohlraum have affected the target before the shock arrived? Despite such challenges, lasers offer the only path currently available for such investigations at pressures greater than 10 megabars, where many theoretical uncertainties linger.

Turbulent Fluid Movement

In contrast to the smooth, orderly behavior of fluids in laminar flow—as visible in a candle flame—rapidly moving fluids tend to become turbulent, the kind of chaotic, disordered state of flow seen in rocket exhausts. Turbulence in swiftly flowing fluids promotes their mixing, such as where fluids of different density border each other.

Scientists study three types of turbulent mixing observed in nuclear weapons: acceleration-induced, when a lighter fluid pushes against a denser fluid (known as the Rayleigh–Taylor instability); shock-induced, when a shock wave passes through the fluid interface (Richtmyer–Meshkov instability); and shear-induced, when two fluids in contact are moving relative to each other (Kelvin– Helmholtz instability). Turbulent mixing is a factor in understanding the operation of both the primaries and secondaries of nuclear weapons.

Experiments on Nova have begun to measure the growth of Rayleigh–Taylor instability in solids. Mounted in a hohlraum, a foil of copper or molybdenum is compressed and shocked while maintained below its melting point. Only after the drive ceases and the metal decompresses does the foil melt, and only then does Rayleigh–Taylor instability appear to develop normally. In other words, the strength of the compressed metal stabilizes the interface. These experiments are directly relevant to primaries, where materials retain strength throughout much of the explosion.

In the familiar low-energy-density world, most fluid flows behave as if incompressible. But weapon physics must deal with the compressible flows that exist under conditions of high energy-density. Understanding the effects of compressibility and radiation flow on hydrodynamic mixing is crucial. Compressibility alters density, affecting the evolution of perturbations and the behavior of mixing.

A recent Nova experiment has investigated turbulent mixing caused by shock-induced Richtmyer–Meshkov instabilities in an environment of high energy-density. The experimental package comprised a beryllium tube mounted perpendicularly to the side of a standard Nova hohlraum (Figure 8). Within the tube nearest the hohlraum was a plastic section, beyond which was a cylinder of low-density foam.

Rapidly heated to very high temperature by the focused laser beams, the hohlraum launched a shock into the plastic. Upon crossing the sawtooth-shaped interface between plastic and foam, the shock induced a mixing flow (Figure 9a). Experimental results agreed well both with simulations and a theoretical model (Figure 9b).

Figure 10 compares three-dimensional surface plots created from data from a recent Nova experiment with a three-dimensional simulation of the event created by the HYDRA three-dimensional simulation code.[4] Both representations

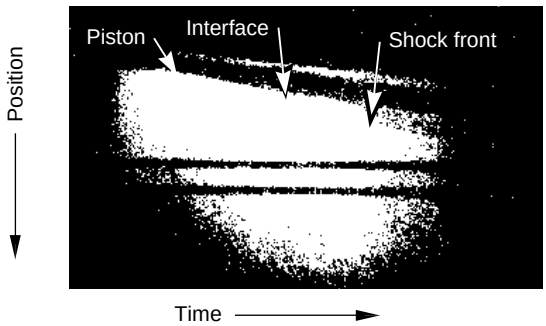

Figure 7. Initial results from an experiment using the Nova laser to measure the equation of state of a plastic. The time-resolved one-dimensional image shows the interface between a plastic piston (doped with bromine to make it opaque to the x-ray backlighter) and the undoped plastic sample being compressed . Note the shock front moving ahead in the plastic.

show a broad bubble surrounding narrow spikes, a shape characteristic of the nonlinear phase of the Rayleigh–Taylor instability. The HYDRA simulation reproduces not only the overall magnitude of the perturbation, but essentially all of the details of the shape, and demonstrates the Laboratory's unique ability to accurately model in three dimensions nonlinear aspects of high-energy-density experiments.

Other Nova experiments are under way, and still others are planned. Nova-class lasers can routinely achieve extreme accelerations, pressures of hundreds of megabars, rapid growth of turbulence, great compression, and high levels of radiation flow and ionization. Powerful lasers can, within certain limits, produce energy-densities that approximate a very-small-scale nuclear detonation.

Opacity and X-Ray Transport

Materials vary in the degree to which they absorb and re-emit radiation of given wavelengths under given conditions, directly affecting the passage of radiation through them. The material's opacity is defined as the measure of how easily it can transmit radiation. Because x rays transport much of the energy in a nuclear weapon, weapon physics is concerned particularly with opacities at x-ray wavelengths.

In the high-temperature plasmas created by nuclear detonation, atoms become highly ionized and the number of possible atomic transitions grows very large. The complicated interaction of radiation with these complex ions makes opacity hard to calculate and forces scientists to rely on approximations. To test such approximations, they have conducted experiments on many different materials at various temperatures and densities. Comparing these data with code calculations can then improve both physical models and computer simulations of opacity.

Because opacity varies rapidly with sample conditions, experiments demand accurate measurement not only of opacity but also of temperature and density. Scientists can obtain such highly precise measurements only if the sample's temperature and density are spatially uniform. Over the past several years, they have devised techniques for doing so within laser-produced plasmas. In a typical experiment, an opacity sample doped with a tracer material with a low atomic number (e.g., aluminum) is sandwiched between layers of plastic and put into a hohlraum. Laser-generated x rays heat and ionize the sample. Constrained by the plastic, the sample expands uniformly and so maintains a constant density.

X-ray backlighting, basically similar to backlighting techniques described earlier, probes the target to provide the required measurements. Two x-ray backlight sources are used. X rays from one backlighter pass through the sample to an x-ray spectrometer, which measures the transmitted spectrum to give the opacity. An experimental setup is shown schematically in Figure 11. The spectrometer also records the absorption spectrum of the tracer material. From the degree of tracer ionization, the sample's temperature can be determined to better than 5% accuracy. The other backlighter illuminates the sample from the side, allowing the width of the expanding sample to be measured and its density to be computed. Figure 12 compares opacity data obtained with the Nova laser with results obtained using a new opacity code.

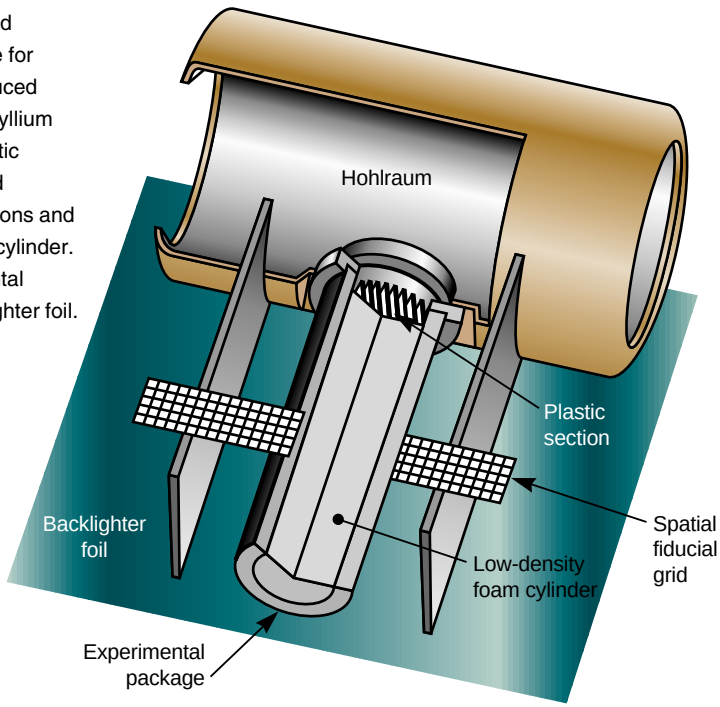

Figure 8. Cutaway view of the hohlraum and attached experimental package for measuring shock-induced mixing. Within the beryllium shock tube is the plastic section with machined sawtoothed perturbations and the low-density foam cylinder. Behind the experimental package is the backlighter foil.

Other Nova Experiments

Opacity alone will not suffice to calculate radiative processes in a weapon. Scientists also require detailed physical models of heat transport and must understand interactions between radiation and matter. Radiative heat and particle transport experiments truly of value to weapon scientists working on stockpile stewardship demand more laser energy than Nova can furnish. Preliminary experiments on Nova, however, have

helped develop research techniques and increase understanding of the basic physics in this area.

In one type of experiment, a thin opaque foil replaces part of the hohlraum wall. Laser-generated x rays inside the hohlraum blow off the foil's inside surface, driving a shock back into the foil. The shock traverses the foil and breaks out its back surface. An ultraviolet telescope, coupled with an optical streak camera, is focused on the foil's back side to measure the time of shock breakout, from which the temperature inside the hohlraum can be inferred.

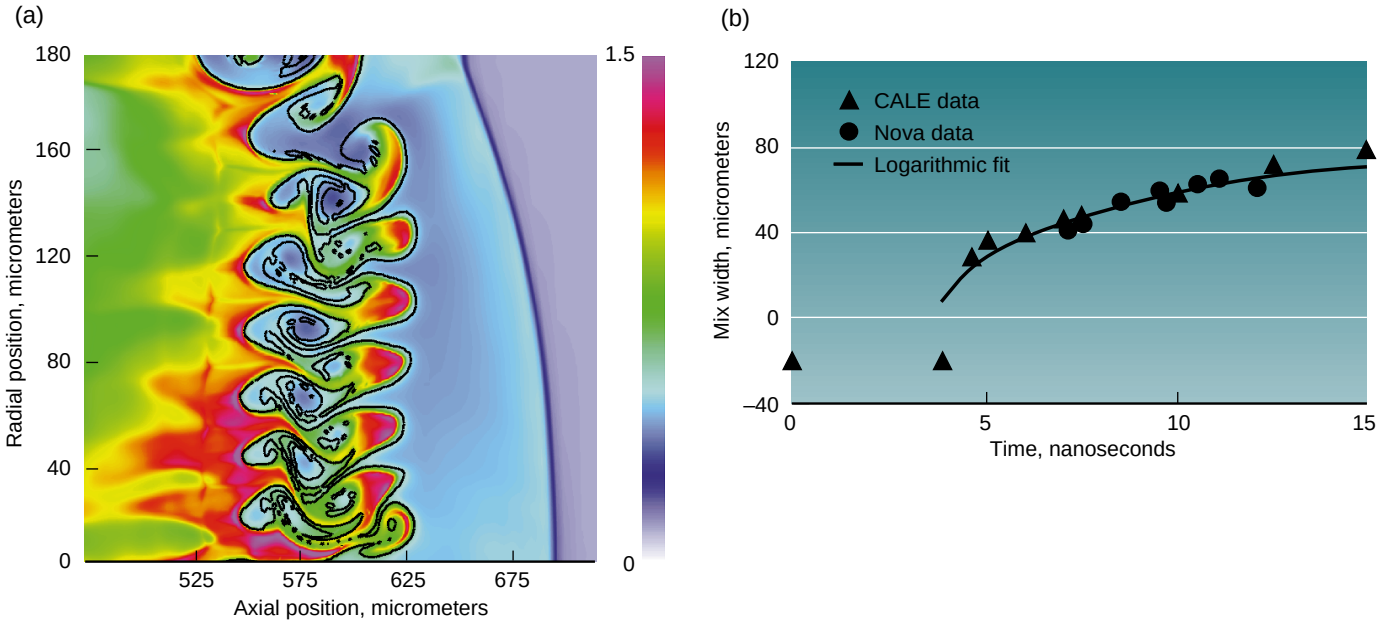

Figure 9. (a) Mixing flow showing density and material contours 7.5 nanoseconds after shock delivery, as modeled by the two-dimensional CALE computer code. (The bar to the right is the logarithm of density.) (b) The width of the mixing region evolves logarithmically with time. The circles represent measured widths from Nova experiments; the triangles represent data points calculated using the CALE code. Good agreement between experimental data and numerical simulation promotes confidence in the code.

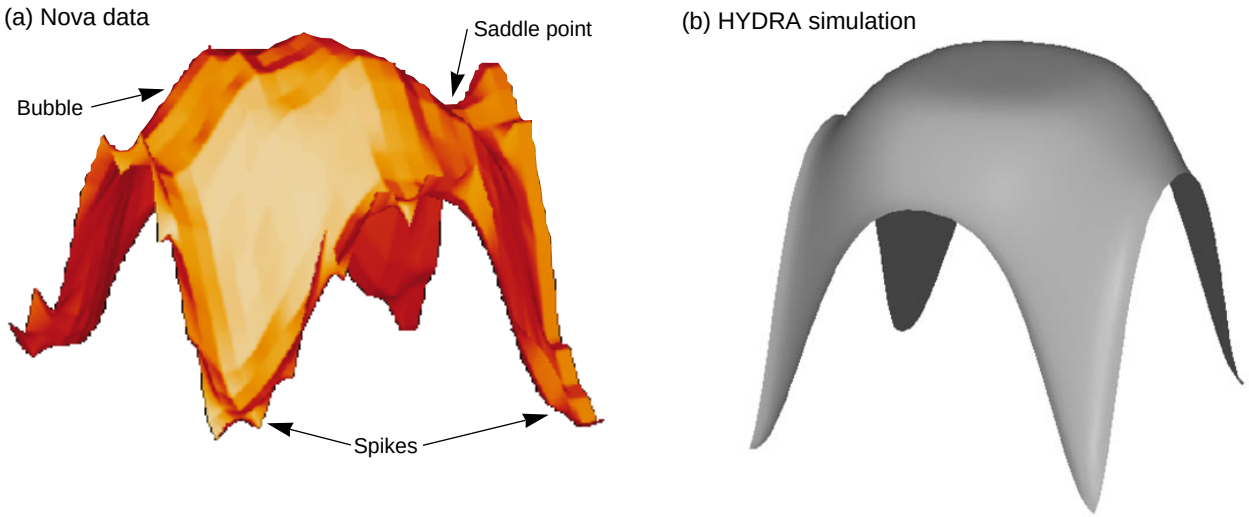

Figure 10. Comparison of (a) the three-dimensional surface plot of data from a Nova experiment 4.3 nanoseconds after shock delivery with (b) a three-dimensional simulation of theat event using the HYDRA computer code shows an excellent correlation between experimental data and code calculation.

The radiation field inside the hohlraum also drives a radiative heat wave through the shocked foil material. The breakout of this heat wave on the foil's back side is recorded by a streak camera. By using different types and thicknesses of foils, scientists can attempt to understand the different effects of opacity, temperature drive, and radiative heat transport.

In a similar type of experiment, a thick sample of low-density foam replaces the thin foil. At low enough densities, the heat front will precede the shock front, permitting scientists to study heat transport through unshocked material. This type of experiment also allows viewing the sample from the side; x-ray backlighting techniques allow the shock position through the sample to be measured as a function of time. This technique gives a great deal more information than the simple shock breakout experiment.

Not all physics experiments fall neatly into the categories of radiation and hydrodynamics. Some are designed to be so complex that they must be modeled with computer codes that take into account the full range of hydrodynamic and radiative processes that would formerly have been involved in a nuclear test. These so-called integrated experiments are intended to validate the integrated physical model and to test the scientist's ability to model extremely complex behavior. Other experiments supported by the weapons program aim at developing diagnostic techniques. Still others are directed toward enhanced understanding of basic science.

One set of experiments that began as basic scientific inquiry resulted in a very useful diagnostic tool—x-ray lasers. Intense brightness, narrow bandwidth, small source size, and short pulses give x-ray lasers many advantages over conventional x-ray illumination devices as imaging systems for experiments not only in physics, but also in inertial confinement fusion and biomedicine.

The Value of NIF

Over a decade of operation has proved the Nova laser's value in studying weapon physics. Nova experiments have already helped improve computer codes through

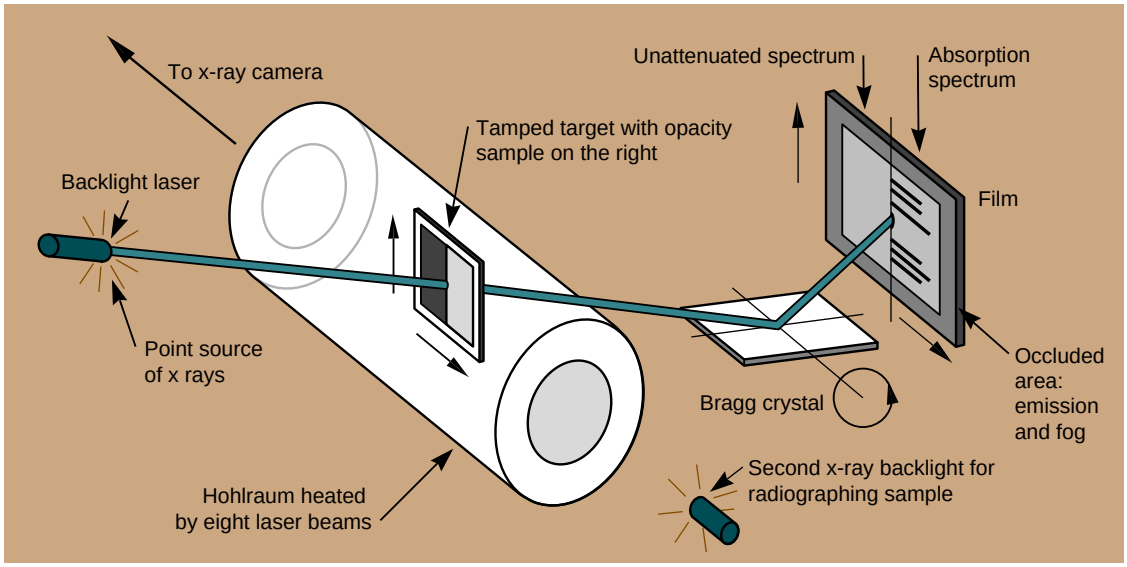

Figure 11. Schematic of point-projection spectroscopy for opacity measurements. The laser-produced backlight x rays are imaged after passing through the target. The image is spatially and spectrally resolved by a Bragg crystal, while temporal resolution is provided by backlight duration.

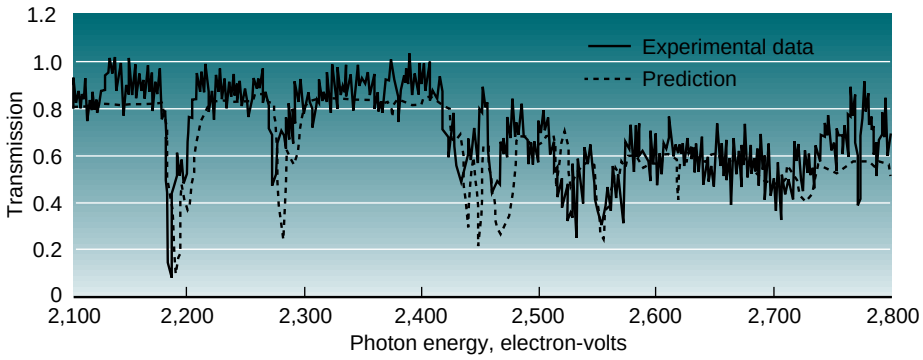

Figure 12. Experimental opacity data compared with calculations. The solid line shows measured x-ray transmission through a niobium sample. The dashed line shows the similar results calculated using an opacity code recently developed at Livermore. Good agreement with experimental data bolsters confidence in the opacity calculations and their underlying theory.

better knowledge of processes like turbulent mixing and properties like x-ray opacity. In the future, such experimentally based knowledge will matter even more. The ability to tie these experimental data back to the simulation codes is crucial for stockpile stewardship.

When nuclear testing was an option, scientists' inability to calculate every detail precisely hardly mattered. They could determine what happened by diagnosing an actual detonation. With that option gone, however, the ability to calculate the effects of each detail, some not calculated at all in the past, assumes major importance. Doing so requires new computer codes, which must then be verified by experiment.

Useful though Nova has been, it lacks the power to meet the future data needs of nuclear weapons scientists. Its energy comes up short in some aspect of every research area. In equation-of-state experiments, Nova cannot reach high enough pressures. In hydrodynamic instability experiments, it cannot follow instabilities long enough. In x-ray opacity experiments, it cannot attain high enough temperatures. In radiative heat transport experiments, it falls short in temperature and cannot drive the radiation far enough. Overcoming these limits will become possible with the National Ignition Facility.

Although more powerful lasers like NIF will open wider vistas on weapon physics, they remain some years away. Meanwhile, Nova experiments have already provided laboratory access to physical phenomena once thought obtainable only by full-scale nuclear tests. With field-testing ended, they have enabled scientists from all the weapons laboratories to continue improving codes through enhanced knowledge of such basic processes as equations of state, mixing, and radiation opacity.

In coming years, Nova will continue to demonstrate, as it has for more than a decade, that in studying the physics of nuclear detonation, powerful lasers can, at least in part, provide code validation data formerly derived from underground nuclear tests.

—Bart Hacker

Key Words: equation of state, Hugoniot, hydrodynamic instability, National Ignition Facility (NIF), Nova laser, opacity, radiative heat transfer, Stockpile Stewardship and Management Program, weapons physics.

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About the Scientists

TED PERRY holds a B.S. in mathematics and physics and an M.S. in mathematics from Utah State University. He also did graduate work at Princeton University, where he received an M.A. and Ph.D. in physics. He joined Lawrence Livermore National Laboratory in 1981, and between 1981 and 1991, he worked in the nuclear test program at the Laboratory, performing experiments on seven underground nuclear tests. In 1991, he became one of the program leaders for weapons physics experiments in A Division of the Defense and Nuclear Technologies Directorate. His recent work has focused on weapon physics experiments using the Nova laser. He received the Department of Energy's Excellence in Weapons Research Award in 1985 and 1994.

BRUCE REMINGTON received a B.S. in mathematics from Northern Michigan University in 1975 and a Ph.D. in physics from Michigan State University in 1986. He joined the Laboratory as a postdoctoral associate in 1986 doing nuclear physics research and became a permanent staff physicist in the Laser Programs Directorate in 1988. Currently as leader of the hydrodynamics group of the Inertial Confinement Fusion Program, he initiates and manages direct- and indirect-drive hydrodynamics experiments on the Nova laser related to high- energy-density regimes, compressed solid-state regimes, fluid dynamics, and astrophysics.

Transforming Explosive Art into Science

For centuries, intuition and trial and error dominated the development of high explosives. Now, high-explosives researchers at Lawrence Livermore are imposing more rigorous scientific structure and techniques upon their work.

FEW products typically take years of effort to synthesize yet disintegrate in a few millionths of a second when used. Despite their brief lifespan, energetic materials, particularly high explosives, are in demand as never before by the Department of Energy, Department of Defense, and industry for their unique properties: shock waves producing pressure up to 500,000 times that of Earth's atmosphere, detonation waves traveling at 10 kilometers per second, temperatures soaring to 5,500 kelvin, and power approaching 20 billion watts per square centimeter.

Explosives have been around since Chinese gunpowders appeared during the 11th century. However, until the past 15 years, their development has been characterized by an approach based largely on intuition and trial and error. Now high-explosives scientists are imposing more rigorous scientific structure and techniques upon all aspects of their work.

Lawrence Livermore National Laboratory

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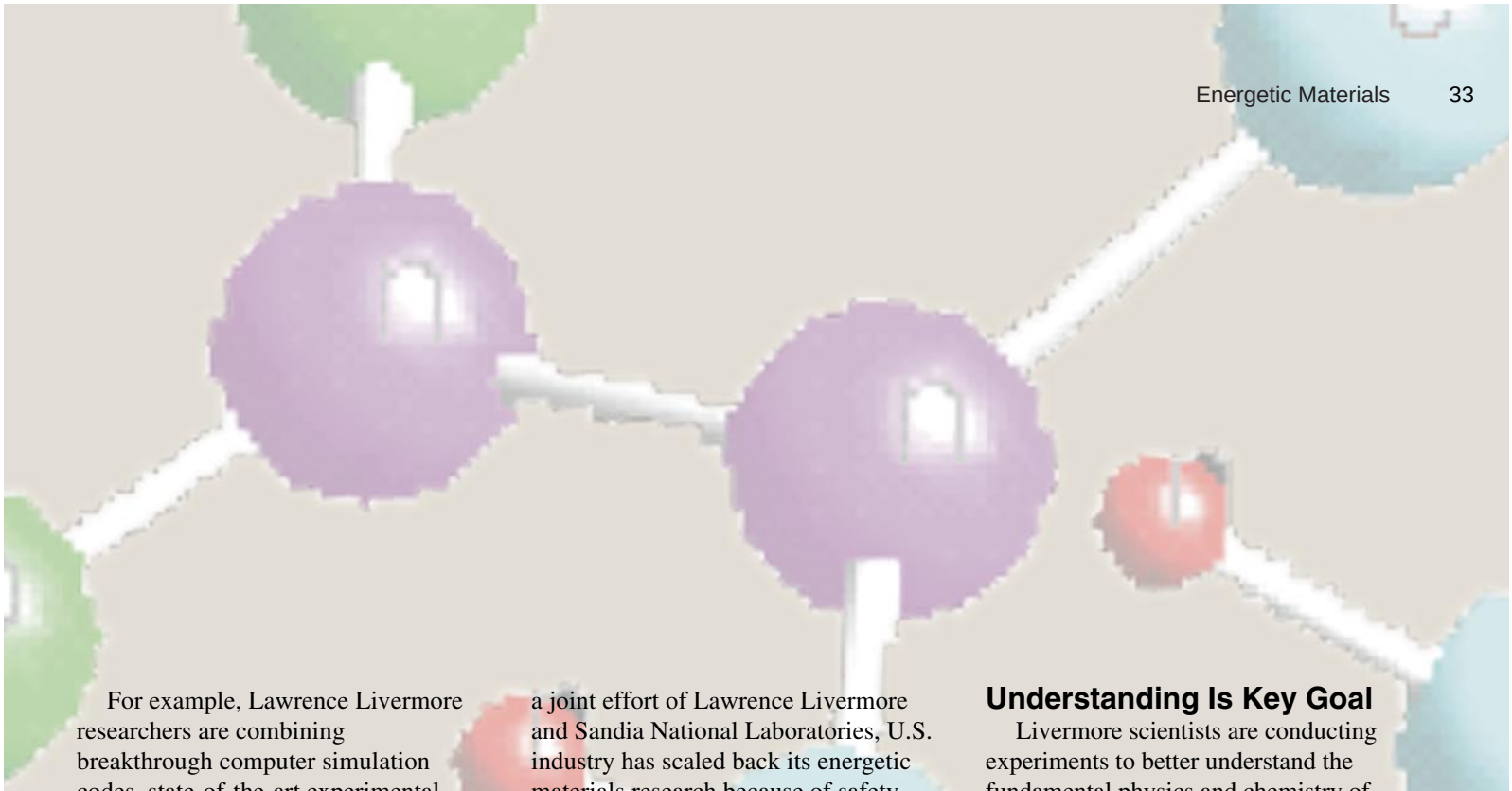


For example, Lawrence Livermore researchers are combining breakthrough computer simulation codes, state-of-the-art experimental diagnostics, and a culture in which theoretical, synthesis, and experimental chemists and physicists work alongside each other. At the same time, they are working more closely with their partners in the energetic materials community, from DOE's Pantex Plant in Texas to the Air Force's Wright Laboratory at Eglin Air Force Base, Florida, to small explosives companies in the San Francisco Bay Area.

Advances in energetic materials, which include high explosives, propellants, and pyrotechnics, benefit DOE's Office of Defense Programs, DoD's warheads and propulsion efforts (especially the 12-year-old DOE/DoD "Memorandum of Understanding on Conventional Munitions"), NASA's space exploration programs, the Federal Aviation Agency's explosive detection efforts, and many industries, including mining, oil exploration, and automobile. The continuing demand is driving a search for better theoretical models of the behavior of energetic materials and an improved diagnostic capability to measure the complex chemical and hydrodynamic processes during detonation.

According to Ron Atkins, director of the Energetic Materials Center (EMC), a joint effort of Lawrence Livermore and Sandia National Laboratories, U.S. industry has scaled back its energetic materials research because of safety and financial considerations. Likewise, the Department of Defense's own energetic materials research faces significant budget pressures, while academia does not have the costly facilities to carry out such research. As a result, says Atkins, "the national labs are becoming the country's most important repository of energetic materials expertise." Atkins is heading a task force representing several Livermore directorates in work to ensure that the Laboratory will remain a national resource for energetic materials expertise over the next decade and beyond.

Livermore researchers have studied and synthesized high explosives for decades because they are an integral element of every nuclear weapon. Today, under the EMC umbrella, their work encompasses a wide range of basic research and programmatic activities. Lawrence Livermore chemists are synthesizing new compounds that yield more energy, are safer to store and handle, and are less expensive and more environmentally friendly to produce. They also are designing new paths to synthesizing existing energetic molecules that are cheaper and easier on the environment.

Understanding Is Key Goal

Livermore scientists are conducting experiments to better understand the fundamental physics and chemistry of energetic materials, particularly with regard to their stability, sensitivity, and performance. "Despite a century of work, scientists still do not understand what happens in a detonation wave thoroughly enough to predict all the details of how a given explosive will behave under various conditions," says Randy Simpson, head of the Energetic Materials Section in the Chemistry and Materials Science Directorate.

Simpson and his colleagues are also involved in fundamental surveillance activities associated with the maintenance of the nation's nuclear weapons stockpile. Performance and safety testing (see *Science & Technology Review*, December 1996, pp. 12–17) assures that the high explosives in nuclear warheads will remain dependable despite decades of storage. Another aspect of stockpile stewardship work is developing safe and environmentally sound methods for dismantling and disposing of thousands of kilograms of high explosives removed from retired nuclear weapons. Going a step further, Livermore chemists are investigating processes that would permit the reuse of these high-quality, expensive materials in the commercial marketplace.

Table 1. Codes used in developing energetic materials.

Code	Function
ALE3D	Hydrodynamic code used in safety analyses such as "cookoff" simulations spanning a remarkably wide time span. (Developed at LLNL.)
CHEETAH	Transforms predicted formation energy and density of molecules into performance measures such as detonation velocity, pressure, energy, impulse, and impetus. (Developed at LLNL.)
GAUSSIAN	Determines the three-dimensional shape of the molecule and the energy binding its atoms.
MOLPAK	Packs molecules together into a low-energy configuration.
TOPAZCHEM, PALM	Predict changes in thermal and chemical properties caused by different accident, battlefield, and aging scenarios. (Developed at LLNL.)

Guiding all of these activities are computer codes that mimic energetic materials and the very rapid physical and chemical processes that govern their detonation (Table 1). The codes reflect longstanding Livermore expertise in simulating extremely short-lived events such as nuclear detonations. Continually refined by experimental data, the codes are paving the way for an unprecedented understanding of energetic materials at the molecular level.

The work is headquartered in the High Explosives Applications Facility (HEAF) at Livermore, which represents the state of the art in high-explosives research with regard to both technical capability and safety (Figure 1). Work at HEAF is complemented by activities some 15 miles away at Site 300, where large-scale high-explosives processing and testing are carried out.

Searching for New Materials

Simpson notes that in a world accustomed to daily announcements of important scientific advances, breakthrough high-energetic materials

Figure 1. (above) Livermore's High Explosives Applications Facility (HEAF), completed in 1989, is playing a major role in developing and characterizing high explosives. (right) Specially designed containment vessels are used to safely detonate high explosives in quantities as large as 10 kilograms of TNT-equivalent.

have been few despite steady progress in explosive power and insensitivity over the past century. The last energetic material to "hit it big" was HMX (cyclo-tetramethylene-tetranitramine), discovered during World War II as a contaminant in a batch of another explosive material. Since then, Simpson says, there have been TATB (triamino-trinitrobenzene, a highly insensitive high explosive for nuclear weapons) during the 1970s and a few specialty materials, but certainly nothing used as widely as TNT (trinitrotoluene) (Table 2).

The reason for the paucity of new energetic materials is the fact that they must meet so many different requirements such as high energy density, insensitivity to mechanical insults, resistance to chemical decomposition, inexpensive synthesis from readily available reagents, and the ability to be formulated with other materials for fabrication into practical devices.

Despite the difficult requirements, Livermore chemists are optimistic that they can improve the safety and performance of current and future weapons systems. It is a balancing act because the compounds must be powerful enough to do the job and at the same time insensitive enough to prevent accidental explosion. For some applications, the priority is on improving safety, especially with nuclear weapons and with explosives stored on ships.

For other applications, higher power and energy are of greatest interest. (Energy is the capacity of an explosive to do work, whereas power is the rate of energy release, or how rapidly the explosive can accelerate metal. Energy is measured in joules, power in joules per second.) In this area, several new Livermore explosives have been developed for Air Force weapons directed at penetrating "hard targets" such as underground reinforced concrete bunkers. In the same performance arena, smaller shaped charges using Livermore formulations are demonstrating velocities up to 10 kilometers per second to penetrate thick steel armor plate some 6 to 8 times the diameter of the shaped charge.

Developing new energetic materials is a complicated process in which many candidate molecules are considered, a few synthesized, even fewer formulated, and only a small handful adopted by the military or industry. The laborious process involves computer modeling, plenty of laboratory work, and thorough testing.

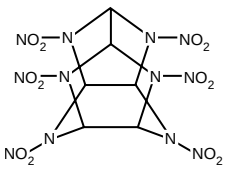
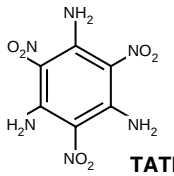
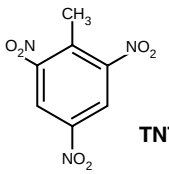
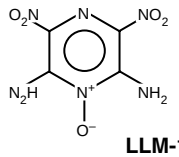
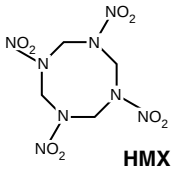
Starting at the Chalkboard

The road to a new high explosive begins the old-fashioned way, when candidate molecules are drawn on a chalkboard by both theoretical and synthesis chemists. Theoretical chemists tend to suggest more "flamboyant" molecules than the synthesis chemists because they have less experience in the laboratory, quips theoretical chemist Larry Fried. Once a group of candidates is agreed upon, Fried and his colleagues take over, screening the molecules with a host of computer codes.

The codes help guide the synthesis chemists by predicting the inherent characteristics of the cyber-compounds. Fried says the process is similar to that found in the pharmaceutical industry. In that business, too, trial and error and human hunches used to be predominant, but now sophisticated computers are helping to point the way to prime-candidate molecules for synthesis.

Livermore high-end workstations do simulations with the speed that approaches a supercomputer's. The software program GAUSSIAN (used widely in the chemical and pharmaceutical industries) is first

Table 2. Molecular structure of important energetic materials.

Material	Molecular Structures
TNT (trinitrotoluene) HMX (cyclo-tetramethylene-tetranitramine), TATB (triamino-trinitrobenzene) LX-19 (2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane, which is CL-20, plus a polymer binder) LLM-105 (2,6-diamino-3,5-dinitropyrazine-1-oxide)	 **CL-20 in LX-19**  **TATB**  **TNT**  **LLM-105**  **HMX**

employed to determine the three-dimensional shape of the molecule and the energy binding its atoms. The molecules are then "packed together" into a low-energy configuration for greatest stability by another widely used program called MOLPAK.

Finally, CHEETAH transforms the molecules' predicted thermodynamic energy and density into explosive performance measures such as detonation velocity, pressure, and energy (Figure 2). CHEETAH, developed by Fried and his colleagues, is a thermochemistry code derived from more than 40 years of experiments on high explosives at Livermore. With libraries of hundreds of reactants and 6,000 products in its code, the program is now used throughout the world and has become DOD's preferred code for designing new explosives and, to a lesser extent, propellants and pyrotechnics (see *Science & Technology Review*, June 1996, pp. 6–13). The capabilities of the massively parallel computers in DOE's Accelerated Strategic Computing Initiative (ASCI) at the Laboratory are being used to assist with modeling the hydrodynamics of candidate explosives, and plans call for ASCI's use in creating advanced predictive models of the chemical reactions that occur when candidate molecules explode.

Assuming the software programs validate the chemists' premise that the candidate molecule offers significant potential, the material is ready to be synthesized.

Synthesis Can Be Tough

While it takes about one week to screen a candidate molecule by computer, its actual synthesis in the laboratory can require a year or even longer of painstaking effort.

"It takes a lot of trial and error to get the synthesis reactions to go," says organic chemist Phil Pagoria (Figure 3). "The chemist must constantly evaluate whether the project is progressing or whether the molecule, as planned, is impossible. It is an iterative process, depending largely on the knowledge, abilities, and intuition of the chemist. Many times, a synthesis scheme cannot be considered for full-scale production because it ultimately requires too many steps or reagents that are too costly."

Much of the synthesis effort is devoted to developing new energetic materials that possess an energy density (the energy that can be released from a specified volume of material) at least 15% greater than that of HMX, the high-energy high explosive against which candidate materials have long been evaluated. HMX replacements are needed for a host of volume-fixed armaments such as so-called smart, or precision-guided, munitions.

Many have been developed at Livermore. One formulation, LX-19, is the highest power material in the world but somewhat more sensitive than

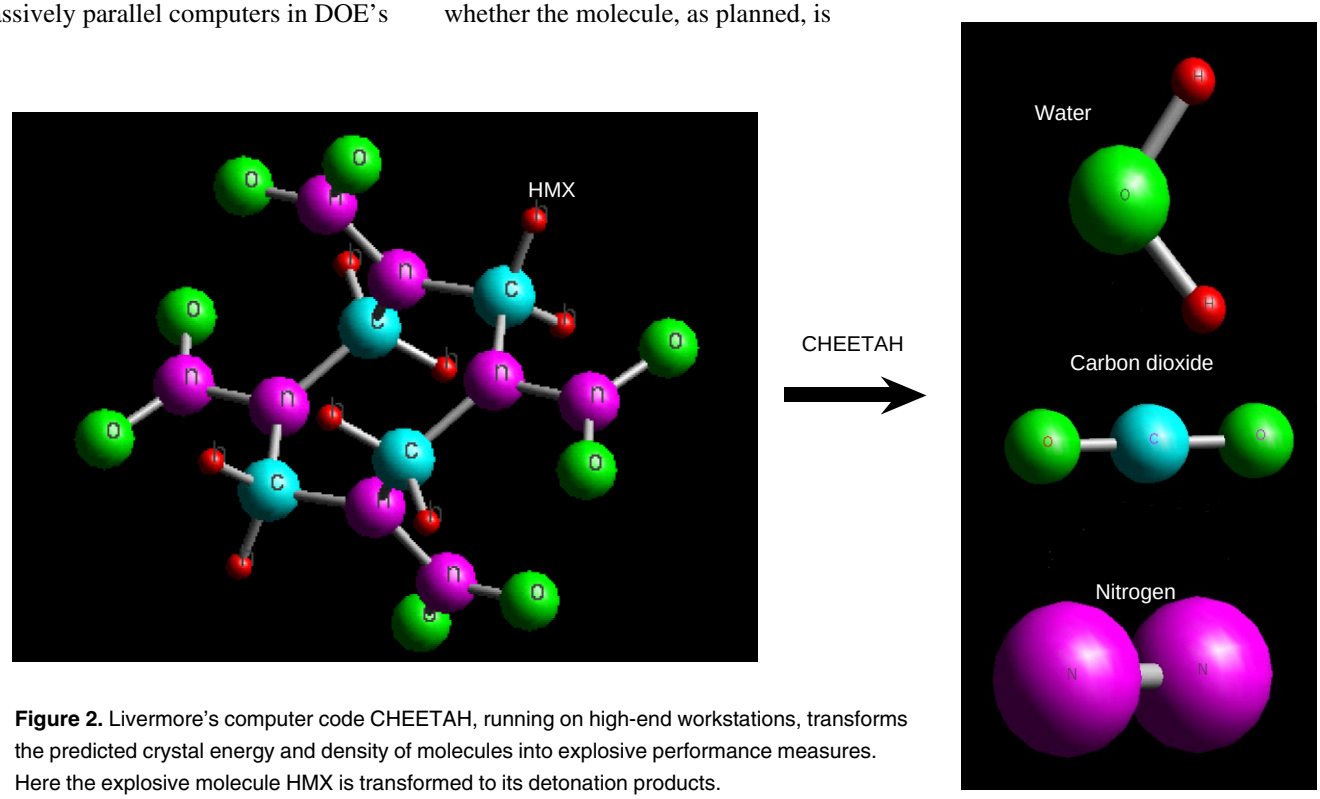


Figure 2. Livermore's computer code CHEETAH, running on high-end workstations, transforms the predicted crystal energy and density of molecules into explosive performance measures. Here the explosive molecule HMX is transformed to its detonation products.

HMX-based materials.* LX-19 is based on CL-20 (developed at the Naval Weapons Center, China Lake, California). Working with the Navy, Livermore experts determined many of the characteristics of CL-20 and performed the first scale-up to kilogram quantities at the Laboratory's Site 300 test area.

A similar effort is aimed at synthesizing materials with more energy than TNT, the best known high explosive in the world and one that offers less power (but better sensitivity) than HMX. For this effort, Livermore has synthesized LLM-105, an insensitive energetic material with 60% more energy than TNT. The new material is under evaluation by Ron Lee and his colleagues in Livermore's Defense and Nuclear Technologies Directorate.

In the process of developing new compounds and more efficient pathways for synthesizing existing compounds, the synthesis group has developed an innovative and cost-effective approach called the VNS (vicarious nucleophilic substitution) method for producing TATB. The procedure eliminates the need for chlorinated compounds, which have adverse environmental effects. (See the November 1996 *Science & Technology Review*, pp. 21–23.) Livermore and DOE's Pantex Plant recently began a four-year effort to apply the VNS method in order to establish a lower-cost industrial supply of TATB.

Once a few grams of a material have been synthesized, they are passed on to experimental chemists for a battery of safety tests (Figures 4 and 5). The tests determine the material's sensitivity to

Figure 3. Organic chemist Phil Pagoria synthesizes a new high-energetic compound inside a glovebox to guard against unwanted moisture.

Figure 4. Scientific Associate Chet Lee measures the burn rate of a high explosive under high pressure, a standard safety test.

Figure 5. Chemist Rosalind Swansiger remotely controls a performance test of a promising high explosive.

* Experimental molecules are designated by an LLM number for Lawrence Livermore molecule. Experimental formulations are designated by an RX number for research explosive. Once the material is in production, it acquires an LX designation for Livermore explosive. DoD experimental munitions receive an XM number.

impact, heat, friction, electrostatic discharge, and shock. Most candidate materials fail at this point. Those that pass are sent on to other chemists for incorporation in a mixture of ingredients called a formulation. Simpson acknowledges that the process is "still largely an art" but adds that it is becoming "more precisely scientific all the time."

A World of Tradeoffs

Formulating high explosives for unique applications may require a medley of ingredients, including energetic crystalline powders, energetic liquids, inorganic oxides, metals, and binders such as thermoplastics, thermosets, and gels. The binder, which takes up as little as 2% and as much as 40% of the volume, can serve several purposes: it can make the explosive easier to fabricate into useful shapes, aid in desensitization to shock, or modify the high explosive's performance characteristics.

Formulations chemist Mark Hoffman acknowledges the role of artistry in arriving at a sound formulation but notes that Livermore people can tap 45 years' worth of experience with high explosives. Much of the artistry is spent juggling the tradeoffs among sensitivity, performance, and cost. As a formulation increases insensitivity to explosion (for safety considerations, for example), performance typically suffers. Hoffman notes: "It does no good to have a weapon on board a tank that does not possess enough power to destroy or incapacitate an opposing tank. But it's inappropriate to carry a weapon that's so sensitive that it explodes in response to a few bumps in the road."

Formulators work closely with other chemists, who can quickly obtain safety and performance measurements using different quantities of a formulation. With as little as 1 to 2 grams, chemists can only perform critical safety tests. With 50-gram quantities, they can evaluate how well the ingredients of a formulation come together to form the new explosive. As formulations are scaled up to kilogram quantities, important tests of performance, thermal

Spotlight on Safety

The very destructive power of high explosives places a premium on all aspects of their safety, including manufacture, transportation, storage, and handling. Likewise, much of Lawrence Livermore's high-explosives work involves determining the sensitivity of existing high explosives and rocket propellants to fire, accident, and terrorist attack.

Safety has also come under the purview of computer codes. "We would like to do predictions of safety at the start of the development process, much as we determine other characteristics of candidate molecules," says theoretical chemist Larry Fried, who is exploring using the widespread computer code GAUSSIAN to determine how much energy it takes to break a molecular bond as an indicator of sensitivity to accidental detonation. He is also exploring the conversion of intermolecular phonons (quanta of vibration energy) to intramolecular vibrational states as part of a computational model that could eliminate inherently unstable molecules from consideration before they are synthesized.

Fellow theoretical chemist Al Nichols has been working with computational scientists from the Defense and Nuclear Technologies Directorate to transform ALE3D, a three-dimensional hydrodynamic, explosive-safety code developed at Livermore (see figure on p. 11). With the ALE3D team, Nichols has added thermal and chemical capabilities to the code so it can answer safety questions about high explosives, in particular a stringent military thermal safety test called "cookoff." Thanks to ALE3D, Livermore is the first research center to simulate cookoff by depicting a remarkably wide time span. The code models deformations in a heated explosive device from the time they begin at the rate of millimeters per day to the instant of explosion when deformation rates increase to kilometers per second.

Safety efforts include working with the Air Force on its missile propellants. One study, a part of the Titan IV program, is looking at the safety ramifications of solid propellant falling from an errant rocket launch, as happened earlier this year when an Air Force Delta rocket blew up at Cape Canaveral, Florida, raining propellant down on the ground below. Another study concerns the propellants of the Air Force Minuteman III missile.

In performing the safety studies, says experimental chemical engineer Jon Maienschein, Livermore chemists are doing business differently by modeling every experiment before it is conducted. In that respect, says Energetic Materials Section leader Randy Simpson, Livermore scientists do a smaller number of experiments than are done at other sites, but they thoroughly instrument each one and precede major experiments with computer simulations.

Maienschein notes that Livermore personnel are working more closely with colleagues and sponsors in DoD. "Both they and we recognize that we can do more by teaming up with each other." The process, he says, encourages creative thinking about, for example, a new generation of transducer-based systems that continuously monitor important safety data such as temperature in high explosives.

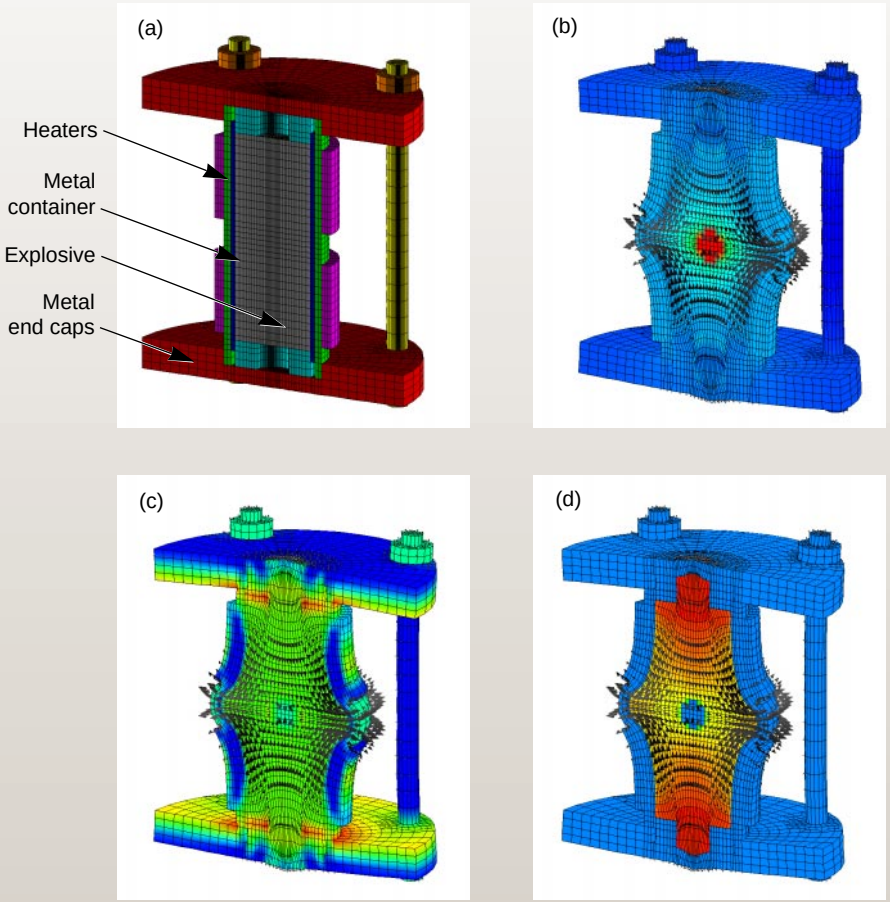
Energetic Materials Center Director Ron Atkins notes that in a world of diminished federal outlays, collaboration is clearly the way to achieve important advances with the greatest cost-efficiency. "We're working hard to build bridges to the armed services, DOE centers like the Pantex Plant in Texas, and other national labs," he says.

stability, and mechanical and physical properties assist designers in evaluating a formulation and determining appropriate use in specific devices. Chemical reactivity tests, for example, identify incompatibilities between device components and a formulation. Because a major objective in formulation is incorporation of the formulated explosive into a device, any possible incompatibility between device components and the formulation must be corrected early.

Atkins notes that obtaining accurate data from experiments at the extreme temperature, pressure, and time regimes of high explosives presents enormous challenges. Many of the tests use diagnostic tools originally developed for underground nuclear weapons tests at the Nevada Test Site. Others were developed more recently. One such tool is the multibeam Fabry–Perot velocimeter, designed by Livermore scientists (July 1996 *Science & Technology Review*, pp. 12–19). This device provides high-resolution, continuous velocity data about the behavior of materials traveling up to 3,000 meters per second. With the multibeam system now producing more meaningful data about the power of explosives—the rate at which they are capable of releasing energy—modeling codes become increasingly accurate. The device also allows more efficient use of budgeted funds because one experiment provides many sets of velocity data, thus taking the place of five separate experiments.

Computer simulations have also strengthened formulation activity and testing. CHEETAH is once again called into play, this time to suggest how the various formulation ingredients will affect performance. In addition, TOPAZCHEM-2D/3D, PALM, and more recently, the ALE3D code (see box, below) augment safety testing by predicting changes in thermal and chemical properties caused by different accident, battlefield, and aging scenarios.

Encouraging results from experiments and computer simulations lead to still



The ALE3D computer code is capable of simulating a "cookoff" safety test by modeling the rate of deformations in a slowly heated high explosive over a wide time span. (a) A model of the test at setup. The high explosive is encased in steel and aluminum and bolted between two metal end caps. Heaters surround the metal container and heat the 7.6-centimeter-tall device at the rate of 3.3°C per hour. (b), (c), and (d) are snapshots of the simulation of the material's deformation as a function of (respectively) temperature, pressure, and chemical change after 50 hours of heating. ALE3D simulations such as this tell energetic-materials scientists in great detail and in slow motion how, when, and with what violence new high-explosive compounds deform when burned. In (b), (c), and (d), the velocity of deformation is 80 meters per second.

larger-scale formulations of 400 grams or greater done at Site 300. When the material properties are optimized, the formulation process is developed for scale-up to production quantities for final technology transfer.

Livermore chemists are also working to improve efficiencies in the production world. They are exploring the use of injection molding equipment much like that used to make plastic toy parts. Such machines could be ideal for making shaped charges, which typically contain a number of complex folds that are difficult to fashion using standard production machinery (Figure 6).

Leaving the Iron Age

Simpson describes the Iron Age as a time when builders were limited to a few

Figure 6. At Site 300 facilities, injection-moldable explosives are developed as part of an effort to enhance production methods. (a) Mark Hoffman formulates a moldable high explosive. (b) Hoffman and Kirk Pederson pour the explosive to a transfer funnel, from which it is poured into a deaerator–loader. (c) Frank Garcia operates the deaerator–loader to remove air from the explosive before loading it into the explosive device. (d) Mike Kumpf displays the finished precision explosive device.

metals for construction. Now builders have a host of different materials from which to choose. "We're leaving the Iron Age of energetic materials because military planners are no longer limited to TNT and HMX," he says. "We're seeing specific new materials for specific military applications."

The driving force is the ascendancy of smart munitions. Because these weapons routinely hit their targets, small improvements in the lethality of the warheads can significantly increase their effectiveness. What's more, fewer and smaller munitions mean that more expensive energetic materials may be used.

As part of this new effort, Livermore chemists are working with the Navy to adapt LX-19 and similar CL-20 formulations to the military's XM-80 program. Multiple small submunitions, each containing about 10 grams of explosives, will be grouped in shells and shot out of Navy guns. Capable of traveling long distances, the shells, which have a propulsion system guided by global positioning satellites, will accurately destroy enemy fortifications.

Simpson is confident that computer codes will continue to become more sophisticated so that a code such as ALE3D will be used as a design tool to model safety elements of energetic devices as diverse as rockets or automobile air bags. It is a safe bet that with other aspects of high explosives, as well, Livermore researchers will play a large part in the new age of high explosives.

—Arnie Heller

Key Words: ALE3D, CHEETAH, Fabry–Perot velocimeter, GAUSSIAN, high explosives, High Explosives Applications Facility (HEAF), HMX (cyclo-tetramethylene-tetranitramine), MOLPAK, PALM, stockpile stewardship, TATB (triamino-trinitrobenzene), TNT (trinitrotoluene), TOPAZCHEM.

For further information contact Randall Simpson (925) 423-0379 (simpson5@llnl.gov).

About the Scientists

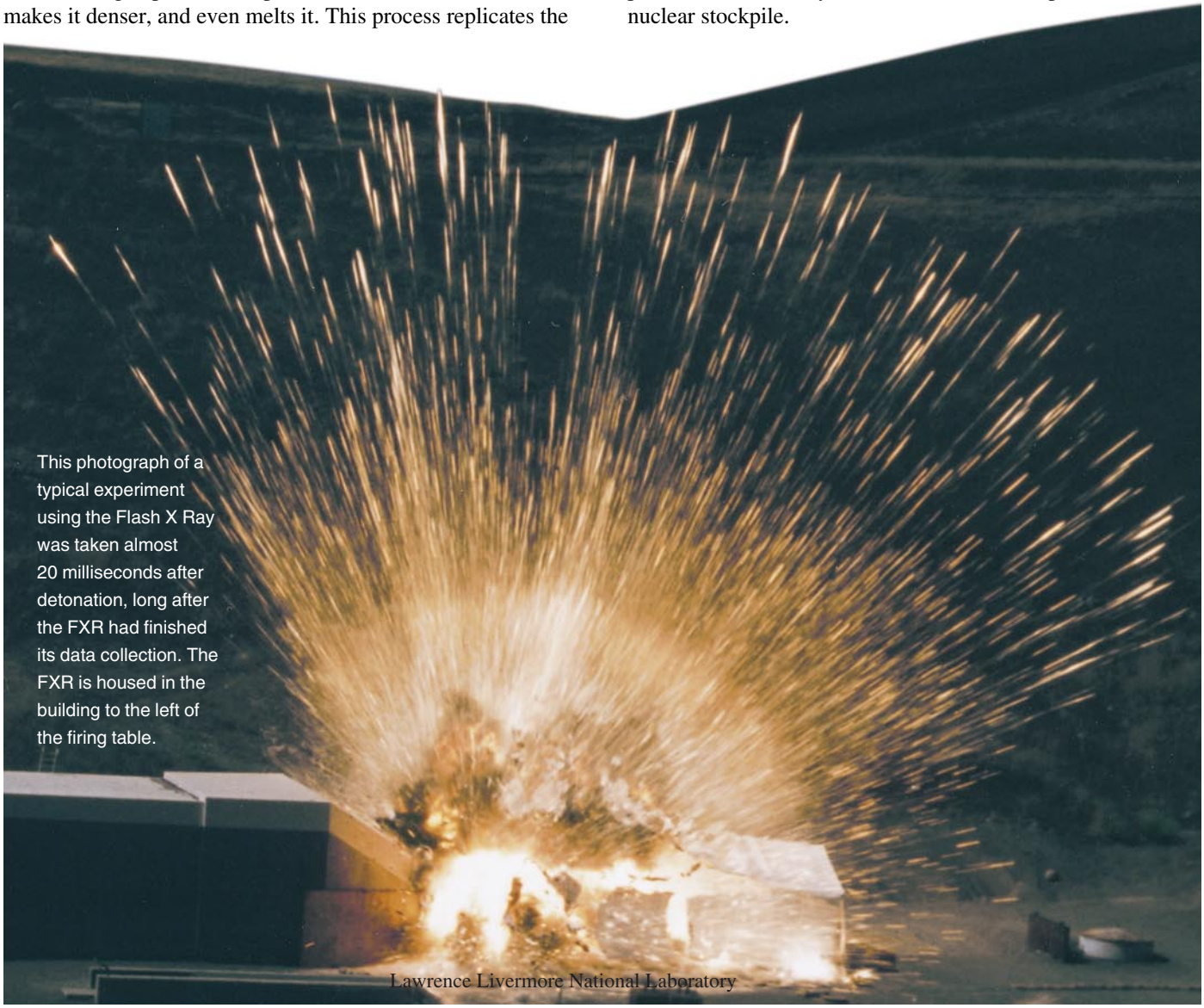
The research, development, and testing of new energetic materials done at the Laboratory's High Explosives Applications Facility is, like all science done at Livermore, a multidisciplinary team effort. In this instance, the team members operate under the auspices of the Energetic Materials Center (EMC), sponsored jointly by Lawrence Livermore and Sandia national laboratories. Chief contributors to the new science of high explosives being done at Livermore are (left to right): ALBERT NICHOLS, a theoretical chemist currently working to model safety aspects of high explosives used in nuclear and defense applications; RANDALL SIMPSON, an experimental chemist who develops new energetic materials and characterizes their initiation and detonation properties; RONALD ATKINS, director of the EMC and coordinator of the team's work; RONALD LEE, a physicist who develops new explosive initiation systems; JON MAIENSCHEIN, an experimental chemical engineer involved in computer simulations of the safety of energetic materials before their testing; MARK HOFFMAN, a formulations chemist responsible for formulating high explosives for unique applications within strict safety, performance, and compatibility guidelines; LAWRENCE FRIED, a theoretical chemist who screens candidate high-explosives molecules using advanced computer codes; and PHILIP PAGORIA, an organic chemist, who is expert in synthesizing new high-energetic compounds.

Better Flash Radiography Using the FXR

IMAGINE a very powerful x-ray machine, several billion times more powerful than the one your dentist aims at your jaw. X rays can penetrate more than a foot of steel and record the motion of materials moving at ultrahigh speeds, making it an excellent tool for peering into the interior of a nuclear weapon's imploding primary stage.

Non-nuclear hydrodynamic experiments reveal the behavior of a nuclear weapon from ignition to the beginning of the nuclear chain reaction. These experiments consist of wrapping inert (nonfissile) material in a high explosive that is then detonated. The resulting explosive compression deforms the material, makes it denser, and even melts it. This process replicates the effects in the core of a nuclear device. High-speed radiographic images of the implosion process are taken with the powerful x-ray machine known as the Flash X Ray, or FXR, which was developed by scientists at Lawrence Livermore National Laboratory in the early 1980s'.

Data from the FXR's x-ray images are used to verify and normalize Livermore's computer models of device implosions. In the absence of nuclear testing, scientists must rely on these computer calculations to develop the judgment necessary to certify the safety and reliability of nuclear weapons, a critical part of the Laboratory's role in the stewardship of our nation's nuclear stockpile.



This photograph of a typical experiment using the Flash X Ray was taken almost 20 milliseconds after detonation, long after the FXR had finished its data collection. The FXR is housed in the building to the left of the firing table.

Lawrence Livermore National Laboratory

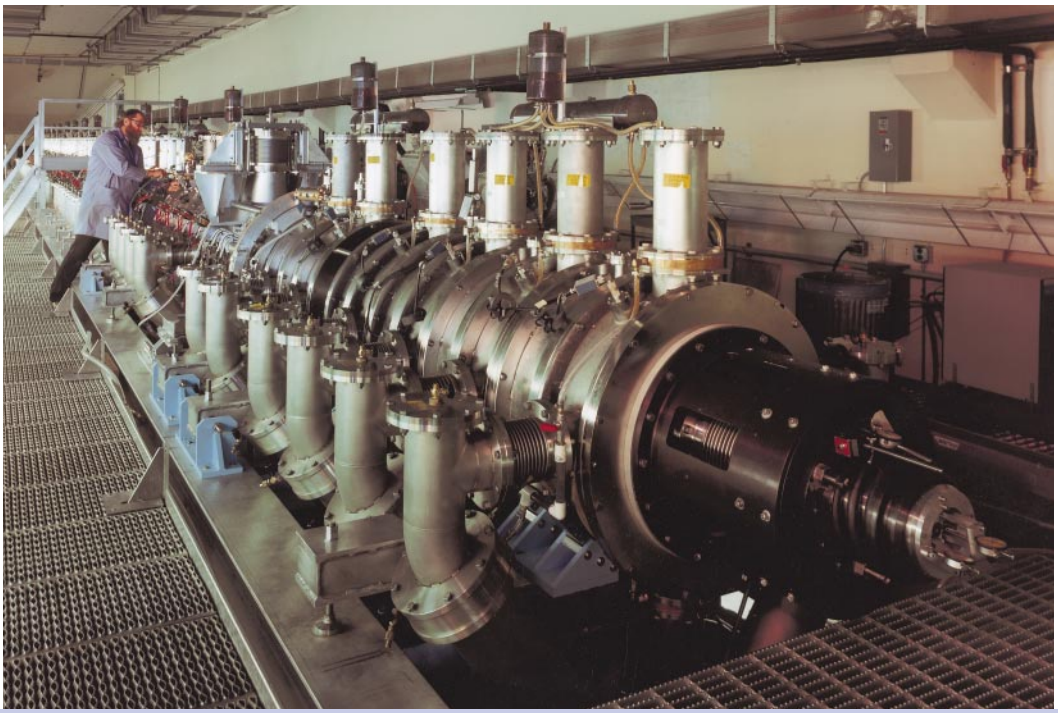
Reprinted from May 1997 *Science & Technology Review*

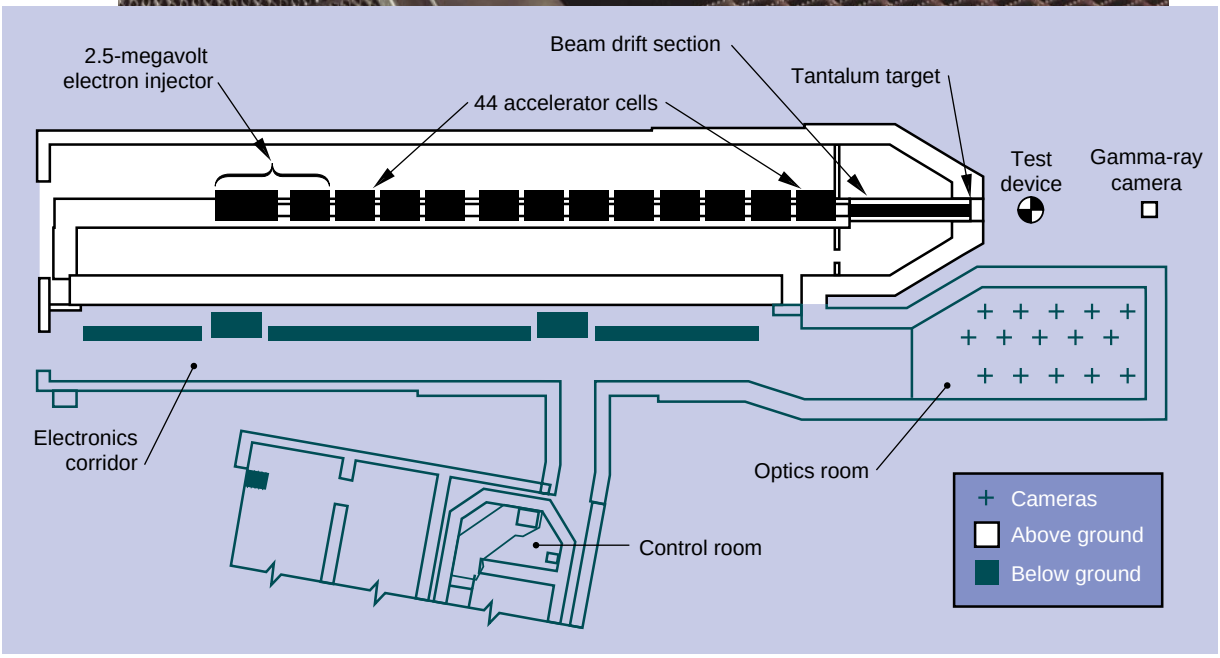
To improve capabilities for science-based stockpile stewardship, Lawrence Livermore has been upgrading many diagnostic facilities at Site 300, the Laboratory's experimental test site. The FXR was already the most sophisticated hydrodynamic flash radiography system in the world. In response to the need for data supporting ever more exact computer modeling codes, it has been made more powerful and capable of producing sharper, more useful radiographs.

The FXR in Action

The FXR is an induction linear accelerator specifically designed for diagnosing hydrodynamic tests and radiographing the interior of an imploding high-explosive device. Its x rays penetrate and are scattered or absorbed by the materials in the device, depending upon the density and absorption cross section of the various interior parts. The x rays that are neither absorbed or scattered by the device form the image on photographic emulsions or on the recording surface in a gamma-ray camera.

An injector introduces an electron beam into the FXR accelerator. After passing through the accelerator, the beam enters a drift section that directs it toward a 1-millimeter-thick strip of tantalum, called a target. As the high-energy electrons pass through the target, the electric field created by the stationary charged particles of the heavy tantalum nuclei causes the electrons to decelerate and radiate some of their energy in the form of x rays. The product of this slowing process is called bremsstrahlung (braking) radiation.





The Flash X-Ray beam area is on the same level as the firing table outside the building. The electronics corridor, optics room, and control room are underground, one level below the beam area and offset from the accelerator as shown in this schematic. Several of the accelerator cells can be seen in the photograph to the right.

The x-ray photons travel toward the exploding device, where most are absorbed. The photons that make it to the camera are the image data.

A Better Radiographic Process

The upgrades to the FXR centered on improving the quality of the beam and adding a new gamma-ray camera system that is 70 times more sensitive than radiographic film. In this camera, designed by Livermore scientists, the beam hits an array of bismuth–germanate crystals with which the x rays interact to generate visible light. This light is recorded on photographic film.

The first task in increasing FXR beam quality was to improve the magnetic field that transports the electron beam through the accelerator. New focus solenoids and printed-circuit magnetic steering coils were installed in each of the accelerator and injector cells. Transverse magnetic forces that had been pulling the beam out of alignment were reduced by a factor of 10 to 20.

The next task was to double the injector beam voltage from 1.2 megavolts to 2.5 megavolts. At the same time, the injector electron beam current was increased from 2.2 kiloamperes to 3 kiloamperes. The number of cells in the injector was increased from six to ten, and the electron diode and the injector magnetic transport solenoids were redesigned.

With the completion of these upgrades, the FXR is producing a higher overall x-ray dose and
a smaller spot size. Today, the central portion on the x-ray spot is twice as intense compared with pre-upgrade levels. Because tuning the FXR is an ongoing process, improvements in performance are expected to continue.

Prior to the addition of the gamma-ray camera, the size of the beam where it hits the tantalum target was a major concern; a smaller "spot size" increases the sharpness and clarity of the radiographs. Achieving a smaller effective spot size was accomplished by passing the x rays through a small hole in a thick plate near the target, a process known as collimation. But because x rays emitted outside the collimation diameter are lost to the radiographic process, collimating the beam meant that thicker materials could not be studied.

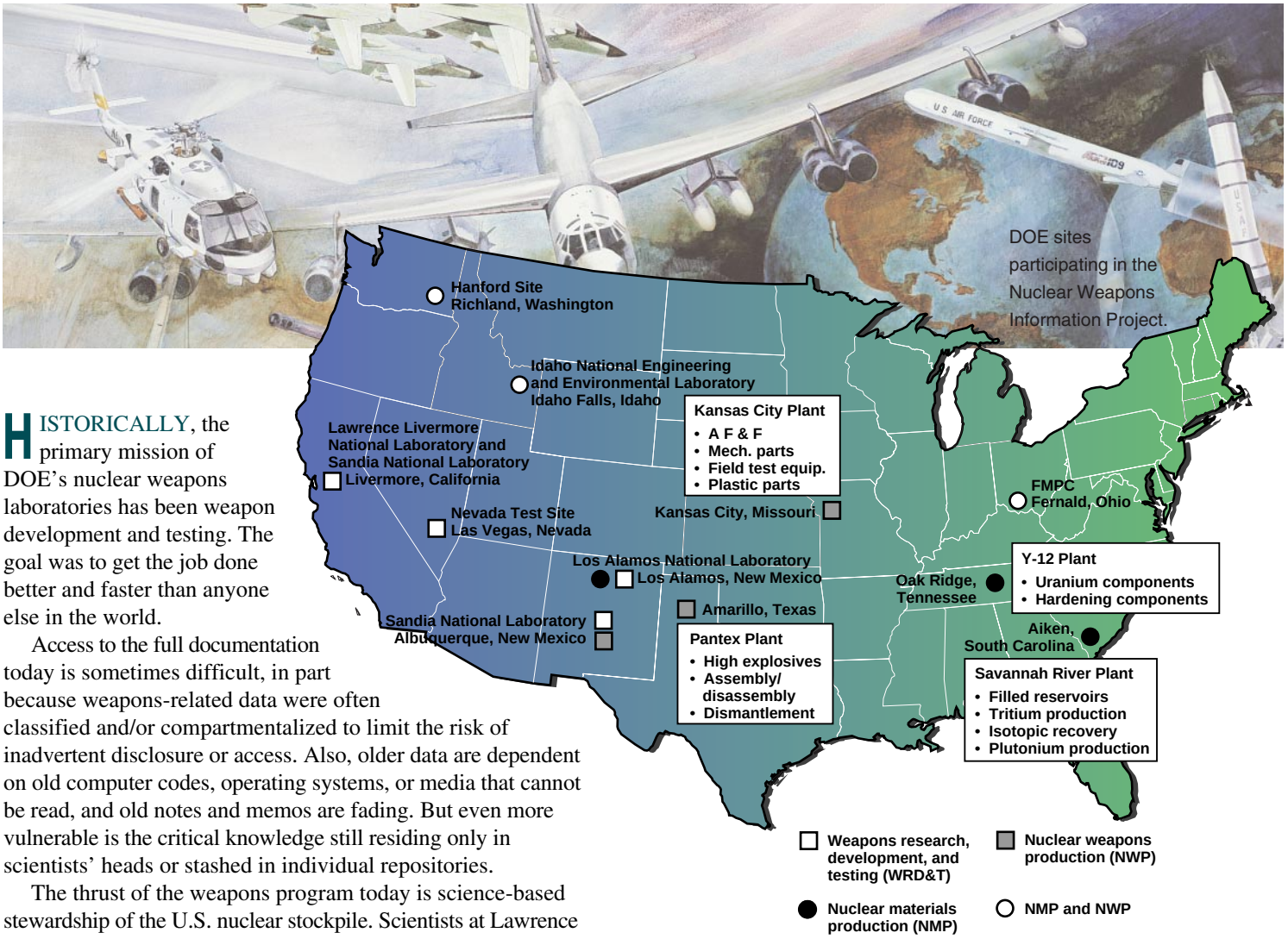
Today, however, the increased sensitivity of the gamma-ray camera and the increased current density of the central portion of the electron beam combine to more than compensate for the losses due to collimation. The gamma-ray camera can produce much sharper, clearer images than before even with a lower available dose. The camera's sensitivity combined with the newly increased x-ray dose at the target means that collimation can be used for experiments involving even higher density materials. Preliminary results indicate that the FXR upgrade—in conjunction with the gamma-ray camera—have significantly improved the radiographic capability at Livermore.

In the near future, the Laboratory will be adding a double-pulse feature to the FXR to provide two radiographs of a single explosion–implosion separated by 1 to 5 microseconds. Researchers can use this information to follow the time evolution of an implosion and learn more about how an implosion progresses. Restoring single-shot, full-energy operation will require simply setting the pulse interval to zero. Livermore scientists are also developing a two-frame gamma-ray camera to capture the fast successive images of double-pulsed FXR radiography and record them on a charged-coupled device camera. Work on the double-pulse feature and the two-frame camera is expected to be complete in 1998.

Key Words: flash x radiography (FXR), gamma-ray camera, hydrodynamic testing, induction linear accelerator, pulsed electron beam, pulsed x-ray source, stockpile stewardship.

For more information contact Ray Scarpetti (925) 422-8502 (scarpetti1@llnl.gov).

Preserving Nuclear Weapons Information



HISTORICALLY, the primary mission of DOE's nuclear weapons laboratories has been weapon development and testing. The goal was to get the job done better and faster than anyone else in the world.

Access to the full documentation today is sometimes difficult, in part because weapons-related data were often classified and/or compartmentalized to limit the risk of inadvertent disclosure or access. Also, older data are dependent on old computer codes, operating systems, or media that cannot be read, and old notes and memos are fading. But even more vulnerable is the critical knowledge still residing only in scientists' heads or stashed in individual repositories.

The thrust of the weapons program today is science-based stewardship of the U.S. nuclear stockpile. Scientists at Lawrence Livermore National Laboratory are responsible for four of the nine weapon systems in the enduring U.S. stockpile, including the only ones that incorporate all modern safety features. Maintaining and managing those systems will be Livermore's responsibility for years to come.

With rare exceptions, the people who will manage the stockpile in the next century will do so without the direct knowledge that comes from having designed and tested a nuclear weapon. Because the generation of designers responsible for the current stockpile is reaching retirement age, "downloading" essential information from their heads is critical for future scientists.

Scientists and engineers at Livermore, proud of their work, enthusiastically embraced the Nuclear Weapons Information Project (NWIP), an archiving effort established in early 1993 to rescue at-risk data and knowledge. Bill Bookless, Principal Deputy Associate Director in the Defense and Nuclear Technologies Directorate, is the project leader. Late in 1993, the Defense Nuclear Facilities Safety Board issued Recommendation 93-6, which emphasized retaining safety-related capabilities and capturing weapons knowledge. That directive enhanced the visibility and priority of NWIP work.

The Nuclear Weapons Information Project will preserve Livermore's portion of the Department of Energy's Stockpile Stewardship and Management Program. It will also preserve data for training future scientists, engineers, and technicians and will provide immediate critical information for emergency response to nuclear weapon incidents.

The information archived in NWIP will support proliferation analyses to deter the spread of nuclear weapons to other countries and to terrorist organizations. And the database will provide the fundamental information necessary to resume weapons design, development, testing, and production if required by changes in a volatile world situation.

Because scientists at Livermore depend on access to information at all DOE nuclear weapon facilities, in 1994 Livermore also took a leading role in implementing an information preservation collaboration across the DOE weapons complex. The Nuclear Weapons Information Group (NWIG) today includes participants from the DOE sites shown in the figure, the Department of Defense's Defense Special Weapons Agency, and the United Kingdom's Atomic Weapons Establishment.

The Task at Hand

When work began on the DOE project, the most critical needs were learning what information existed and how to get appropriate access to it. Some DOE sites have as many as 300 different databases or catalogs of relevant data. And some data shelved in unmarked boxes have never been catalogued. Consequently, the initial focus of the group was on "metadata," which are data about data—typically bibliographic data—and on standardization efforts.

Terminology has changed over time, and various organizations across the DOE complex use different terms for the same thing. Local glossaries have been developed and are being shared and integrated, and a categorization system is being developed to define common subject areas. Livermore leads the working group that is developing metadata standards and has led the pilot implementation of searches in and across multiple catalogs.

Capturing documents and data is actually the easy part of the project. Capturing the knowledge that is in people's heads and that cuts across program boundaries is more difficult. Videotapes are being made of panel discussions, tours, lectures, and operations to save undocumented anecdotal technical information and historical perspectives.

Livermore has already adopted the NWIG standards and methods for access by implementing commercial "browser" software to provide access to its electronic archives. A pyramidal need-to-know model is also being implemented, such that individuals authorized at the top of the pyramid may have access to nearly everything while those authorized at other levels have access only to information in a particular domain or perhaps about specific weapon systems. By enhancing its classified network infrastructure, Livermore can balance the increased access to information against the increased threat of compromise.

Translating archived files into such standard formats as HyperText Markup Language (HTML) and Portable Document Format (PDF) minimizes the number of platform-sensitive formats that must be translated indefinitely as the technology changes. Settling on a few standard formats also allows the search engine to index every word of every document for retrieval. Links can then be made to the actual archived online documents, or for catalog searches, the search engine can indicate where the documents can be found.

Cutting-Edge Technologies

Several advanced technologies are being applied to the Nuclear Weapons Information Project at Livermore. An example is the online video search and retrieval system, which will provide authorized users of the archives access to videotaped information through a search of the automatically generated transcripts. A search will yield both words in the transcript and matching video images.

The access control mechanisms work together with state-of-the-art identification and encryption technology to ensure authorization, authentication, and secure delivery of information on distributed classified networks. Administrators in weapons-related divisions at Livermore are also making use of this new commercial technology to better protect sensitive unclassified information. Livermore is leading the effort across the DOE complex to establish and implement access control policies and procedures.

Information Is a National Asset

Downloading the knowledge from scientists' heads and archiving those stashed personal files—plus organizing and categorizing more accessible data—are essential tasks. The project team is establishing the archives so that this accumulated information, an important national asset, is preserved for the long term and readily accessible whenever needed. The success of much of DOE's Stockpile Stewardship and Management Program depends on these new archives.

Key Words: archives, Nuclear Weapons Information Project, Stockpile Stewardship and Management Program.

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Site 300's New Contained Firing Facility

Protecting the environment, worker health and safety, and our nation's nuclear arsenal—the CFF will be a building for the 21st century.

Figure 1. The Contained Firing Facility is in the design phase. Construction will begin in 1998.

SOMETIME in 2000, far fewer loud "BOOMS" will resonate from Site 300, the Laboratory's explosives test complex. Lawrence Livermore National Laboratory's new Contained Firing Facility (CFF) will begin operation that year to provide indoor testing of high explosives, and most open-air experiments at Site 300 will be discontinued.

The new Contained Firing Facility (Figure 1) will be an important adjunct to Livermore's science-based stockpile stewardship program.* Without the validation provided by underground nuclear tests, Livermore scientists must still assure the safety and reliability of our nation's nuclear stockpile as weapons age beyond their originally planned life. Computer modeling supplies a wealth of information about how the explosives and assemblies in nuclear weapons will behave, but improved hydrodynamic testing of certain components is necessary to validate the computations.

Situated in the hills between the cities of Livermore and Tracy, Site 300 has been used since 1955 to perform experiments that measure variables important to nuclear weapon safety, conventional ordnance designs, and possible accidents (such as fires) involving explosives. The CFF will drastically reduce emissions to the environment and minimize the generation of hazardous waste, noise, and blast pressures. Although emissions from open-air testing at Site 300 are well within current environmental standards, the CFF is an "insurance policy" that will allow continued high-explosives testing should environmental requirements change. Future residential development in an area less than a mile away will also benefit from the facility's environmental precautions.

The new $50-million facility is currently in the final design stage, under the leadership of Livermore's Charles F. (Joe) Baker, who is project manager for the CFF project. Holmes

* For more information on Livermore's stockpile stewardship program, see *Science & Technology Review,* August 1996, pp. 6–15.

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and Narver Inc. of Orange, California, completed the conceptual design,[1] and the Parsons Infrastructure and Technology Group of Pasadena, California, started the final design in February 1996.

Construction of the new containment facilities at Building 801, scheduled to begin in April 1998, will require complete shutdown of operations at the building. According to Baker, "Even on an accelerated schedule for construction, equipment installation, final testing, and activation, downtime is estimated to be 28 months. With careful planning and early integration of acceptance testing with construction, we are working to minimize downtime and get testing at Building 801 back on line as quickly as possible."

CFF Design

Upon completion, the CFF will be a permanent, state-of-the-art firing chamber constructed on the site of Building 801's present open-air firing table. About 2,500 square meters will be added to Building 801, also the site of LLNL's recently upgraded 18-megaelectron-volt flash x-ray (FXR) machine. Building 801 contains a variety of other advanced, high-speed optical and electronic diagnostic equipment that together constitute a unique capability to diagnose the behavior of high-explosives-driven assemblies.

The CFF additions consist of four components: a firing chamber, a support area, a diagnostic equipment area, and an office/conference module, as shown in Figure 2.

The heart of the CFF is the firing chamber. Slightly larger than half a small gymnasium (16 by 18 meters and 10 meters high), the firing chamber will contain the blast overpressure and debris from detonations of up to 60 kilograms (kg) of cased explosive charges. The inside surfaces of the chamber will be protected from shrapnel traveling as fast as 1.5 kilometers per second with 38-millimeter-thick mild steel plates. To permit repetitive firings, all main structural elements of the firing chamber are required to remain elastic when subjected to blast. Detonations will be conducted above a 150-millimeter-thick steel firing surface (the shot anvil) embedded in the floor.

All main structural elements of the firing chamber must be able to withstand repetitive firing as well as meet design safety standards. These criteria require the structure to withstand a 94-kg TNT blast, which is the equivalent to 60 kg of high explosives. During the testing phase of the project, "overtests" will be run using 75 kg of high explosives to assure that the building can withstand planned 60-kg detonations.

A key aspect of the new facility is that the rectangular concrete firing chamber will be made with low-cost, conventional reinforcement, as opposed to the labor-intensive, laced reinforcement commonly found in many blast-resistant structures. From a materials standpoint, a spherical chamber shape would be more blast efficient, but a slightly heavier, rectangular shape is cheaper to construct, provides easier and more desirable setup and working surfaces, and encompasses existing diagnostic systems. The thickness of the reinforced concrete walls, ceiling, and floor of the chamber will be 1.2, 1.4, and 1.8 m, respectively.

The support area, which measures about 1,500 meters^2, is for preparing the nonexplosive components of an experiment and also for equipment and materials storage, personnel locker rooms, rest rooms, and decontamination showers. It also houses filters, scrubbers, and a temporary waste-

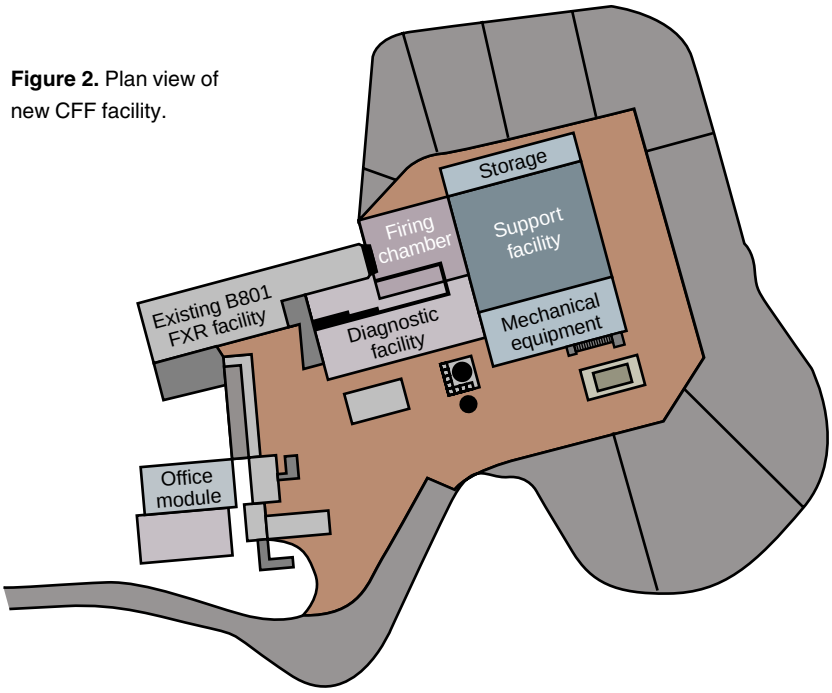

Figure 2. Plan view of new CFF facility.

accumulation area for the waste products from testing.

The diagnostic equipment area (about 600 meters^2) will accommodate a multibeam Fabry-Perot velocimeter to measure velocity–time histories from as many as 20 points on an explosively driven metal surface.[2] The velocimeter optical equipment will take measurements through 12 horizontal optical lines of sight into the firing chamber. There are already 11 vertical optical lines of sight from the existing camera room, which is now beneath the open-air firing table and will soon be under the new contained firing chamber.

LLNL Blast-Effects Testing

After reviewing the conceptual design report, Baker and his engineering staff identified three design issues related to blast effects that would benefit from further investigation: shrapnel mitigation, close-in shock loading, and total structural response.[3] Staff from Livermore and Site 300 performed additional testing in these areas to verify the planned approach or to modify the design as required. Together these tests confirmed that with proper protection, a rectangular firing chamber constructed of low-cost, conventionally reinforced concrete will be acceptable.

Shrapnel Mitigation

High-velocity fragments from cased explosives could do significant damage to the pressure liner in the firing chamber and thus compromise the containment and sealing of hazardous gases and particulates. Worst-case shrapnel-producing experiments at Site 300 were monitored and documented to evaluate various general-purpose shrapnel-protection schemes. (See Figure 3.) The resulting design is a replaceable, 5-centimeter-thick multilayer system of steel plates, to be installed on the inside concrete surfaces of the firing chamber walls and as “throw rugs” on the floor.

From this testing program, three important design modifications were identified:

- Still more local shielding will be required on an as-needed basis near those experiments that use materials such as shaped charges. Local shielding will permit the overall general-purpose shielding to be thinner, resulting in a cost saving.
- General-purpose shielding will be made from mild steel instead of armor plate to cut roughly half the shielding cost yet provide about 85% of the penetration resistance of armor plate.
- Multilayer technology—thinner shrapnel-mitigation plates separated by air spaces—will be used, permitting the total thickness of shielding to be reduced and facilitating replacement and repair.

Close-In Shock Loading

The highest shock loading that the Contained Firing Facility must withstand will occur on the floor just below the 60-kg shot anvil. Currently, because of the diagnostic requirements of the FXR and the desired optical lines of sight, the distance from the top of the shot anvil to the floor is 1.22 meters. (See Figure 4.) This short distance results in high blast loading on the reinforced concrete floor of the chamber. Because floor damage has been a common problem for many blast chambers used by the Departments of Energy and Defense, close-in blast

Figure 3. Shrapnel damage to a steel plate after a test to determine how much shielding is necessary for the firing chamber.

loading on the chamber floor was considered to be one of the most critical design issues.

To investigate this concern, a series of 19 experiments ranging from 25 to 200% of anticipated close-in blast loading were conducted on a one-quarter-scale section of the proposed floor design. Strain gages were embedded in the concrete and placed on the reinforcing bars, on the hold-down bolts, and under the anvil surface to measure blast-induced strains.

During these tests, measured strains on the reinforcement, the bolts, and the anvil were all within elastic limits for steel. But tensile strains in the concrete were 10 times those allowable and would be likely to cause severe concrete cracking and pulverizing over the long term. To reduce the measured strains in the concrete to acceptable elastic levels and to prevent pulverizing, a low-cost blast attenuation system placed between the high-explosive and the anvil was developed and tested. Interestingly, of the various blast attenuation systems studied, the least expensive one, a rubber doormat-type material, proved to be the only acceptable option (Figure 5).

Total Structural Response

Once shrapnel protection and shock loading criteria were determined, the engineering staff evaluated criteria for the entire structure of the new firing chamber. The primary design criterion was that the chamber exhibit a totally elastic response to detonations within it, meaning that the chamber must not incur any permanent changes to its size or shape over time. To evaluate the structure, Livermore staff engineered and constructed a one-quarter-scale model based on the conceptual design, and installed instruments such as strain gages, pressure transducers, and temperature gages. Sixteen scaled detonation tests were performed in the model (Figure 6), which exhibited a lightly damped vibrational response that placed the structure in alternating cycles of compression and tension. During compression, both the reinforcing steel and the concrete remained elastic. During tension, the reinforcing steel remained elastic, but the concrete elastic limit was exceeded in two areas, and the concrete cracked in both places.

Overall, the experiments demonstrated that a rectangular, conventionally reinforced, concrete

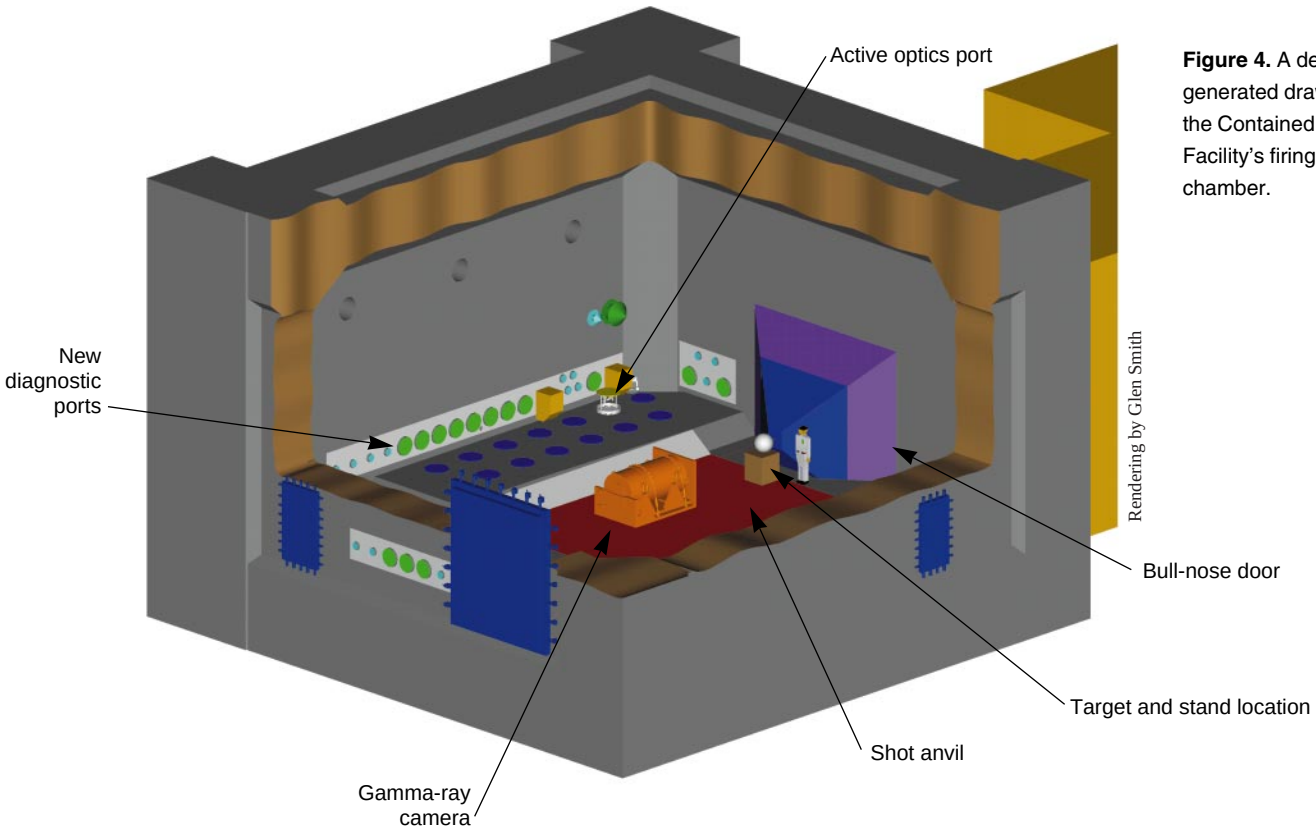

Figure 4. A design-generated drawing of the Contained Firing Facility's firing chamber.

structure can be used as a firing chamber. The final design will incorporate more steel reinforcing to reduce cracking.

Built-in Protection

The design of the Contained Firing Facility incorporates numerous features to ensure the health and safety of those working inside the facility and to protect the outside environment.

Worker Protection

For workers in the facility, decontamination of the firing chamber after testing is very important. Some of the toxic and hazardous products from testing that will be monitored include ammonia, carbon monoxide, hydrogen chloride, hydrogen cyanide, hydrogen fluoride, nitrogen oxides, as well as aerosols of beryllium and other metals. Low-level radioactive aerosols are also expected from depleted uranium used in many tests.

Special mechanical systems will be installed for internal, closed water wash-down of the chamber interior after every test. The air and surfaces inside the chamber will be sampled for contamination, and cleanup will be repeated if necessary. Baker notes, "The goal is for employees to be able to return to the chamber to work after a test without having to wear protective clothing or breathing apparatus." He adds, "Firing chambers tend to be dark and dingy. With the CFF, we are striving to achieve a bright, clean, laboratory-like atmosphere."

Other features address the possibility that an otherwise well-planned experiment in the CFF for some reason might fail to detonate. Robotic systems for defusing and removing the explosive materials already exist and are being incorporated in the facility's design.

Near-Zero Discharge

"Contained firing" implies complete containment of all blast effects associated with the detonation of cased high-explosive materials, including noxious gases, aerosolized and chunky particulate matter, and impulse noise. The CFF project is based on a "near-zero discharge" policy. An occasional, inadvertent discharge would still be well within the limits of more stringent future regulations.

The firing chamber will be a sealed structure to contain not only very high-amplitude, short-duration impulse shock pressures but also the much lower-amplitude and longer-duration quasistatic gas pressures that are typical of explosives detonated in closed firing chambers. Anchored to the inside of the concrete chamber surfaces will be a thin, continuous, mild-steel pressure liner that will seal the chamber and prevent detonation gases from passing through the concrete walls, ceiling, and floor, all of which may develop structurally acceptable hairline cracks as the facility ages. All doors, optical lines of sight, and other intrusions into the firing chamber will have seals that allow the firing chamber to function as a pressure vessel to contain the blast and quasistatic pressure. After the gases cool, blast dampers will open, and ventilation fans will fill the chamber with fresh air. The exhaust gases will be processed through high-efficiency particulate air (HEPA) filters and scrubbers before being released to the environment. Slight negative atmospheric pressures will be maintained afterward in the firing chamber and the support area to reduce the escape of unprocessed airborne hazardous particulates and gases to the environment.

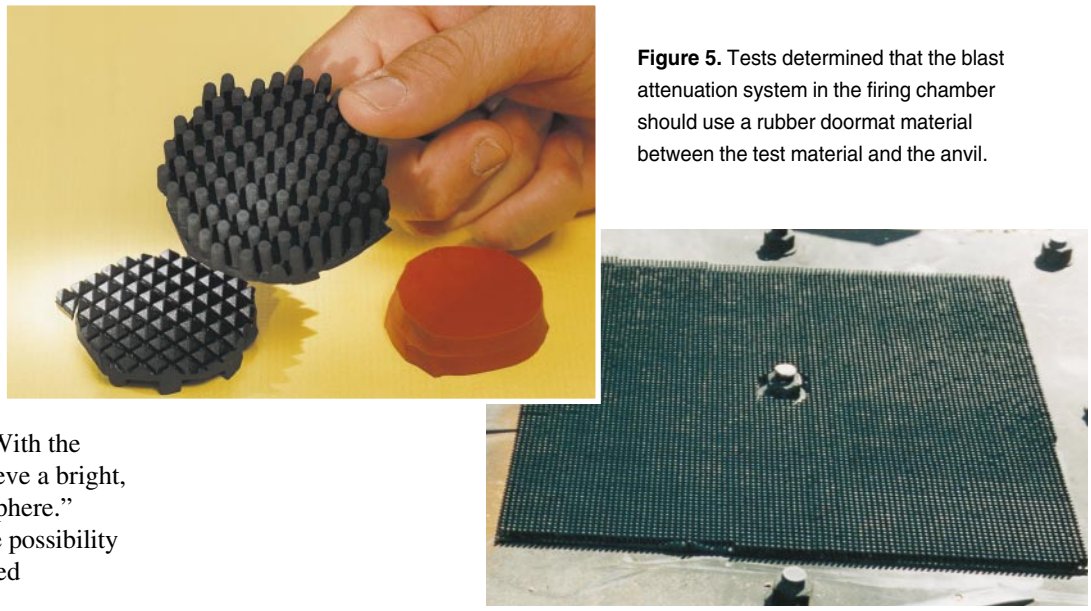

Figure 5. Tests determined that the blast attenuation system in the firing chamber should use a rubber doormat material between the test material and the anvil.

Figure 6. Detonations inside a quarter-scale model were used to determine the facility's total structural response to future tests.

Waste Disposal

Solid wastes and shot debris will be disposed of primarily as low-level radioactive waste, with virtually no mixed (toxic and radioactive) waste anticipated. The wash-down decontamination system will recirculate water spray within the chamber and filter out dust and particulates in the form of sludge, which will be handled appropriately. The elimination of most open-air testing at Site 300 will significantly reduce the amount of contaminated firing-table gravel waste. Livermore estimates that the CFF will reduce total solid waste to about one-tenth the amount generated in comparable shots today.

A New Flexibility

Given the growing importance of LLNL's science-based stockpile stewardship program, the new CFF will give Lawrence Livermore the capability to continue high-explosives testing if environmental standards make open-air testing more difficult. According to Milt Grissom, Site 300 manager, "By the time the Contained Firing Facility is complete in 2000, it will indeed be a building for the 21st century—protecting the environment, worker health and safety, and our nation's nuclear arsenal."

—Katie Walter

Key Words: environment, health and safety; flash x-ray (FXR) machine; high-explosives testing; stockpile stewardship.

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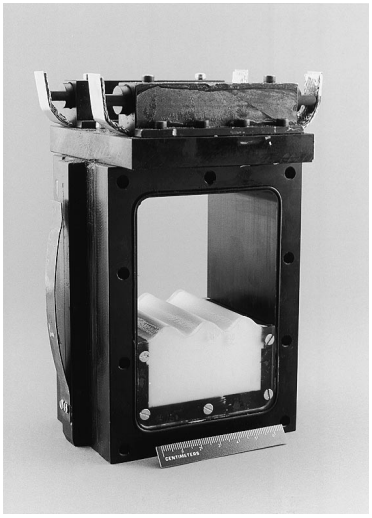
About the Engineer

CHARLES F. "JOE" BAKER received his B.S. in Civil Engineering in 1964 from the Georgia Institute of Technology. He worked for the State of California as a bridge engineer for six years before joining the Laboratory in 1970. Since then he has held a variety of positions in engineering, facilities design, construction management, and program management. Currently, he is Program Manager for the Advanced Hydrotest Facility, the Contained Firing Facility, and the Site 300 Facilities Revitalization Projects. Baker is an expert in designing buildings and structures to resist the effects of high-explosive blasts and is particularly knowledgeable about safety analyses for new facilities, investigations of accidental explosive detonation, and energetic materials testing.

The Linear Electric Motor: Instability at 1,000 g's



WHAT do salad dressing and nuclear fusion have in common, and how can an electric motor further our understanding of both? More than one might suspect.

In both salad dressing and nuclear fusion, materials of different density will mix, which has a great bearing on such things as the uniformity of the dressing or how much energy will be achieved from an inertial confinement fusion (ICF) capsule.[1] To investigate this mixing process, Lawrence Livermore has built a linear electric motor (LEM) that can provide selected acceleration profiles up to 1,000 times Earth's gravity.

"When friends ask what I do, I like to tell them that I'm particularly concerned with what happens when you turn a bottle of salad dressing upside down," quips Guy Dimonte, the Lawrence Livermore physicist who is leading the project to study instabilities in liquids of different densities when they are accelerated by a linear electric motor. "Actually, I'm only half joking, because the principle is the same, whether it's oil mixing with vinegar or a plastic shell mixing with thermonuclear fuel in inertial confinement fusion. We need to understand how hydrodynamic instabilities enhance the mixing of different materials because this information is very important to Lawrence Livermore's stockpile stewardship work," he says.

Perturbations Grow

When fluid of high density is supported against gravity by a less dense liquid, the system is unstable, and microscopic perturbations grow at the interface between the fluids. This phenomenon, called the Rayleigh–Taylor instability, also occurs when a bottle of oil-and-vinegar salad dressing is turned upside down. The instability causes spikes of the dense fluid to penetrate the light fluid, while bubbles of the lighter fluid rise into the dense fluid. The same phenomenon occurs when a light fluid is used to accelerate a dense fluid, causing the two fluids to mix at a very high rate. For example, during the

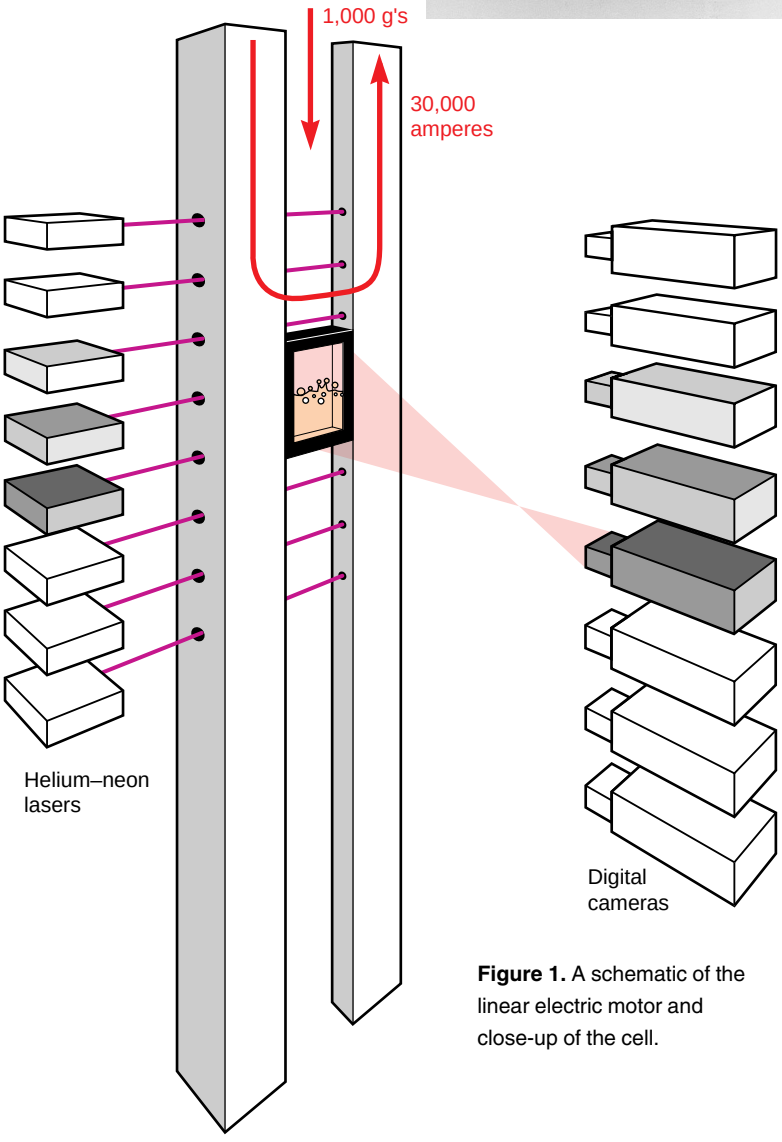


Figure 1. A schematic of the linear electric motor and close-up of the cell.

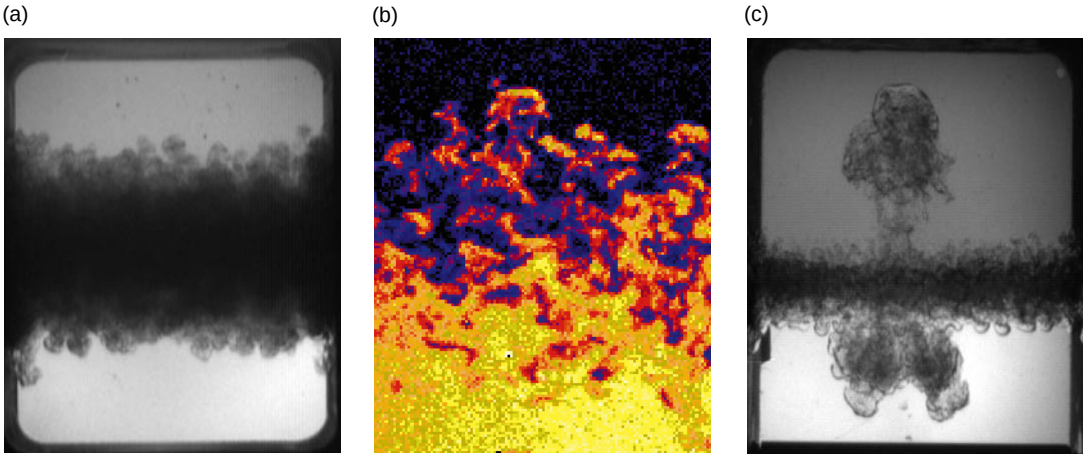


Figure 2. Sample images using (a and c) a flash backlighter and (b) a laser sheet. Images (a) and (b) have a smooth initial interface; (c) has a localized initial disturbance.

implosion of an ICF capsule, this instability can cause enough mixing to contaminate, cool, and degrade the yield of the thermonuclear fuel.

The LEM is an excellent tool for studying this instability, but what is it? Think of a miniature high-speed electric train (the container) hurtling down a track (the electrodes) while diagnostic equipment (optical and laser) photographs it. The configuration is shown in Figure 1.[2]

The LEM, configured by Dimonte and his colleague, physicist Marilyn Schneider, consists of four linear electrodes, or rails, that carry an electrical current to a pair of sliding armatures on the container. A magnetic field is produced that works in concert with the rail–armature current to accelerate the container—just as in an electric motor, but in a linear fashion rather than in rotation. The magnetic field is augmented with elongated coils just as in a conventional electric motor. This configuration also helps hold the armatures against the electrodes to prevent arcing. The electrical energy (0.6 megajoules) is provided by 16 capacitor banks that can be triggered independently to produce different acceleration profiles (i.e., how the acceleration varies with time).

The container that holds the fluid is machined from a block of Delrin, a material that is corrosion-resistant, strong, and nonconducting. The container is $9 \times 9 \times 12$ centimeters (about 4 inches on a side) and has 0.5-cm-thick Lexan windows in the front and back so the liquids can be backlit and imaged. High-resolution optical imaging diagnostics record the inter-fluid mixing. The optical source is either a flash backlighter for photography or a laser sheet for laser-induced fluorescence (Figure 2).

The container trajectory is measured with a laser position detector (LAPD) consisting of eight transverse, 1-milliwatt beams at different positions along the trajectory. When the container intersects these beams, photo diodes send electrical signals that are recorded by digitizers and then trigger the optical diagnostic system. The images are captured electronically using charge-coupled device (CCD) cameras and a desk-top computer using a LABVIEW program. Higher resolution images are taken with remote-controlled 35-millimeter cameras, and the images are digitized later with a photodensitometer. Electrical signals from the LAPD, current monitors, magnetic field loops, and crystal accelerometers are acquired on digitizing oscilloscopes and archived on another desk-top computer. Finally, the container is stopped by a mechanical brake with spring-loaded aluminum drums.

The key to successful operation of the LEM is the sliding armature because it must carry as much as 30,000 amperes of current without arcing. "When we first started, our armatures were flawed, and we melted a lot of copper electrodes with spectacular arcs. After several modifications, we developed an armature that is very reliable, capable of several hundred arc-free shots before the electrodes need to be replaced. The system now works great, but without the exciting fireworks of the early days," Dimonte says.

In a typical experiment, the container is filled with two fluids (such as freon and water) and inserted between the rail.[3] The diagnostic equipment is activated, and the laboratory is then closed and interlocked. From an adjoining control room, the capacitors are charged and fired, sending the container down the rails with a final velocity of about 30 meters per second, depending on the needs of the experiment. Higher velocities are attainable with the energy available in the banks, but they are not required for most experiments. As the container intersects the laser beams, the imaging diagnostics are triggered and electrical signals are acquired. The container then enters the brake region and stops smoothly. "When we are in high gear, technicians Don Nelson and Sam Weaver can fire a shot as quickly as every 10 minutes," Dimonte explains.

Wide Range of Acceleration

"The beauty of using the LEM for these experiments is that we can take very high resolution images of the instabilities over a wide range of acceleration profiles," Dimonte says. "Most alternative drivers like compressed gas

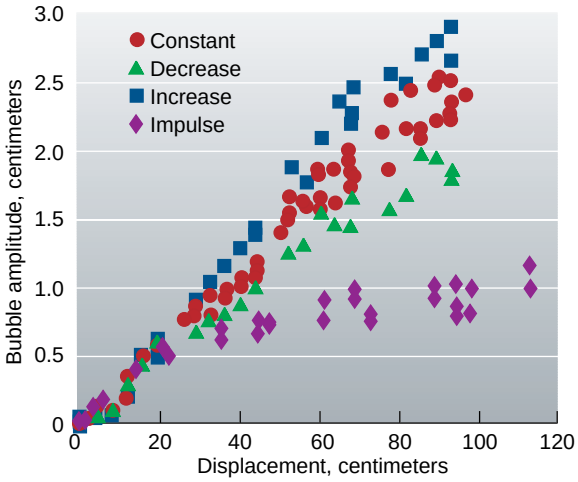


Figure 3. The bubble penetration distance versus the distance traveled by the fluids in a LEM.

or rocket motors do not provide this flexibility. Mixing experiments are performed on Livermore's Nova laser under realistic conditions, but with less relative detail than on the LEM. The LEM is complementary to Nova and a very reliable and cost-effective tool for investigating the fine details of turbulent mixing."

In the example of Figure 2, the fluids have very little viscosity and the mixing is fast and turbulent. Here, scientists are interested in how the random bubbles of light fluid (on top) penetrate the heavy fluid (on bottom) and how the corresponding spikes of heavy fluid penetrate the light fluid. (Remember, gravity has been turned upside down because of the downward acceleration.) The amount of fluid mixing is indicated in Figure 3, which shows the bubble amplitude versus the distance traveled by the container for different acceleration profiles. From these data, Dimonte and Schneider can test turbulent mixing models and full hydrodynamic computer simulations.[3]

In another set of experiments, Dimonte and Schneider are investigating the mixing when the "fluids" have material strength. For example, when an aluminum plate is accelerated by high explosives, the driving pressure is comparable to the yield strength, or the point at which the material would become plastic. In this case, a smooth surface is expected to remain stable indefinitely, whereas a very rough surface would be unstable. They are testing this hypothesis by doing experiments using yogurt because it has enough yield strength to show the effect at the reduced g-forces of the LEM.

Figure 4. Yogurt perturbations after being accelerated by 30 g's. Initial undulations at the interface were 1 millimeter; here they grew to 40 millimeters.

Figure 4 shows an image of yogurt accelerated in the LEM when the initial undulations at the interface were about 1 millimeter in amplitude. The perturbations became very large because of the instability. When the experiment was repeated with a smooth interface, the instability was inhibited by the material strength.

Many more experiments are possible on the LEM with different fluids, diagnostics, and acceleration profiles. "Our strategy is to use small-scale experiments like the LEM, with high-quality optical diagnostics, to investigate the micro-physics of turbulent mixing. Over the next five years, we will test the mixing models with data of unprecedented resolution. When the National Ignition Facility becomes available, the mixing models can then be applied to more realistic conditions in an integrated sense, that is, including the other issues relevant to stockpile stewardship, such as radiation flow and material equation of state," Dimonte says.

—Sam Hunter

Key Words: acceleration, linear electric motor (LEM), Rayleigh–Taylor instability.

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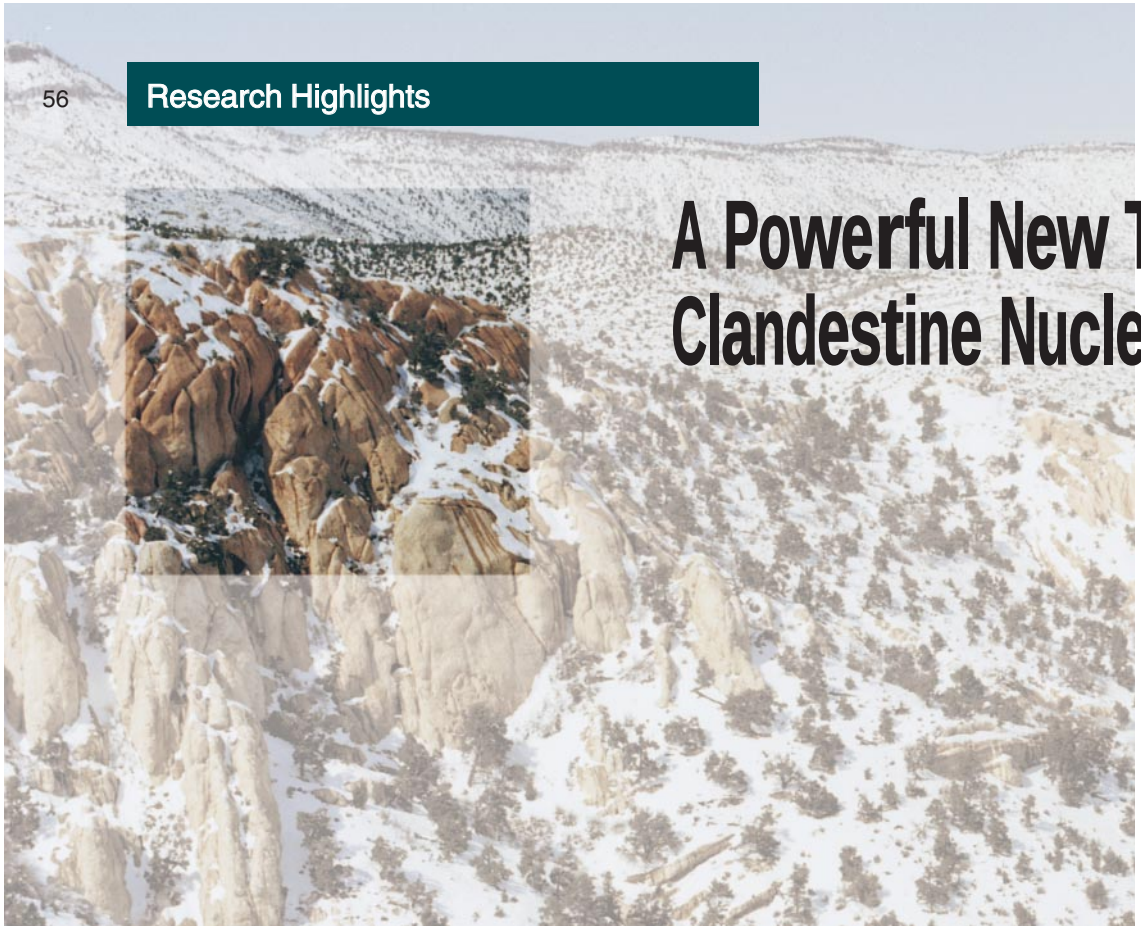
A Powerful New Tool to Detect Clandestine Nuclear Tests



Experiments with the Laboratory's new method of detecting clandestine nuclear tests were conducted on the rocky Rainier Mesa at the Nevada Test Site during periods of low atmospheric pressure, mainly at the beginning of storms, so that tracer gases could rise toward the surface through natural faults and fractures.

WHEN President Clinton and other world leaders signed the landmark Comprehensive Nuclear Test Ban Treaty last September, they served notice that any signatory nation trying to conceal an underground nuclear test would have to elude a vigorous international verification program armed with the latest monitoring technologies. Thanks to the work of a multidisciplinary Lawrence Livermore team, the international community now has a powerful new forensic tool to help enforce the treaty by detecting even deeply buried clandestine nuclear tests.

Under the terms of the treaty, which bans all nuclear weapons test explosions, a system of verification and inspection will be administered by the Comprehensive Test Ban Treaty Organization in Vienna, Austria.

Lawrence Livermore scientists have long played an important role in providing monitoring technologies in support of nuclear treaty verification and on-site inspection. The latest Livermore technology is based on the discovery that minute amounts of rare, radioactive gases generated in underground nuclear detonations will migrate toward the surface along natural fault lines and earth fissures.

Livermore geophysicist Charles Carrigan led the team that included physicists Ray Heinle, Bryant Hudson, and John Nitao and geophysicist Jay Zucca. With the help of results from earlier studies, they theorized that highly sensitive instruments might detect telltale radioactive gases rising during periods of barometric low pressure through natural fissures in the ground above the blast. To test the hypothesis, the team obtained two gases, 0.2 kilograms (7 ounces) of helium-3 and 50 kilograms (110 pounds) of sulfur hexafluoride, as tracers. These nonradioactive gases are ideal tracers because they are present in very low quantities in the natural environment.

As the photo on p. 25 shows, the bottles containing the gases were placed with a 1.3-kiloton charge of chemical explosives into a mined cavity that was 15 meters (50 feet) in diameter and 5 meters (17 feet) high. The cavity was located 400 meters (1,300 feet) below the surface, two to three times deeper than that required for a similar sized underground nuclear test. A somewhat shallower detonation, says Carrigan, might have produced a collapse crater or extensive fractures connecting the cavity with the surface, both telltale signs of an underground explosion. Hence, clandestine tests would very likely be conducted at the greater depth to avoid easy detection of treaty violations.

Simulating a Nuclear Test

The detonation, known as the Non-Proliferation Experiment, occurred on September 22, 1993, in the rocky Rainier Mesa of the Nevada Test Site, where some of the nation's nuclear tests

were conducted until a testing moratorium went into effect in 1992. The chemical explosion simulated a 1-kiloton underground nuclear detonation, which, as expected, did not produce any visible new cracks in the Earth.

Over the year and a half following the blast, team members, including technical support personnel from Test Site contractors EG&G and REECo, collected nearly 200 samples of subsoil gases for measurement. At some sampling stations, sampling tubes were driven into the ground to depths of 1.5 to 5 meters (5 to 16 feet) along fractures and faults. At other stations, tubes were simply placed beneath plastic sheeting that was spread on the ground to trap rising soil gases and to limit atmospheric infiltration (see photo, p. 58).

The first positive finding came 50 days after the explosion, when sulfur hexafluoride was detected in fractures along a fault. Interestingly, the much lighter helium-3 showed up 375 days—more than a year—following the explosion. Both gases were first detected along the same natural fissure within 550 meters (1,800 feet) of the blast site.

Over the course of the extended sampling period, virtually all the samples yielding concentrations of the two tracers appeared along natural faults and fractures in the mesa during periods of low atmospheric pressure, mainly at the beginning of storms. The low pressure accompanying storms, says Carrigan, makes it possible for the gases to move toward the surface along the faults. Although over the course of a year the number of low-pressure days equal the number of high-pressure days, the gases are eventually drawn upward. "There's a ratcheting effect," he explains. "The gases don't go back down as much as they go up." (See the simulation on p. 58.)

Carrigan notes that it is counterintuitive that helium-3 takes so much longer to make its way up natural fissures than sulfur hexafluoride, which is 50 times heavier. Computer models developed at Livermore showed that this result occurred because most of the heavier sulfur hexafluoride gas moved directly up the rock fractures. In contrast, the helium-3 diffused readily into the porous walls of the rocks as it slowly moved upward toward the soil surface. Critical to determining why helium-3 behaved as it did was Bryant Hudson's analysis of helium-3 in Livermore's noble gas laboratory, where he used mass spectrometry to measure the presence of helium-3 in soil-gas samples down to parts per trillion.

Modeling the Detonation

Carrigan and Nitao modeled the experiment using a porous-flow simulation software called NUFT (Non-Isothermal Unsaturated Flow and Transport) developed at LLNL by Nitao. In attempting to make the simulation as realistic as possible, the team used actual barometric pressure variation data from the Rainier Mesa weather station. The simulation showed the two gases moving at different rates toward the surface following the detonation. The calculated arrival times at the surface for both tracers were in excellent agreement with the data.

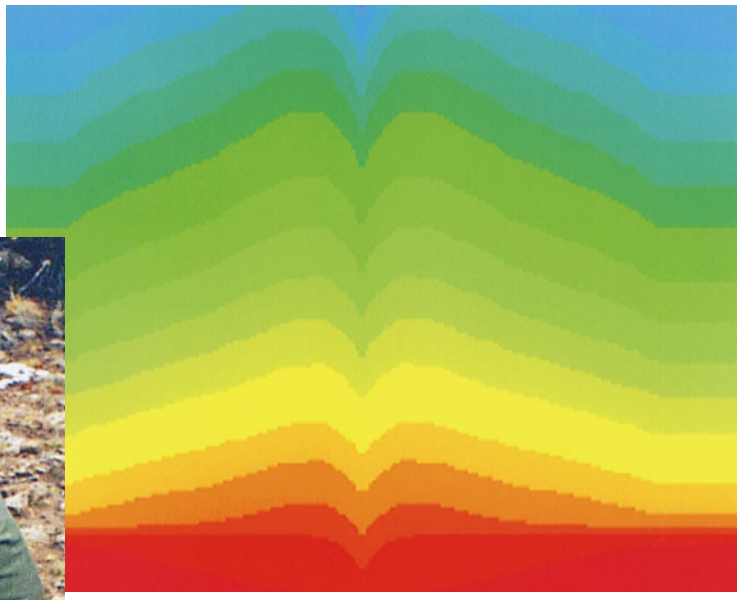
Given the good agreement between the computer model and the observations, the team then used NUFT to simulate the gases released from an underground 1-kiloton nuclear test under atmospheric conditions similar to those that followed the 1993 Non-Proliferation Experiment. The software was used to predict the arrival of detectable concentrations of the rare gases argon-37 and xenon-133 at 50 and 80 days, respectively, after the detonation.

These two isotopes are ideal indicators of nuclear explosions because they are not produced naturally in significant quantities; thus, background levels are extremely low. Also, their short half-lives of 34.8 days and 5.2 days can be used to infer how recently an event had occurred. Other, more long-lived isotopes might still be present in the environment from decades-old tests and would tend to muddy the conclusions of investigators trying to determine whether a clandestine test had recently occurred.

The successful confirmation of the experiment by computer simulation implies that sampling of soil gases for rare, explosion-produced radioactive tracer gases at the surface near a suspected underground test can be an extremely sensitive way

A bottle of sulfur hexafluoride gas is separated from the explosives in a mined test cavity to prevent thermal decomposition of the tracer gas during detonation.

A crew of scientists from Livermore and the Nevada Test Site collect soil-gas samples from tubes inserted to a depth of 5 meters (16 feet) in soils that cover rock containing geologic faults and fractures. The soil gases were detected following a contained, 1-kiloton, underground chemical explosion 400 meters (1,300 feet) beneath Nevada's Rainier Mesa.



Using Livermore's NUFT (Non-Isothermal Unsaturated Flow and Transport) simulation software, the team was able to model gases moving toward the surface following detonation. Shown is a "rainbow" simulation of barometric "ratcheting" of trace gas in the porous walls of a 300-meter- (985-foot-) long, 0.001-meter- (0.03-inch-) wide vertical fracture (centerline of graphic). Concentration decreases from red near the detonation to blue at the surface as surface pressure variations cause the tracer gas to move up and down the fracture until it eventually reaches the surface.

to detect nearby underground nuclear explosions that do not fracture the surface. As a result, says Carrigan, an on-site inspection has a good chance of finding conclusive evidence for a clandestine nuclear explosion for several months afterward.

Putting Treaty Evaders on Notice

"If detected, the radioisotope signals would be unequivocal," according to Bryant Hudson. "They would put treaty evaders on notice that they risk detection if they try to explode a nuclear device underground. We can't absolutely guarantee there won't be cheating, but we've made it more difficult."

Carrigan points out that because of political considerations, it may take some time to get a country to agree to an on-site inspection under the terms of the test ban treaty. The thinking of many experts has been that such inspections need to be conducted within a few days to capture evidence of a test. The Livermore team's work, however, shows that waiting weeks or even months to detect rare gases is not a problem and may well be advantageous, because the gases need time to arrive at the surface.

Team members caution that searching for tracer gases is only one of many detection tools. Other methods that might be used at a suspected test site include analyzing the printouts of seismographs for aftershocks from an explosion, looking for explosion-induced stress in plants and trees, drilling for explosion debris, examining the earth for fractures and craters, and searching for pipes and cables leading underground.

In discussing the work of the team, Carrigan attributes its accomplishments to a confluence of Lawrence Livermore strengths in computer simulation, geophysical theory, nuclear test containment, and radiochemistry. "Interdisciplinary collaboration made this work possible," he says.

—Arnie Heller

Key Words: Comprehensive Nuclear Test Ban Treaty, nuclear proliferation, nuclear treaty verification, NUFT (Non-Isothermal Unsaturated Flow and Transport).

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High Explosives in Stockpile Surveillance Indicate Constancy

Livermore actively seeks to improve the analysis of high explosives in stockpiled nuclear weapons, keeping in mind the purposes of traditional surveillance: to look for defects in materials and processes, to monitor indicators of both constancy and change, and to confirm that design choices did not cause problems.

ANY weapon in the U.S. nuclear arsenal, if ever deployed, must work exactly as intended. Americans expect that assurance even though international relations since 1989 have brought dramatic and fundamental changes to the U.S. nuclear weapons program. Responsibility for assuring reliability, performance, and safety of the nuclear weapons stockpile belongs to the nuclear design and production community, which conducts the wide range of activities in the Department of Energy's New Material and Stockpile Evaluation Program.

Although stockpile evaluation is not new, methods and tests have undergone marked changes since the program's inception almost four decades ago. Today, each of the participating national laboratories—Lawrence Livermore, Los Alamos, and Sandia—is responsible for the extensive and rigorous tests to evaluate the portions and components of the stockpile weapons that each has designed. This overview of Livermore high-explosives (HE) tests of nuclear stockpile weapons illustrates the degree of assurance toward which the laboratories work.

Stockpile Evaluation

"Stockpile surveillance" is the third, or maintenance, phase of a spectrum of special tests that begins during a weapon's design and ends only with its retirement from the stockpile (see box on p. 60 and Figure 1). Such tests now are the principal means of evaluating the condition of U.S. nuclear weapons. For this phase, stockpile laboratory tests provide "indicators of constancy" through comparison with baseline data gathered during weapon development and production.

Stockpile laboratory tests usually begin during the third or fourth year after the weapon's production begins. Sample weapons removed from the stockpile are dismantled, components are inspected and tested, and then the weapons are reassembled and restored in the stockpile. Increasingly, surveillance activities have focused on one central question: How can a weapon's useful service life be predicted?

In addition to checking for materials and production defects, stockpile surveillance involves monitoring potentially damaging changes to a weapon's components caused by aging or environmental factors. Simply because nothing is wrong, the inference cannot be made that the weapon will last indefinitely. Livermore's Enhanced Surveillance Program is currently examining concepts that improve predictive capabilities.

Should problems appear, the increasing body of data will guide the program to accommodate or eliminate adverse effects. Old or damaged parts are replaced or upgraded before a weapon is reassembled for the stockpile. This aspect of surveillance resembles keeping a stored car in driving condition. Regular inspections can spot signs of damage or deterioration before they become too costly to repair. The vehicle can also be upgraded by installing improved replacement parts.

High Explosives

The ideal high-energy explosive must balance different requirements. HE should be easy to form into parts but resistant to subsequent deformation through temperature, pressure, or mechanical stress. It should be easy to detonate on demand but difficult to explode accidentally. The explosive should also be compatible with all the materials it contacts, and it should retain all its desirable qualities indefinitely.

No such explosive existed in 1944. While using what was available to meet wartime demands, scientists at Los Alamos began to develop a high-energy, relatively safe, dimensionally stable, and compositionally uniform explosive. By 1947, scientists at Los Alamos had created the first plastic-bonded explosive (PBX), an RDX*-polystyrene formulation later designated PBX 9205. Although other PBXs have since been successfully formulated for a wide range of applications, only a handful have displayed the combination of adequate energy content, mechanical

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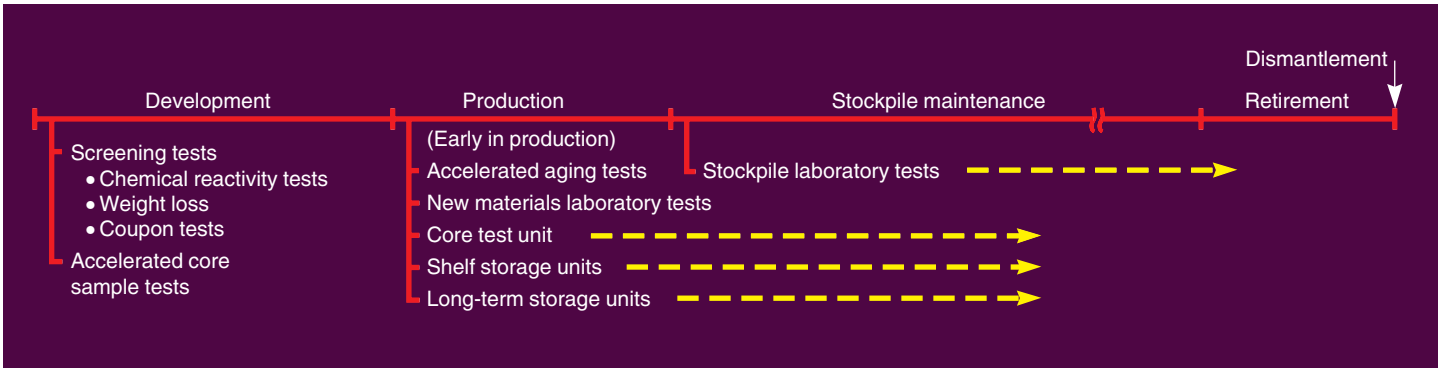


Figure 1. Phases of evaluation in stockpile surveillance.

properties, sensitivity, and chemical stability required for stockpile nuclear weapons. Since the 1960s, Livermore has been researching and developing safer HE for Livermore-designed weapons.

The plastic coating that binds the explosive granules, typically 5 to 20% of each formulation by weight, is what gives each PBX its distinctive characteristics. Pressing a PBX molding powder converts it into a solid mass, with the polymer binder providing both mechanical rigidity and reduced sensitivity to accidental detonation. The choice of binder affects hardness, safety, and stability.

Too brittle a PBX can sustain damage in normal handling and succumb to extreme temperature swings or thermal shocks, while too soft a PBX may be susceptible to creep and may lack dimensional stability or strength. To achieve safe and stable PBXs, the Laboratory uses two main charge explosives based on HMX and TATB.† HMX is more energetic than RDX but retains good chemical and thermal stability, important for long-term storage and survival in extreme environments. Sensitivity of any PBX is a complex characteristic strongly affected by HE particle size distribution, viscoelastic properties, binder-to-HE wetting, and storage environment. Only the TATB-based formulations (Figure 2) of Livermore's LX-17 and Los Alamos's PBX 9502 are considered "insensitive" high explosives (IHE); others are termed "conventional."

HE's Role in a Nuclear Weapon

The nuclear explosive package includes nuclear and non-nuclear components that comprise a primary explosive device and a secondary, both enclosed within a radiation-proof case. A key component of a primary is typically a shell of fissile material—the pit—to be imploded by a surrounding layer of chemical high explosive (HE) termed the main charge.

Stockpile evaluation requires a comprehensive battery of tests that addresses all functional aspects of a weapon throughout its so-called stockpile-to-target sequence, stopping short of actual detonation with nuclear yield. Although the moratorium on underground nuclear testing has precluded detonating a stockpile weapon to assess its reliability, performance, and safety, stockpile evaluation is working to provide an adequate alternative route to the same goal of reliability assessment.

The HE clearly plays a role vital to proper weapon function, but many questions surround the long-term stability of the complex organic molecules of which the HE is composed. To provide assurance that stockpile quality is maintained, Livermore's Stockpile Evaluation team develops diagnostic tests that are performed on the HE in the main charges of stockpile weapons.

Evaluating the Package

Livermore is responsible for surveillance of the stockpile weapons that are based on its own designs. The Engineering Directorate and the Defense and Nuclear Technologies Directorate collaborate on Livermore's Stockpile Surveillance Program. General procedures for the annual evaluation begin with a predetermined number of samples of each weapon type chosen at random from the stockpile. All are disassembled to varying degrees for evaluation, but typically only one weapon has its explosive package reduced to its component parts: pit, explosive, detonators, and secondary.

* RDX is 1,3,5-trinitro-1,3,5-triazacyclohexane.

† HMX is 1,3,5,7-tetranitro-1,3,5,7-tetrazacyclooctane; TATB is 1,3,5-triamino-2,4,6-trinitrobenzene. See *S&TR*, November 1996, for more information on TATB.

Livermore mechanical engineers and materials scientists develop prototype tests, and then Pantex workers perform the tests on actual stockpile weapons components and materials. The tests focus on what would alter the estimated minimum warhead life or require retrofitting.

The complete evaluation entails four major investigations, each with rigorous safety and technical protocols: (1) examining the HE for changes in appearance and texture, including surface discoloration, cracks (using dye penetrant), or tackiness of any materials; (2) measuring physical and mechanical (tensile, compressive) properties, including density and contour; (3) measuring chemical properties, including HE and binder composition, binder molecular weight, and warhead atmosphere analysis; and (4) conducting performance tests, including pin hydrodynamic tests, "snowball" tests, and detonator test firing or disassembly.

In characterizing materials, Livermore surveillance addresses interrelationships among components. Environmental factors such as radiation, heat, and chemical incompatibility can affect the behavior of components and their interfaces throughout the initiation chain: the detonator, booster, and main charge. Explosives could also suffer aging effects in such properties as creep, growth and density gradients, thermomechanical integrity, initiation capability, detonation performance, sensitivity, and safety.

These concerns are addressed during the warhead's development and early production phases, largely through tests using accelerated aging techniques (primarily elevated temperature) to simulate the long-term effects of internal and external environment. The main goal of accelerated aging tests is determining whether materials, parts, and assemblies are compatible with each other and retain their essential properties.

During surveillance, actual aging and environmental effects are evaluated, using new materials laboratory tests and material qualification test results as baseline data.

Tests of Physical Properties

Density and density uniformity are parameters easily measured with high precision. If HE chemical and density distributions remain substantially constant during storage, no significant change is expected in specific energy or detonation velocity.

In both stockpile laboratory tests and accelerated aging tests, density distribution is measured using cored samples. These measurements are then compared with recorded densities from each material lot. Laboratory test results show that accelerated aging conditions do not significantly alter the uniformity of HE density; density actually becomes more uniform throughout the main charge.

Tests of Mechanical Properties

As an integral part of the explosive package's structure, HE must retain its own structural integrity. Therefore, tensile and compressive mechanical properties of HE are monitored (see Figure 3). These mechanical properties were found to be correlated with HE composition and density, as well as the crystallinity and nature of the polymeric binder. Mechanical properties may also be affected by changes in the properties of the explosive–binder interface, but these can only be addressed indirectly.

Tensile strength testing. Tensile tests are performed on LX-17, for

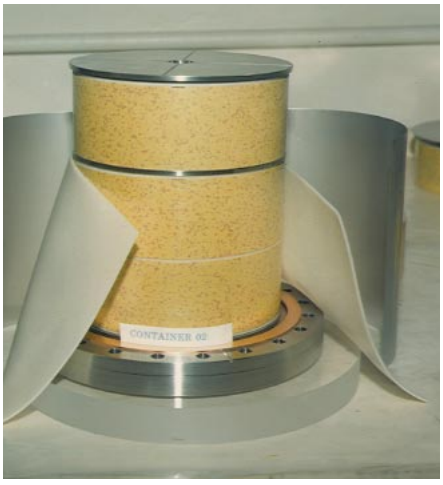


Figure 2. TATB material is being prepared for an aging test.

Figure 3. High-explosives chemist Mark Hoffman sets up HE for mechanical tests.

example, at a low temperature (–20°C) and a slow rate because these conditions simulate the expected worst case (due to thermal expansion mismatches of the materials). This test best shows differences in material quality. Test data for three Livermore weapon systems show no apparent aging trends in LX-17 tensile stress and strain at failure.

Compression testing. For simulating the worst-case conditions for creep (displacement under fixed load) in the warhead, compression tests are performed on LX-17 at an elevated temperature (50°C) and a slow rate (1,440 microstrain per hour).

In surveillance testing, compression values for LX-17 have not failed or fallen outside of material qualification limits. Data on stockpile-aged material from the W87 warhead, however, do show an apparent stiffening of the LX-17 with age (see Figure 4). Although this phenomenon may actually reflect an increase in the crystallinity of the binder, the LX-17 continues to be monitored and will be compared with the behavior in other systems.

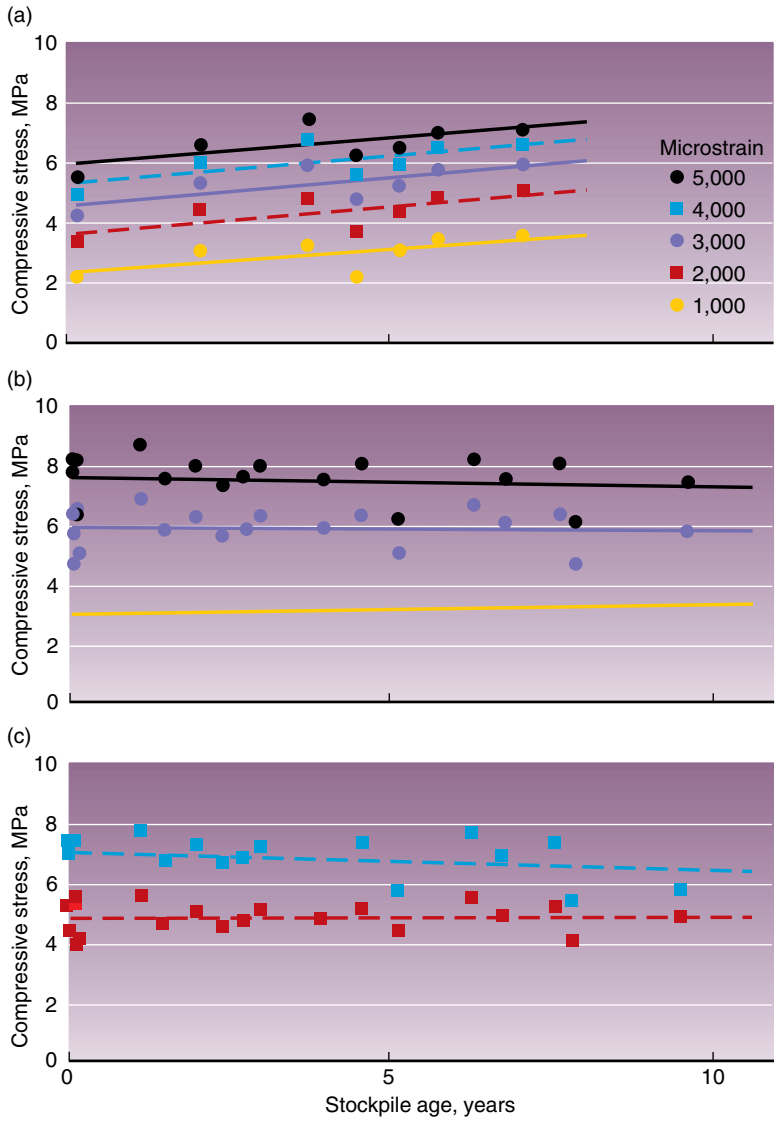


Figure 4. (a) The compressive stress tests for the LX-17 high explosive recovered from the W87 new materials laboratory test (NMLT) units and stockpile laboratory test (SLT) units. The data show a stiffening of the LX-17 at all strain levels, which may be consistent with a gradual increase in the crystallinity of the Kel-F-800 binder. For reasons not clear at this time, this trend is not supported by the observations from the B83 (b) NMLT units and (c) SLT units.

Tests of Chemical Characteristics

As HE ages or degrades, its compatibility with other materials in the primary may suffer. Thus, several types of analysis are employed to evaluate the HE's chemical composition.

Chemical composition analysis. Relative percentages of binder and HE are compared with values obtained from qualification tests of newly produced HE. Percentages of HE different from nominal values could signal significant chemical degradation, which would mean lower energy density for LX-17. To date, however, aging has not affected chemical composition. Changes, if any, remain too subtle for current analytic techniques.

Molecular weight analysis. For this analysis, the polymer binder is extracted from the HE and subjected to gel permeation chromatography (also called size exclusion chromatography). Current techniques have yet to reveal significant aging effects on the molecular weight or molecular weight distribution of LX-17 binder. Small changes in molecular weight that might indicate the onset of degradation, however, are very

difficult to detect and characterize. In Livermore's Enhanced Surveillance Program, methods are being developed to improve the ability to detect aging effects.

Warhead atmosphere gas sampling. Mass spectroscopy and gas chromatography of warhead gas samples can identify material outgassing and ongoing chemical reactions, both of which may indicate degradation or decomposition of the organic compounds in the HE. They also help to verify whether warhead environmental seals have leaked.

Performance Tests

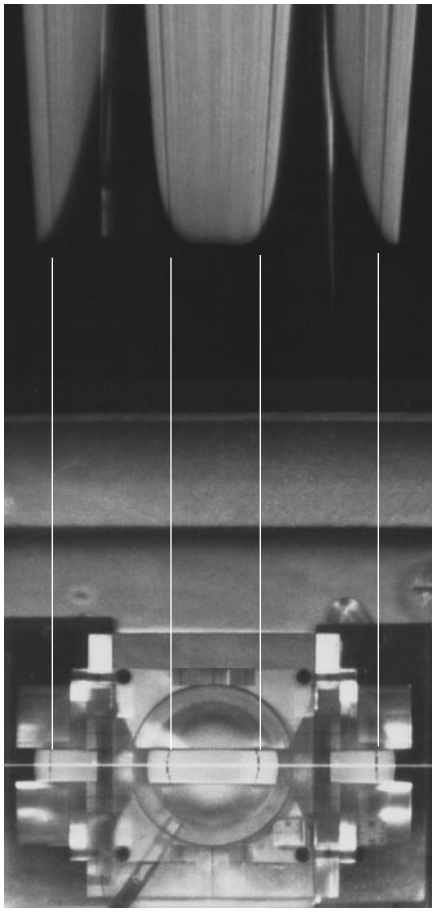
Performance tests tell about the detonation response of the material. Pin hydrodynamic tests check the implosion reliability and performance of the main charge; "snowball" tests help determine the initiation reliability of the booster. Detonators also are test-fired, and certain ones are disassembled for inspection and analysis.

Pin hydrodynamic test. This test monitors changes in the implosion behavior of HE. The test assembly comprises three main subassemblies: a pin-dome assembly, a mock pit, and the HE. The test measures elapsed time from initiation until the explosive drives the mock pit into an array of timing pins, a "pin dome," of known length and location. The HE implodes the mock pit onto the timing pins, which provide data about the temporal and spatial uniformity of implosion. A nonuniform implosion could indicate an HE problem. Excessive density variations, voids, or cracks in the HE, for example, can disrupt the shock-wave propagation from the detonation. To date, surveillance testing has observed none of these problems in stockpile samples.

Snowball test. This test checks reliability of the initiation chain by confirming that the booster initiates the HE. A machined shell of LX-17 is assembled with a booster and detonator to form a "snowball." When this assembly is fired, a streak camera captures spatial and temporal information of the initial, or "breakout," detonation wave on the outer surface of the LX-17 snowball (see Figure 5). The relatively flat curves at the bottom of the image data indicate a good, uniform explosion. Changes in the breakout profile would be used to track the performance of the booster and the condition of the interface with the HE.

Aging tests. So far, surveillance data on HE from the B83, W84, and W87 programs show no evidence of aging effects. Because the W87 system must be requalified for an additional 25 to 30 years, additional data are being gathered and analyzed to improve Livermore's long-term predictive

(a)



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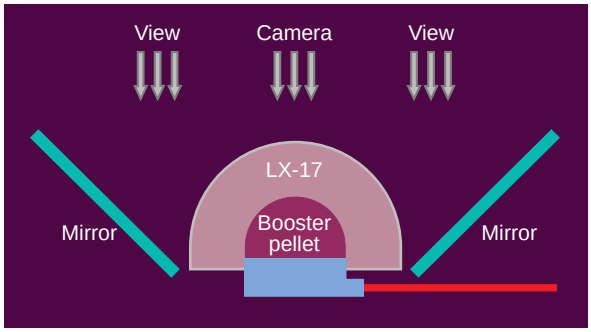

Figure 5. (a) A "snowball" test assembly (bottom) is aligned with samples of snowball test data (top) as recorded by the streak camera. (b) The schematic shows the mirrors that reflect the left and right sets of snowball data.

For illustration, vertical lines are drawn between the photographic breakout record and the markers on the snowball surface. The relatively flat curves at the bottoms of the image data indicate a good, uniform explosion.

capability. Aged LX-17 is being subjected to far more comprehensive testing than usual for stockpile laboratory test units. In essence, properties of control material from various sources are compared to the chemical, physical, mechanical, and performance properties of aged LX-17 for signs of age-induced changes.

Changes, if any, will be studied further in the Enhanced Surveillance Program. Should no changes be discovered, confidence in the projected longevity of the W87's HE materials will be scientifically supported.

A compatibility program initiated during W84 warhead production is paying dividends by serving as a source of aged materials for advanced study. Some specimens of LX-17, UF-TATB (ultrafine TATB) boosters, and LX-16 pellets from W84 production are already being subjected to accelerated aging in a weapon-like atmosphere for ten years.

The Next Step in Surveillance

Continually sought to improve the analysis of HE in weapons in the stockpile, technologies must still fulfill the purposes of traditional surveillance. First, early in a weapon's stockpile life, materials and processes are scrutinized for defects, and then they are monitored to confirm that design choices do not cause problems.

Other improvements are being evaluated for inclusion in the program: (1) fundamental understanding of aging mechanisms in stockpile materials, (2) better selection of stockpile samples for testing and evaluation, (3) better uses of available materials (stockpile-aged materials, such as those from retired and dismantled weapons), and (4) peer review of surveillance data.

Accordingly, the Livermore Stockpile Surveillance Program has proposed revisions in the surveillance mission to achieve the following capabilities:

- Detecting and identifying changes in stockpile-aged materials that previous surveillance methods may not have discovered.
- Predicting—not simply monitoring—any identified age-induced changes in materials through the use of models.
- Providing information on aged materials to weapons designers, who can assess effects on weapons performance.
- Verifying the safety of aged materials via testing and modeling.

These changes will help improve an already successful Livermore stockpile evaluation program. They will enhance surveillance techniques to assure the nation and its armed forces that Livermore-designed weapons can be safely stored and transported and that they can work exactly as intended throughout their stockpile life.

Key Words: accelerated aging, high explosive (HE), LX-17, nuclear weapon, PBX, pin-dome test, predictive capability, snowball tests, stockpile evaluation, stockpile surveillance, TATB.

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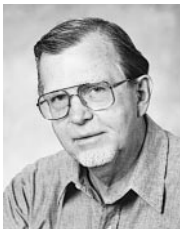
About the Scientist



ANDERS W. LUNDBERG has supported nuclear weapons engineering and testing at Lawrence Livermore since 1961. He received both his B.S. and M.E. in mechanical engineering from the University of California at Berkeley in 1959 and 1961, respectively. At Livermore, he has been a project engineer and group leader in the Weapons Program and the Nuclear Test Program; currently, he is group leader for Stockpile Surveillance in the Mechanical Engineering Department.

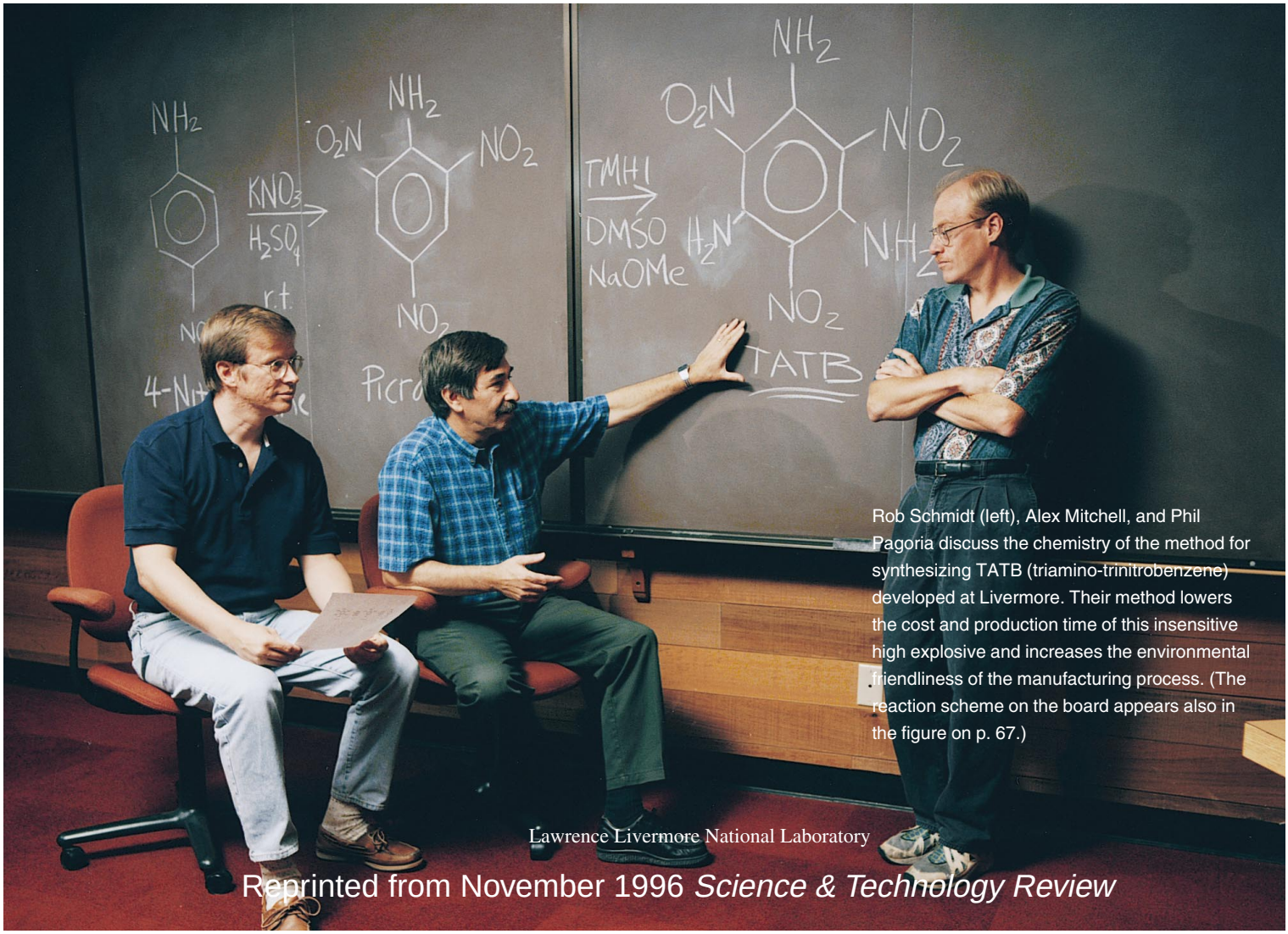
Addressing a Cold War Legacy with a New Way to Produce TATB

ONE of the most important accomplishments made by weapons laboratories' chemists in the past two decades has been the formulation of powerful conventional high explosives that are remarkably insensitive to high temperatures, shock, and impact. These insensitive high explosives (IHEs) significantly improve the safety and survivability of munitions, weapons, and personnel. The Department of Energy's most important IHE for use in modern nuclear warheads is TATB (triamino-trinitrobenzene) because its resistance to heat and physical shock is greater than that of any other known material of comparable energy.

The Department of Energy currently maintains an estimated five-year supply of TATB for its Stockpile Stewardship and Management Program (see the August 1996 *Science & Technology Review*, pp. 6–15), which is designed to ensure the safety, security, and reliability of the U.S. nuclear stockpile. The Department of Defense is also studying the possible use of TATB as an insensitive booster material, because even with its safety characteristics, a given amount of that explosive has more power than an equivalent volume of TNT.

In addition to its military uses, TATB has been proposed for use as a reagent in the manufacturing of components for liquid crystal computer displays. There is also interest in employing the explosive in the civilian sector for deep oil well explorations where heat-insensitive explosives are required.

Despite its broad potential, the high cost of manufacturing TATB has limited its use. Several years ago, TATB produced on an industrial scale in the U.S. was priced at $90 to $250 per kilogram. Today it is available to customers outside DOE for



Rob Schmidt (left), Alex Mitchell, and Phil Pagoria discuss the chemistry of the method for synthesizing TATB (triamino-trinitrobenzene) developed at Livermore. Their method lowers the cost and production time of this insensitive high explosive and increases the environmental friendliness of the manufacturing process. (The reaction scheme on the board appears also in the figure on p. 67.)

Lawrence Livermore National Laboratory

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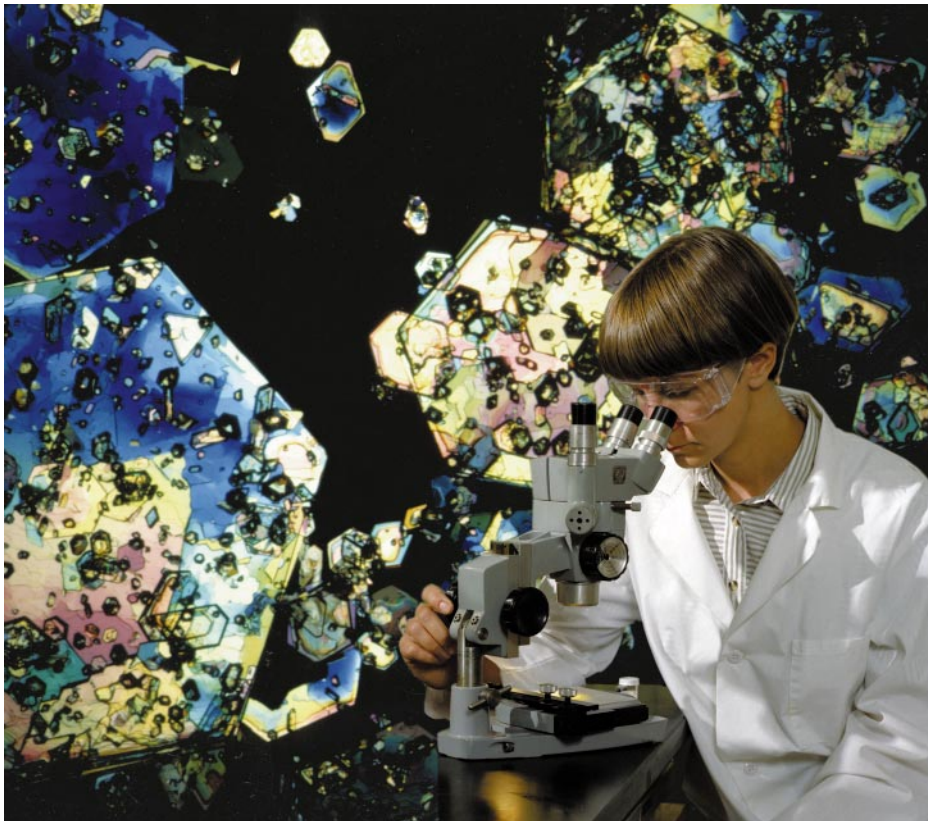
about $200 per kilogram. In response to a need for a more economical product, chemists at Lawrence Livermore have developed a flexible and convenient means of synthesizing TATB as well as DATB (diamino-trinitrobenzene), a closely related but less well known IHE developed by the U.S. Navy. The initial phase of this work was funded by the Department of Defense (U.S. Navy) to explore the chemical conversion of surplus energetic materials to higher value products as an alternative to detonation.

The Lawrence Livermore process—also called the VNS (vicarious nucleophilic substitution) process—should be able to produce TATB for less than $90 a kilogram on an industrial scale in about 40% less manufacturing time. The process also offers significant advantages over the current method of synthesis in environmental friendliness, for example, by avoiding chlorinated starting materials. What's more, the process uses either inexpensive, commercially available chemicals or surplus energetic materials from both the former Soviet Union (UDMH, a rocket propellant) and the U.S. (Explosive D, a high explosive).

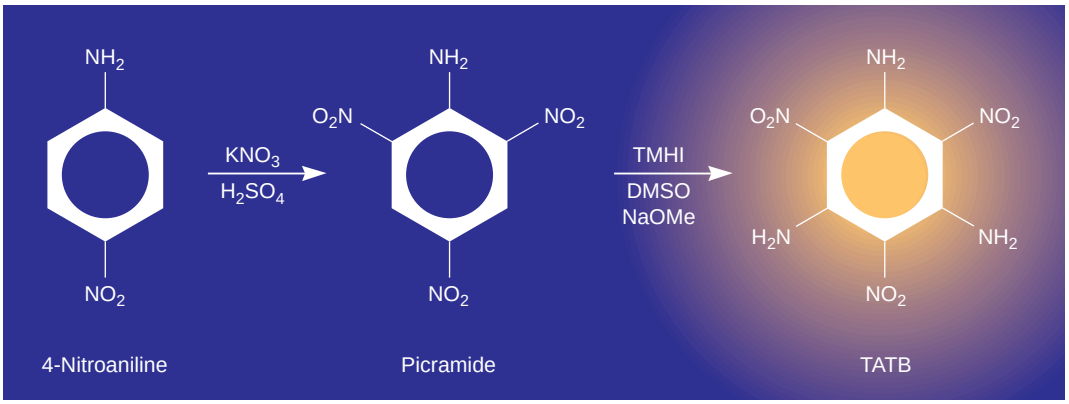
By using UDMH (*uns*-dimethylhydrazine) and Explosive D (ammonium picrate), this process disposes of energetic materials left over as a legacy of the Cold War in an environmentally responsible manner. It allows the use of surplus energetic materials as unique feedstocks to make more valuable materials such as higher value explosives or other products. Indeed, the new chemistry is also applicable to the synthesis of chemicals that are important intermediates in the preparation of numerous pharmaceutical and agricultural chemicals.

Current Process Produces Impurities

The currently accepted method for manufacturing TATB in the U.S. involves a reaction sequence that starts with the relatively expensive and domestically unavailable chlorinated compound TCB (trichlorobenzene). Elevated temperatures of 150°C are required for two of the reaction steps leading to TATB. The major impurity produced is ammonium chloride; in addition there are low levels of chlorinated reaction side-products.



Fran Foltz examines crystals of TATB (triamino-trinitrobenzene) under a microscope. The background photograph shows TATB crystals at high magnification.



The process of synthesizing TATB (triamino-trinitrobenzene) from picramide using TMHI (trimethylhydrazinium iodide) as expressed in this reaction scheme may result in a large decrease in the cost of TATB.

The VNS process is more environmentally friendly than the current synthesis. It employs mild reaction conditions and eliminates the need for chlorinated starting materials. The latter characteristic is especially important in light of the growing movement to eliminate chlorinated compounds from the industrial sector altogether because of their possible adverse environmental effects.

The VNS process depends on two key materials, TMHI (trimethylhydrazinium iodide) and picramide (trinitroaniline), which can be obtained from either inexpensive starting compounds or surplus energetic materials available from demilitarization activities. TMHI can be prepared directly from hydrazine and methyl iodide, or it can be synthesized by reacting UDMH with methyl iodide. Some 30,000 metric tons of UDMH rocket propellant are located in the former Soviet Union, where they await disposal in a safe and environmentally responsible manner.

Two U.S. companies have received congressional funding to demilitarize UDMH in Russia using a chemical process that produces lower value products (ammonia and dimethylamine). In contrast, the VNS process converts UVMH to TMHI, which will be used for the production of higher value products such as TATB.

TMHI reacts with picramide in the presence of a strong base to give TATB at a yield of over 95%. Picramide may be obtained from low-cost, domestically available nitroaniline. Or, as in the synthesis of TMHI, picramide may be synthesized from a surplus munition, in this case, Explosive D. Several million kilograms of Explosive D are available for disposal in the U.S.

New Process to Increase TATB Availability

The availability of relatively inexpensive TATB using the improved synthesis will facilitate its use, both for military and civilian applications. At the same time, the VNS process provides a new avenue for disposing of large quantities of energetic materials that are a legacy of the Cold War. The process reflects a new perspective within both the Department of Defense and the Department of Energy—treating surplus energetic materials as assets to be recycled whenever possible.

This new approach to the synthesis of TATB and other insensitive energetic materials is still in the development stage. Over the next year, the synthesis will progress from the 10-gram scale at the Laboratory's state-of-the-art High Explosives Applications Facility to the kilogram-pilot-plant scale at Site 300. During this stage, the necessary performance and sensitivity tests will be conducted to qualify the synthesis in terms of ease of use, purity, particle size, and cost. The process will also be evaluated for environmental friendliness and waste reduction. At the conclusion of the study, the technology will be ready for transfer to an industrial partner for commercial scale-up.

Key Words: insensitive high explosives (IHE), stockpile stewardship, TATB (triamino-trinitrobenzene).

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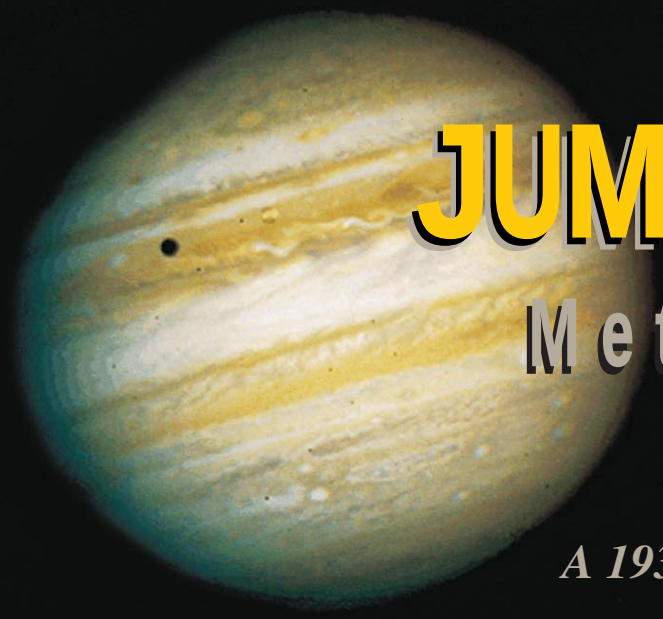
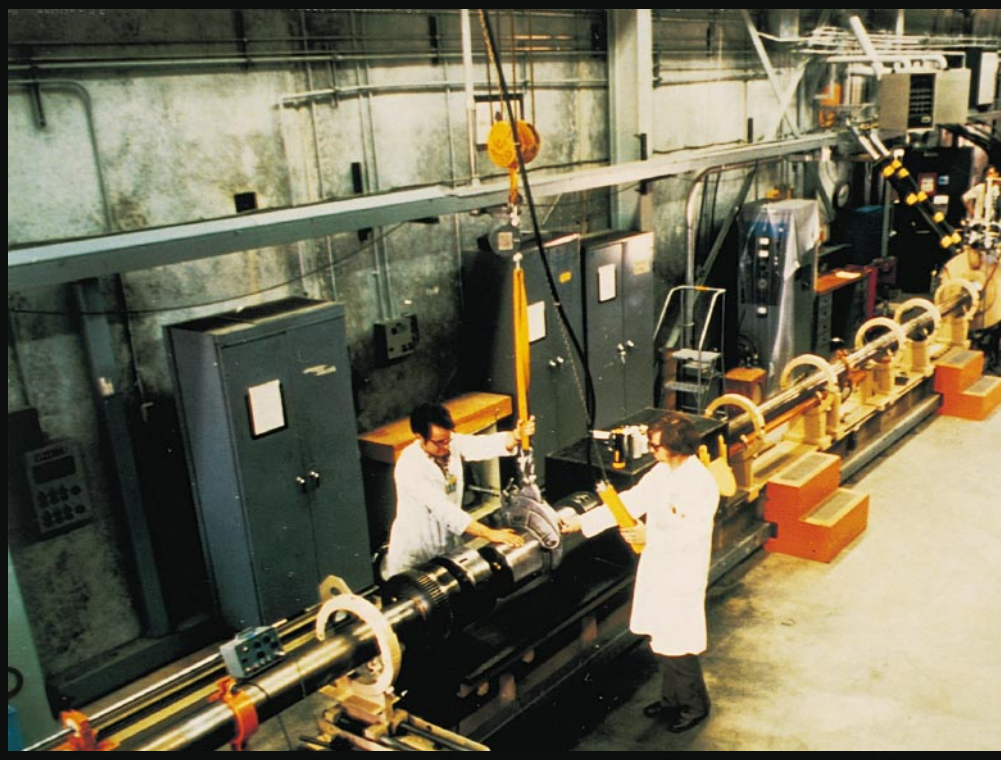


JUMPIN' JUPITER!

Metallic Hydrogen

A 1935 theory predicted that hydrogen becomes metallic when enormously intense pressure is applied. But the theory remained unproved for some 60 years until a Lawrence Livermore team tried a "shocking" idea.



The Laboratory's two-stage light-gas gun was instrumental in the shock compression experiments that metallized hydrogen.

Reprinted from September 1996 *Science & Technology Review*

HYDROGEN is the simplest and most abundant of elements. Composed of one proton and one electron, it makes up 90% of our universe (by number of atoms). On Earth, hydrogen is commonly found as a diatomic molecular gas. But on Jupiter, where interior pressure is millions of times greater than that at our planet's surface, the hydrogen molecule is theorized to exist as a superhot liquid metal.

The theory that hydrogen turns metallic under extreme pressure was first advanced in 1935 by Eugene Wigner, who would go on to win a 1963 Nobel Prize in physics for his work in quantum mechanics. Finding experimental evidence of Wigner's hydrogen metallization theory, however, has proven to be extremely difficult for the scientific community. While studies of the universe's lightest material led to discovery of hydrogen's solid and liquid phases, metallic hydrogen remained out of reach—until recently.[1]

At Lawrence Livermore National Laboratory, in a series of shock compression experiments funded by Laboratory Directed Research and Development grants, we successfully ended a 60-year search for hard evidence of metallic hydrogen and the precise pressure at which metallization occurs at a particular temperature.

Our success in metallizing hydrogen would not have been achieved without the shock-wave technology built up over more than two decades to support Lawrence Livermore's nuclear weapons program. It represents the integration of the Laboratory's broad capabilities and expertise in gas-gun technology, shock physics, target diagnostics, hydrodynamic computational simulations, cryogenics, and hydrogen and condensed-matter physics.

Knowing what happens when matter, such as hydrogen, encounters enormously high pressure and temperature is critical for the success of the Laboratory's research in areas relevant to our science-based stockpile stewardship mission, such as nuclear explosives, conventional high explosives, and laser fusion, as well as for our collaborative efforts in planetary science research. For more than two decades, we have been helping improve that understanding through shock-compression studies using our two-stage light-gas gun (see the box on p. 69).

The gas gun permits us to fire hypervelocity projectiles into highly instrumented targets (Figure 1), shocking matter to extreme conditions for a millionth of a second or less. These experiments create pressures of a million-plus atmospheres, temperatures up to thousands of degrees depending upon the material being shocked, and densities several times that of a material's solid state.

In addition to hydrogen, we have performed shock compression experiments on other liquefied gases such as nitrogen, water, carbon dioxide, oxygen, carbon monoxide, deuterium (an isotope of hydrogen), helium, and argon, and on solids such as aluminum, copper, tantalum, and carbon (graphite). Data from such experiments are used to determine a material's equation of state (EOS expresses the relationship between pressure, density, and temperature), to validate theories, and to generate reliable computational models of a material's behavior under a wide range of thermodynamic variables.

Quest for Metallic Hydrogen

Under normal conditions on our planet, molecular hydrogen functions as an insulator, blocking electrical flow. Apply sufficient pressure, theory said, and hydrogen turns metallic, becoming an exceptional conductor of electricity. Theory predicted that metallization would occur when the insulating molecular solid would transform to a metallic monatomic solid at absolute zero—0 degrees kelvin (K) or –460°F. For early metallic hydrogen theorists, "sufficient pressure" was thought to be 0.2 megabars (1 bar is atmospheric pressure at sea level; a megabar, or Mbar, is a million times atmospheric pressure at sea level). Subsequent predictions pushed metallization pressure to as high as 20 Mbar. At the time our experiments were conducted, the prevailing theory predicted 3 Mbar for solid hydrogen at 0 K.

For 35 years after Wigner proposed his theory, studies on metallic hydrogen were relegated to the theoretical realm because there was no way to approach the subject experimentally. By the 1970s, however, the tools of science had reached a point where it became possible to construct experiments aimed at creating conditions that theory said were required for metallization. At Lawrence Livermore, for example, one research approach[2] used an explosively driven system that compressed a magnetic field and, in turn, a small sample of hydrogen to megabar pressures without shocking the hydrogen, and thus the temperature of the sample was kept very low. The early Livermore experiments generated pressures similar to those we recently reached (about 2 Mbar). While electrical conductivity was measured, the approach did not provide necessary evidence of metallization; the measurement system was only sensitive to conductivity values much less than that of a metal.

In recent years, researchers at other laboratories have attempted to achieve metallization by crushing micrometer-sized samples of crystalline hydrogen in a diamond anvil cell. This small mechanical press creates very high pressures in a nanogram-sized sample when the small flat faces of two flawless diamonds are forced together, exerting megabar pressure on the sample trapped between them.[3] While diamond anvil studies of hydrogen resulted in an initial claim of optical evidence for metallization, this claim was later found to not hold up.[4] Significantly, there was no establishment of metallic character using optical probes. Metallic character is most directly established by electrical conductivity measurements, which are not yet possible in diamond anvil cells with hydrogen samples at any pressure.

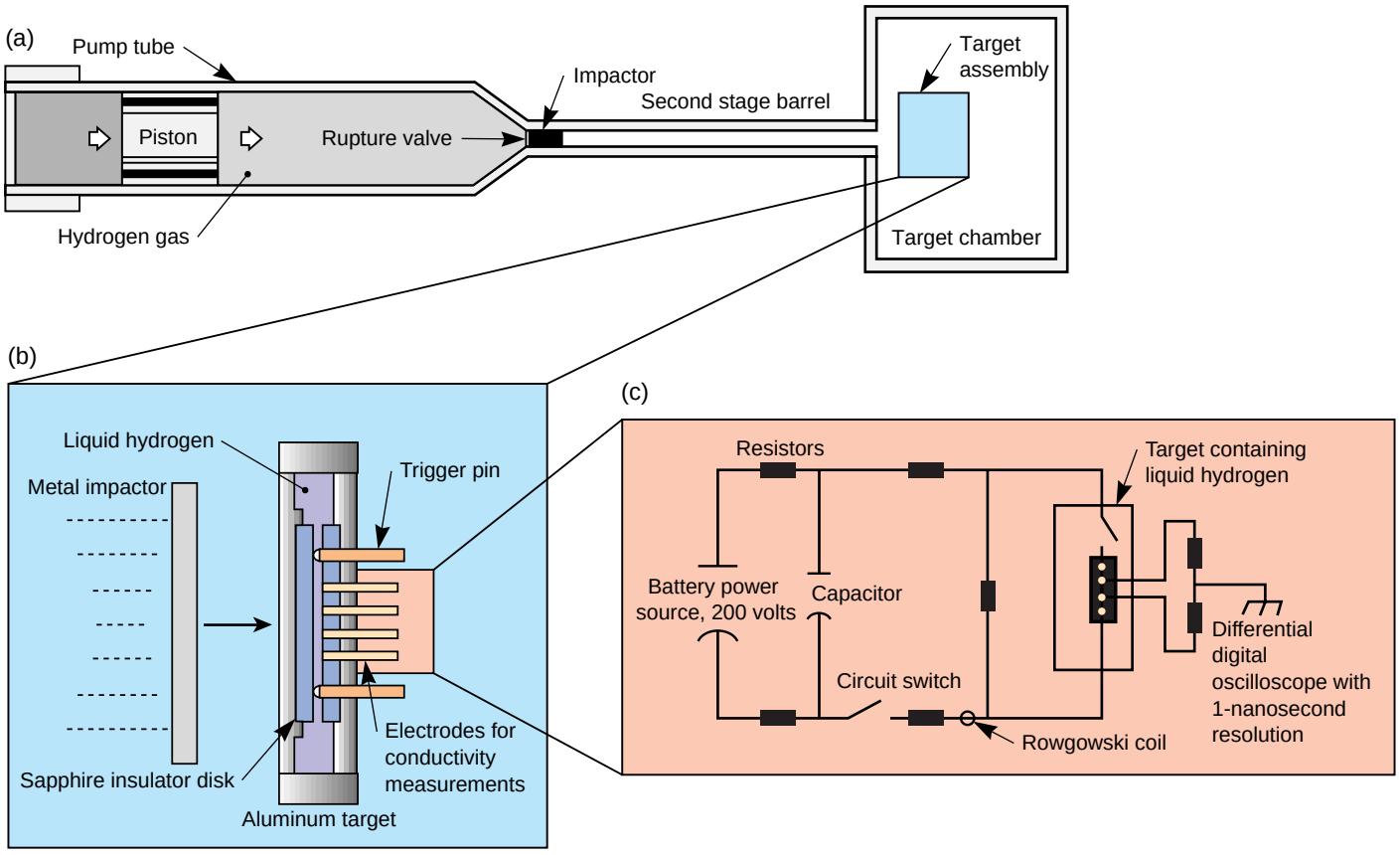


Figure 1. Our success in metallizing hydrogen came during a series of experiments to understand the electrical properties of shocked liquid hydrogen. (a) Our two-stage light-gas gun accelerates plastic-encased aluminum and copper impactor plates to velocities of up to 8 kilometers per second (18,000 mph), sending a shock wave into (b) the target assembly containing a 0.5-millimeter-thick sample of liquid hydrogen. Electrical resistivity/conductivity is measured using (c) a four-probe constant-current circuit. Trigger pins turn on the data-recording equipment when hit by the initial shock wave, and a Rowgowski coil measures current. The circuit is connected to a differential digital oscilloscope, which instantaneously records the electrical quantities during the test.

Our Approach

In 1991, we began a series of experiments to determine how compression affected the electrical properties of diatomic or molecular hydrogen and deuterium both of which are insulators at ambient temperatures and pressures. Our specific objective was to advance fundamental understanding of the way hydrogen transitions from an insulator to a conductor at shock-test pressures and temperatures. Evidence of actual metallization was an unanticipated result of our experiments. It was unexpected for several reasons: (1) we used liquid hydrogen, rather than solid hydrogen that conventional wisdom indicated was required; (2) we applied a methodology—shock compression—that had never before been tried in order to metallize hydrogen; and (3) we were working at higher temperatures (3,000 K) than metallization theory specified.

For our experiments, we used liquid hydrogen at an initial temperature of 20 K (–423°F) because: (1) it is easier to liquefy hydrogen than it is to solidify it in our experiments, (2) shock compression dramatically increases temperatures and turns solid hydrogen into liquid, so it made sense to begin with a liquid, and (3) only fluid hydrogen, not solid, is present in high-pressure and high-temperature systems that matter to the "real world"—in superhot, hydrogen-rich planets like Jupiter and Saturn and in fusion energy experiments like those conducted at Livermore where laser beams compress tiny spherical targets of liquid deuterium and tritium, both isotopic forms of hydrogen.

As in any shock-wave experiment involving liquids, we confined the liquid hydrogen (or in some cases liquid

How Our Gas Gun Works

Our shock compression studies use a 20-meter-long, two-stage light-gas gun built by General Motors in the mid-1960s for ballistic missile studies; the gun has been in operation at the Laboratory since 1972.

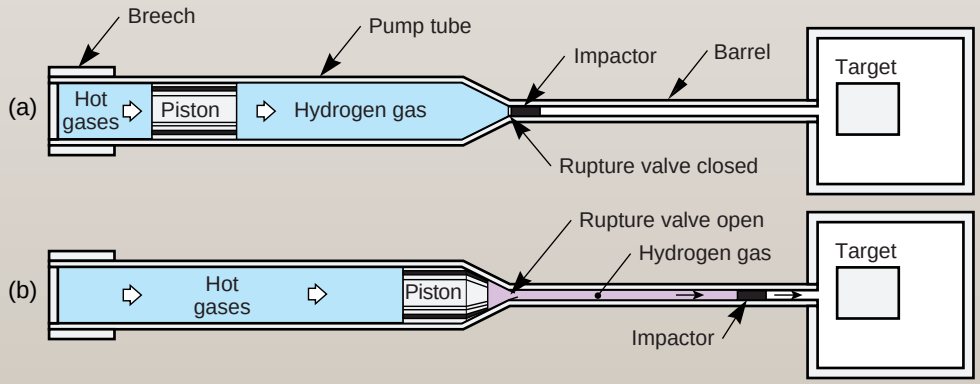
The gun consists of a first-stage breech containing up to 3.5 kilograms of gunpowder and a pump tube filled with 60 grams of hydrogen, helium, or nitrogen gas; and a second-stage evacuated barrel for guiding the high-velocity impactor to its target.

Hot gases from the burning gunpowder drive a heavy (4.5- to 6.8-kilograms) piston down the pump tube, compressing the gas. At sufficiently high pressures, the gas eventually breaks a rupture valve and enters the narrow barrel, propelling a 20-gram impactor housed in the barrel toward the target.

When the impactor hits the target, it produces a high-pressure shock wave. In a fraction of a microsecond, the shock wave reverberates through the target. Diagnostic equipment, triggered by the initial wave, measures the properties of the shocked material inside the target during this extremely brief period.

Projectile velocity can range from 1 to 8 kilometers per second (up to 18,000 mph). The preferred velocity is achieved by selecting the appropriate type and amount of gunpowder, driving gas (hydrogen for velocities at or above 4 kilometers per second, helium and nitrogen for lower velocities), pressure required to open the rupture valve, diameter of the barrel, and the metal and mass of the impactor.

The velocity of the shock wave, when combined with the initial conditions (impactor velocity, known densities, equation of state of the projectile and target materials) yields a precise measure of the pressure, density, and energy attained.



(a) In the first stage of the gas gun (blue shading), hot-burning gases from gunpowder drive a piston, which in turn compresses hydrogen gas. (b) In the second stage (pink shading), the high-pressure gas eventually ruptures a second-stage valve, accelerating the impactor down the barrel toward its target.

deuterium) in a suitable target container that separated it from the vacuum of the target chamber. (Refer to Figure 1b.) The target walls had the required flat impact surface and were made of a material for which we have an accurate equation of state (aluminum) so that we could compute the pressures, densities, and temperatures reached during the experiments. The liquid hydrogen (or deuterium) was a half millimeter thick, and the target was cryogenically cooled.

We sandwiched the target between two single-crystal sapphire anvils that provide stiffness and electrical insulation for the four steel electrodes implanted at the surface of the liquid hydrogen inside the target. These electrodes are used to measure the changes in the sample's electrical resistivity/conductivity during shock tests. Two of the electrodes introduce current to the inertially confined hydrogen sample, and two measure voltage across the sample. A trigger pin in the target produces an electrical signal when struck by the initial shock wave, turning on the data recording system (Figure 1c) at the proper moment. The conductivity of the shocked hydrogen is thus measured before the pressure wave reaches any external surface, that is, before the sample holder blows up when the shock reaches its external surface.

We mounted the anvils on aluminum plates that serve as the front and rear walls of the target, initially at 20 K. At that low temperature, the aluminum remains strong and ductile. Finally, we carefully wrapped the target with 50 layers of aluminized mylar to reduce the heat losses that would boil away the liquid hydrogen and cause our sample to literally

disappear. The impactors aimed at these target samples were made of aluminum and copper embedded in plastic.

Using these impactors in the gas gun, we shocked the hydrogen samples to pressures ranging from 0.9 to 1.8 Mbar and temperatures from 2,000 to 4,000 K. We designed our conductivity experiments to consist of an initial weak shock in the hydrogen followed by a series of very weak shocks reverberating between sapphire anvils, between which our hydrogen sample was sandwiched. In this way, the temperature was kept about ten times lower than it would be for a single sharp shock to the same final pressure. Each data point we recorded using the diagnostics illustrated in Figure 1c represents a measurement taken in about one ten-millionth of a second, which is more than sufficient for the sample to come into equilibrium, that is, reach a stable pressure, density, and temperature. Electrical signal levels of a few hundredths of a volt and currents of about 1 ampere lasted about 200 nanoseconds (200×10^{-9} seconds), indicating that, indeed, metallization had occurred.

Our Results

As shown in Figure 2, we found that from 0.9 to 1.4 Mbar, resistivity in the shocked fluid decreases almost four orders of magnitude (i.e., conductivity increases); from 1.4 to 1.8 Mbar, resistivity is essentially constant at a value typical of that of liquid metals. Our data indicate a continuous transition from a semiconducting to metallic diatomic fluid at 1.4 Mbar, nine-fold compression of initial liquid density, and 3,000 K.

Some theorists have speculated that metallic hydrogen produced under laboratory conditions might remain in that state after the enormous pressures required to create it are removed. However, metallization in our experiments occurred for such a brief period of time, and in such a manner, that questions about hydrogen's superconducting properties and retention of metallic form could not be answered.

At the relatively low temperature, the fluid hydrogen remained almost essentially molecular, rather than breaking into individual atoms. As a result, electrons in the sample freely flowed from molecule to molecule in a fashion that is characteristic of metals. At metallization, we calculate that only about 5% of the original molecules have separated into individual atoms of hydrogen, which means that our metallic hydrogen is primarily a molecular fluid. (Observation of this molecular metallic state in our experiments was unexpected. Only the monatomic metallic state was predicted by theory.)

In looking at the insulator-to-metal transition, we focused on the changes in electronic energy band-gap (measured in electron volts) in hydrogen under shock compression. The value of the electronic band-gap is the energy that must be absorbed by an electron in order for it to contribute to electrical conduction. A zero band-gap is characteristic of a metal; a positive, nonzero band-gap is characteristic of an insulator. Thus, the magnitude of the band-gap of an insulator is a measure of how far away the insulator is from being a metal.

At ambient pressure, condensed molecular hydrogen has a wide band-gap (about 15 electron volts), making it a

Figure 2. As shock compression increases pressure, liquid molecular hydrogen's electrical resistivity falls dramatically, a decrease of almost four orders of magnitude from 0.9 to 1.4 megabars before plateauing between 1.4 and 1.8 megabars where resistivity (and conversely, conductivity) is essentially constant at a value typical of that of a liquid metal. Our experiments used molecular hydrogen and deuterium, which have different densities.

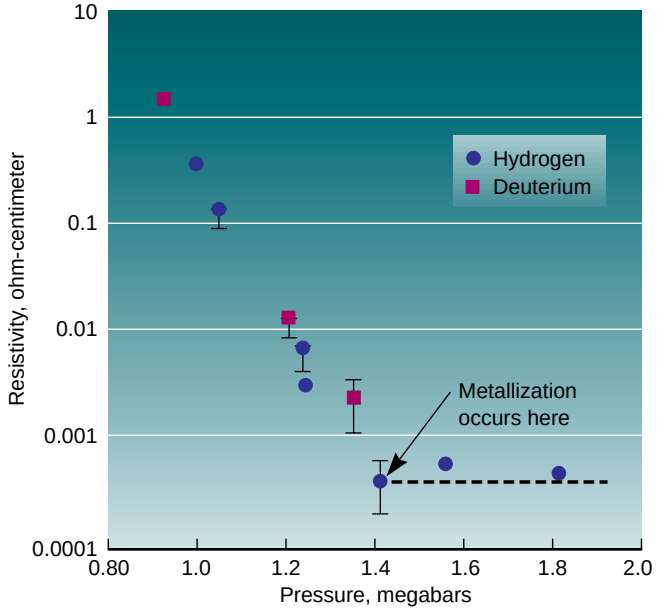


Figure 3. We examined electronic band-gap changes as molecular hydrogen makes the transition from insulator to conductor. At ambient pressure, condensed molecular hydrogen has an electronic energy band-gap of 15 electron volts (eV), making it an excellent insulator. In previous single-shot shock compression experiments (at up to 0.2 megabars pressures and 4,600 degrees kelvin), measurements yielded an energy gap of 11.7 eV.[5] The results of our new shock compression studies (shown by the solid part of the curve) indicate that molecular hydrogen becomes metallized when the band-gap is reduced to about 0.3 eV.

transparent insulator, like glass. Theory said that when hydrogen is squeezed by tremendous pressure, the gap would close to zero (the band-gap of metals, which are nontransparent conductors). Our studies show that when shocked multiple times in a very cold liquid state, hydrogen becomes first a semiconductor and then a fluid metal when, as its density increases, its temperature becomes equal to the band-gap at about 0.3 electron volts (Figure 3). At this point, all the electrons that can be excited by the shock to conduct electricity have been excited. Insensitive to further decreases in band-gap, the conductivity stops changing. Our conductivity data for hydrogen are essentially the same as those for the liquid metals cesium and rubidium at 2,000 K undergoing the same transition from a semiconducting to metallic fluid. The comparison is shown in Figure 4.

Implications/Future Research

Our gas-gun experiments enhance collective knowledge about the interiors of giant planets. Our earlier studies of temperature measurements of shock-compressed liquid hydrogen led us to conclude that Jupiter's molecular envelope is cooler and has much less temperature variation than previously believed. Further interpretation of those data suggests that there may be no distinct boundary between Jupiter's core and mantle, as there is on Earth.[6]

Jupiter, which is almost 90% hydrogen, is not the only planet rich in metallic hydrogen. Hot metallic hydrogen is believed to make up the interior of Saturn and may be present in other large planets discovered recently outside our solar system. The presence of metallic hydrogen in these planets has a pronounced effect on their behavior. On Jupiter, given its extreme internal pressures, the bulk of hydrogen is most likely in the fluid metallic state; in fact, given the pressure at which hydrogen metallizes, much more metallic hydrogen—the equivalent of 50 times the mass of Earth—exists in Jupiter than previously believed. We also assume this metallic hydrogen is the source of Jupiter's very strong magnetic field, the largest of any planet in our solar system.

The results of our experiments lend credence to the theory that Jupiter's magnetic field is produced not in the core, but close to the Jovian surface (Figure 5). Based on our data, it appears that the band of conductivity producing the magnetic field is much closer to the planet's surface than was thought to be the case.[7]

We anticipate that laser fusion scientists, who use the compressibility of hydrogen to tune laser pulses, also will find the results of our metallic hydrogen experiments extremely useful. Our experiments provide new insight into the behavior of deuterium and tritium, isotopic forms of hydrogen used in laser fusion targets. Higher fusion-energy yields could result from an improved understanding of the temperature–pressure relationship in hydrogen and its isotopes. Indeed, our hydrogen metallization studies suggest strongly that the revised computation of the equation of state of hydrogen at intense pressures will help in perfecting the hydrogen-isotope-filled targets being designed for the National Ignition Facility, making their performance range broader and more flexible. This is also encouraging news for the science-based

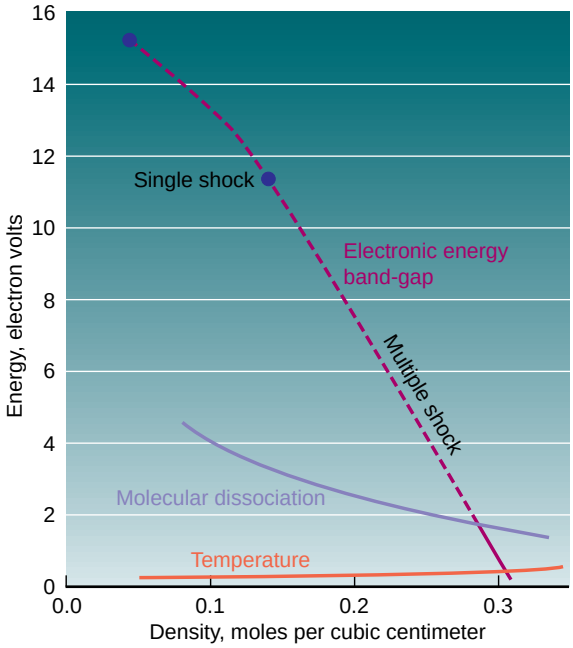
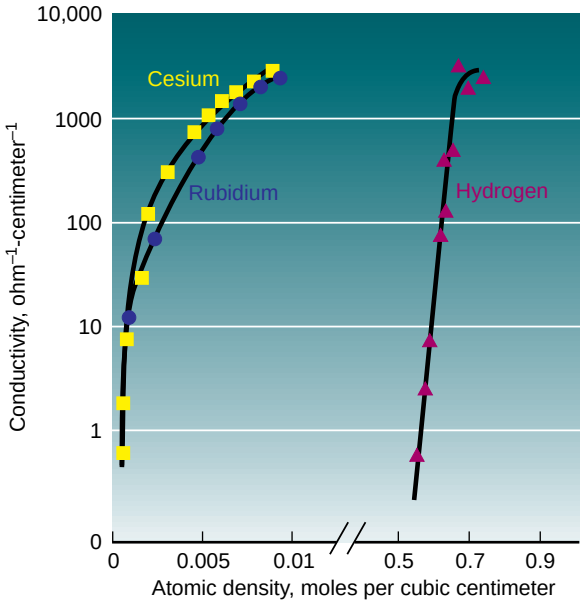


Figure 4. At 2,000 degrees kelvin, conductivity for hydrogen is about the same as that of the metals cesium and rubidium. Liquid molecular hydrogen becomes conducting at a higher density than do those metals.



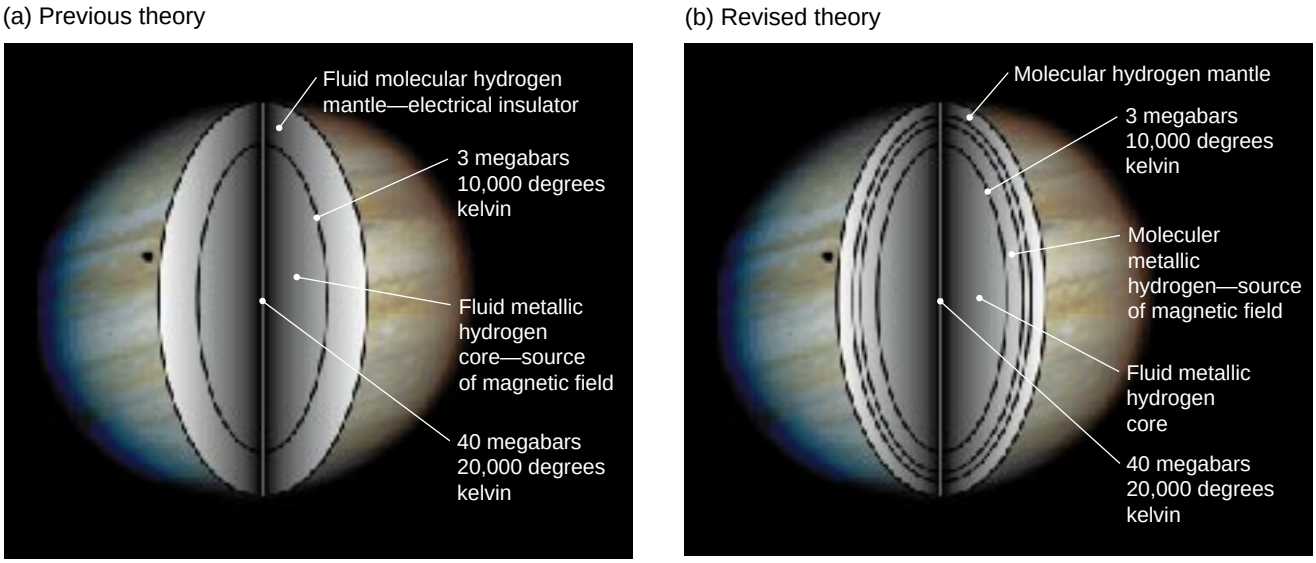


Figure 5. Our work has allowed us to calculate the electrical conductivity in the outer region of Jupiter. The planet's magnetic field is caused by convective dynamo motion of electrically conducting metallic hydrogen. Our results indicate that in Jupiter, the magnetic field is produced much closer to the planet's surface (Figure 5b) than was thought previously (Figure 5a).

stockpile stewardship research that will eventually be performed on NIF.

Future experiments will focus on (1) using various hydrogen isotopes—molecular hydrogen, deuterium, and hydrogen–deuterium—to determine the temperature dependence of the electronic energy gap, (2) exploring higher pressures up to 3 Mbar, and (3) probing effects in similar liquids such as molecular nitrogen and argon.

Key Words: gas gun; hydrogen—fluid, liquid, metallic; Jupiter; National Ignition Facility; shock compression tests; stockpile stewardship.

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About the Scientist

Physicist WILLIAM NELLIS joined the Laboratory in 1973. His specialty is the investigation of condensed matter both during and after high-pressure shock compression. The highlight of this work is the observation of the metallization of fluid hydrogen at 1.4 megabars pressure and nine-fold compression. He has delivered invited talks at 44 professional conferences since 1979 and is the author or co-author of more than 100 papers. A fellow of the American Physical Society's Division of Condensed Matter Physics, Nellis holds M.S. and Ph.D. degrees in physics from Iowa State University. He received his B.S. in physics from Loyola University of Chicago.

Keeping the Nuclear Stockpile Safe, Secure, and Reliable

In the absence of nuclear testing, the Department of Energy's Stockpile Stewardship and Management Program will use enhanced computational and experimental capabilities to help assess the status of the stockpiled weapons and predict, detect, evaluate, and correct problems affecting them. For Lawrence Livermore, the program represents a fundamental change from its historic nuclear weapons mission.

Vic Reis, Department of Energy's Assistant Secretary of Defense Programs, visited Lawrence Livermore last October to underscore the importance of the Stockpile Stewardship and Management Program. While at LLNL, Reis visited the preferred site of the National Ignition Facility, a key component of the program.

IT is not often that the Department of Energy's Assistant Secretary of Defense Programs visits the Laboratory to deliver a pep talk on a newly announced national security program of paramount importance to the department and the country. But that's what happened last October when Vic Reis told a packed assembly of more than 350 employees that the "awesome responsibility" for decisions regarding the safety and reliability of the nation's nuclear weapon stockpile "has been put right back where it belongs—with the labs."

Reis was referring to the DOE's far-reaching plan to make every effort possible to ensure that the nation's nuclear force remains safe, secure, and reliable without new weapon development or the use of underground testing. The plan, formally called the Stockpile Stewardship and Management Program (SSMP), is the result of close collaboration among the DOE and scientists from Livermore, Los Alamos, and Sandia National Laboratories. Indeed, in his address to employees, Reis credited LLNL Director Bruce Tarter and many top Livermore managers for their work to delineate for President Clinton, the Joint Chiefs of Staff, and the Congress the viability of the program, based on the projected capabilities and resources of the DOE weapon laboratories.

The SSMP will use enhanced computational and experimental capabilities to help predict, detect, evaluate, and correct problems affecting nuclear weapons in the national arsenal but without additional nuclear testing. For Lawrence Livermore, the program represents a fundamental change from its historic mission of nuclear weapon development, nuclear testing, and

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surveillance. Stewardship of the U.S. nuclear stockpile is now this laboratory's "foremost responsibility," according to Tarter.

Specifically, the ambitious goals of the nation's SSMP are to:

- Provide the capabilities for the maintenance, assessment, and certification of the stockpile, including sources of nuclear weapon expertise to provide independent, critical reviews.
- Provide the capability to address the full range of stockpile problems that may arise.
- Minimize to the greatest extent possible the risks involved in maintaining the U.S. nuclear stockpile under the constraints of no additional nuclear testing, no new-design weapon production, and limited budgets.
- Preserve the essential technical expertise unique to nuclear weapons.
- Provide a supply of tritium to replenish the inventory reduction caused by radioactive decay of tritium in existing weapons.
- Support U.S. nonproliferation, arms control, and nuclear weapon-related intelligence efforts.
- Provide the ability to reconstitute U.S. nuclear testing and weapon production capacities, should national security so demand in the future.

This new program addresses the U.S. nuclear stockpile, which is shrinking dramatically from Cold War levels. In the desire to conclude the Comprehensive Test Ban Treaty (CTBT), the U.S. has unilaterally halted the development and deployment of new nuclear weapon systems, begun closing elements of the nuclear weapon production complex no longer needed for a much smaller stockpile, stopped underground nuclear testing, and been involved in unprecedented nuclear arms limitation agreements between the U.S. and the nations of the former Soviet Union.

The program received powerful support last fall when President Clinton said that his decision to pursue a CTBT was based on assurances that the DOE nuclear weapon labs can meet the challenge of maintaining the nuclear deterrent under a CTBT through a Stockpile Stewardship and Management Program that does not include nuclear testing. This April President Clinton reaffirmed his determination to achieve a worldwide CTBT in a joint declaration with Russian President Boris Yeltsin.

The Human Factor: Preserving Key Skills and Assuring Sound Judgment

The Stockpile Stewardship and Management Program (SSMP) places a premium on skilled, experienced people. As Lawrence Livermore Director Bruce Tarter said in April, "Stewardship of an aging stockpile is a heck of a different job than innovative research and design. It will rely—even more than in the past—on people throughout the Laboratory, the universities, and industry."

However, nuclear weapon science is a highly circumscribed field; there exists no broad industrial or university base from which to draw nuclear weapon expertise. U.S. weapon scientists have no true peers other than their colleagues at the three DOE weapon laboratories.

In the last few years, many of LLNL's most experienced weapon scientists and engineers have retired or left the Laboratory, and further retirements of experienced staff are expected in the next 10 years. To prepare for this situation, Livermore, Los Alamos, and Sandia are archiving their nuclear design data, knowledge, and skill bases. Lawrence Livermore, for example, is videotaping classified interviews of retired weapon designers explaining their craft and the steps leading to key design decisions. Scientists and engineers new to the weapon program will be able to draw upon archival data as well as their experienced colleagues as they acquire the expertise to maintain the enduring stockpile in a time of no nuclear testing or new weapon development.

The SSMP places a premium on expert judgment in another important way. Throughout the history of the U.S. nuclear weapon program, interlaboratory peer review has helped to compensate for incomplete knowledge about nuclear weapon physics. Without nuclear testing, an independent review process is even more important.

Livermore and Los Alamos continue to be responsible for the weapon systems each laboratory originally designed, while Sandia has responsibility for the non-nuclear components and integration of all systems. At the same time, under a process called dual revalidation, Livermore and Los Alamos (aided by Sandia) formally examine and assess the safety and reliability of each other's weapon systems under the auspices of the Project Officer Groups of the Departments of Defense and Energy. The program offers another layer of confidence in safety, security, and reliability provided by some of the best researchers in the nation.

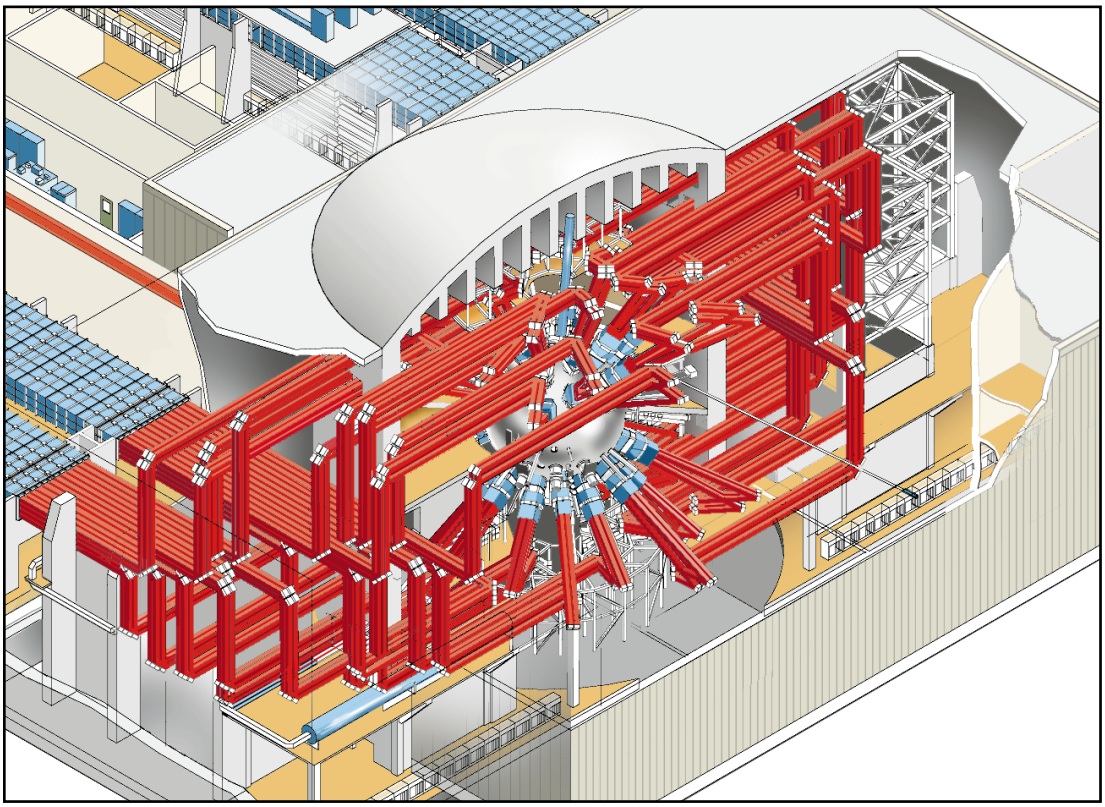
Urgency, Risk Underlie Program

An urgency underlies the program that can best be understood by realizing that the average age of the weapons in the U.S. stockpile next year will be greater than at any time in the past and will continue to increase until it soon exceeds the base of experience of the nation's weapon scientists. This is because the U.S. has no new weapons planned or in production to replace the oldest stockpile weapons.

Also, it must be anticipated that the reliability of the stockpile may degrade as the weapons age beyond their designed lifetimes. Problems could be caused, for example, by radioactive decay, slow chemical changes, or incompatible materials. Serious consequences could arise from common-mode failures, ones that occur when similar materials or fabrication processes are used in several weapon systems. Because recently concluded arms control agreements have sharply reduced the number of weapons, such common-mode failures can affect a larger portion of the stockpile than in previous eras.

It seems likely that problems will arise over the next few years. Of the nuclear weapon systems introduced into the U.S. stockpile since 1970, nearly half have required post-development nuclear testing to verify whether a problem existed, or to resolve or fix ones relating to safety or reliability. Furthermore, all of the weapon systems that are candidates for the enduring stockpile (those weapons permitted as a result of the START II agreement with Russia) have already been retrofitted to some degree, including the replacement of major nuclear components in some cases.

Weapon scientists must be able to accurately evaluate the severity of problems and devise the right "fixes," whether they be a remanufactured component, modification to a component to extend its lifetime, or substitution of a more reliable or safer part. In the past, the extent of a problem or the effectiveness of a "fix" could be determined with an underground nuclear test at the Nevada Test Site. If the problem proved to be particularly severe, a new warhead or weapon system could be developed. With nuclear testing and new weapon development no longer options, stockpile stewardship must rely on an



The target chamber of the National Ignition Facility (NIF). When operational in 2002, the NIF will permit experiments with conditions of pressure, temperature, and density close to those that occur during the detonation of a nuclear weapon.

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improved understanding of nuclear weapons based on greatly improved facilities and computational models.

In addition to urgency, some areas of risk were folded into the President's decision. It is known that in some cases there is no adequate substitute for nuclear testing. The weapon recertification process will take these risks into account.

Key Thrust Areas

The national stockpile stewardship program has three main thrusts: laboratory experiments, computer simulations, and stockpile inspections. In each, Lawrence Livermore has particular responsibilities.

Upgrading Experimental Facilities and Capabilities

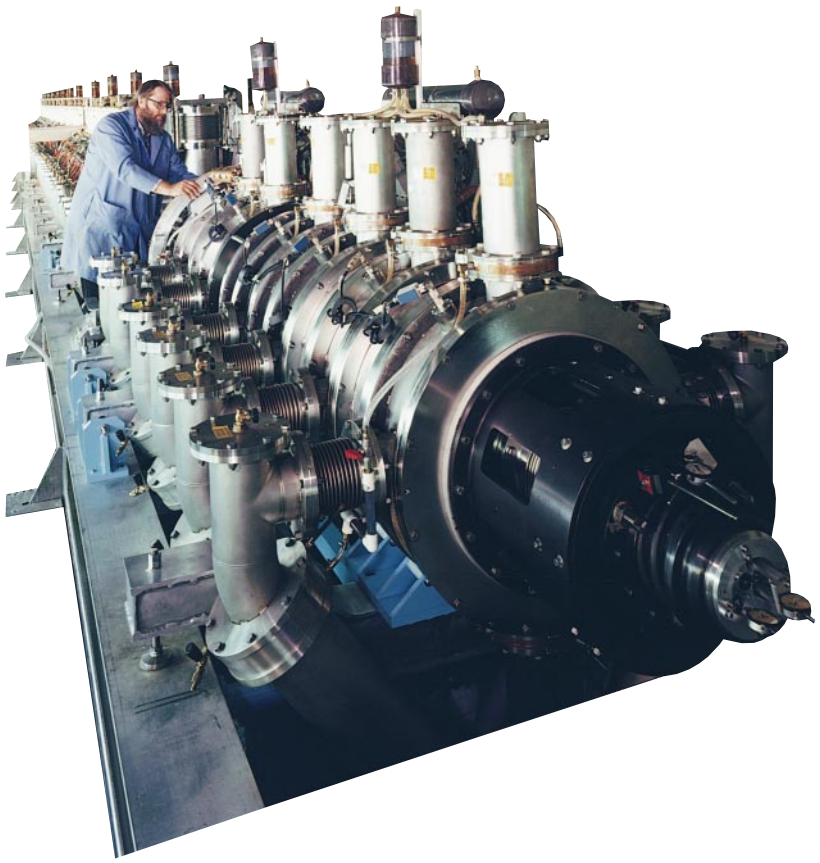
Defining the stockpile stewardship program has required extensive cooperation and coordination among Livermore, Los Alamos, and Sandia weapon experts. They recognize that the science of nuclear explosives is extremely complex. Even after more than four decades of work by hundreds of very capable scientists, gaps remain in understanding nuclear weapon behavior.

As a result, to provide needed data and simulations capability, a major thrust of the program is to upgrade existing experimental and computational capabilities at the three weapon laboratories and to design and construct several new facilities by providing insight into specific physics regimes. These strengthened capabilities will compensate, to the greatest degree possible, for the absence of nuclear testing. Together, the facilities will give the ability to investigate most phases of nuclear weapon operation. (See the box on p. 80 for a list of key facilities.)

Enhanced experimental facilities will provide the ability to evaluate safety and performance issues that could have significant stockpile consequences. The new data will be combined with past data from experiments and nuclear tests and used to validate new and evolving computational models. Also, enhanced experimental and computational capabilities will help the weapon laboratories maintain the knowledge and skill base that are essential for training new people and assuring continued support for stockpile stewardship.

It must be remembered that laboratory experiments cannot duplicate a nuclear test. Even the most advanced non-nuclear experiment can access only a small portion of the physics regimes or materials dynamics relevant to nuclear weapons. Scientists and engineers face the new challenge of interrelating and extrapolating data from many different experiments to provide an overall evaluation of weapon safety and performance.

Also important to the DOE and its laboratories is the planning under way now to develop and build the National



LLNL's Flash X-Ray (FXR) machine, located at Site 300, is a part of the most capable high-explosives test facility in the world. The facility uses powerful x rays to penetrate deeply into dense materials and record the configuration of these materials at a chosen time during the operation of a test device.

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Ignition Facility (NIF), which will provide more than ten times the power of the Nova laser at a greatly decreased unit cost. Site selection will occur after public review of a program-wide environmental impact statement and record of decision are completed later this year. The preferred site for NIF is Livermore, although wherever it is located, all of DOE's nuclear researchers will be using NIF to further understand nuclear weapons.

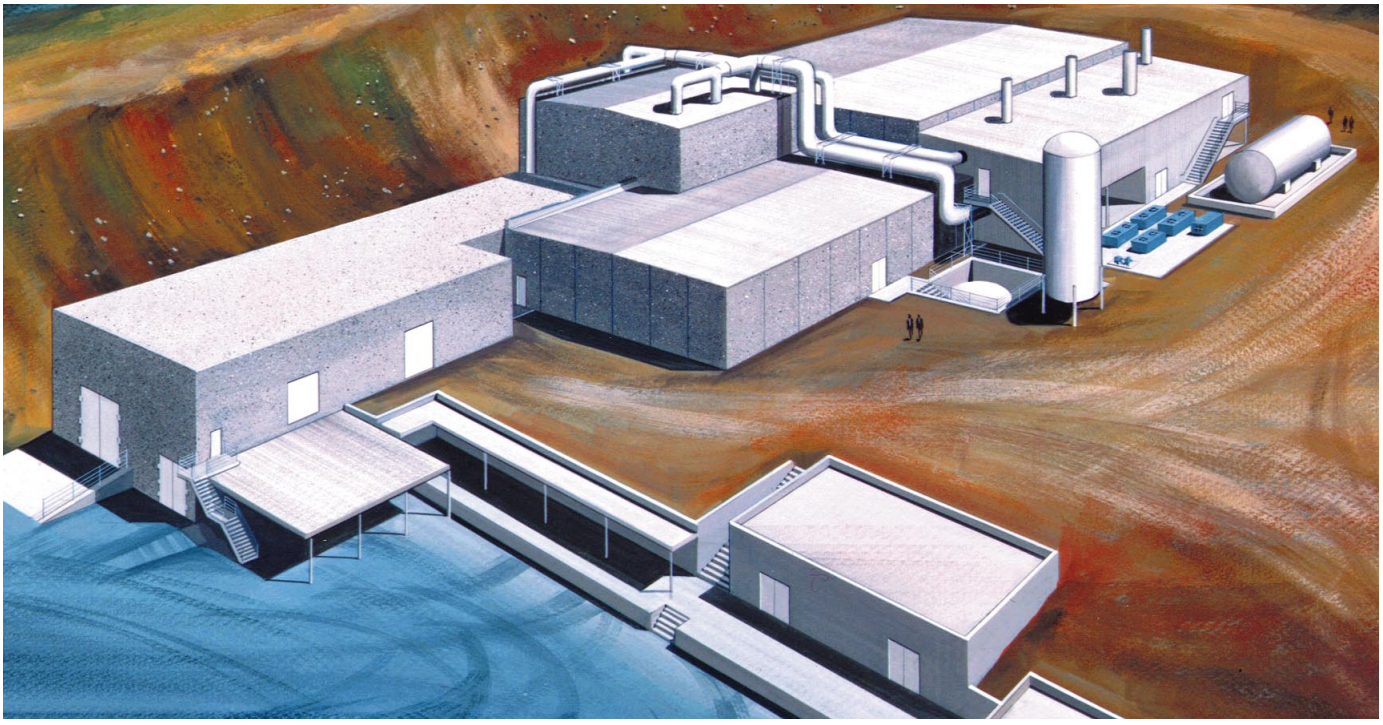
The need to obtain better data on the properties of plutonium and how it performs in an aging nuclear warhead is crucial. Experiments planned by Livermore and Los Alamos will reveal new information about the properties of plutonium at conditions close to those during weapon implosion. LLNL researchers also plan to conduct subcritical experiments on plutonium. Examples of this work include diamond-anvil-cell pressure measurements, equation-of-state studies, and metallurgical evaluations of aged plutonium.

Simulating Nuclear Testing

In the absence of nuclear testing, computer simulation is the only way to assess the performance of a complete nuclear weapon system. Numerical simulation also provides an essential tie to data from past nuclear tests and is an important means of predicting the performance and changes that might occur in the stockpile due to aging, environmental exposure, materials incompatibilities, or other reasons.

However, even today's most advanced supercomputers are not adequate to do the job. Increases of up to 10,000 times in computational speed, network speed, and data storage capacity are needed to provide simulations of weapon safety and performance of the required complexity and detail when testing is not an option. New generations of supercomputers, especially those employing many parallel processors, will greatly increase the accuracy, completeness, and resolution of computer calculations as they simulate nuclear weapon phenomena in three dimensions.

The objective of DOE's Accelerated Strategic Computing Initiative (ASCI) is to vastly improve the weapon simulation capability at the national security laboratories to the level required for stockpile stewardship. The goals are to develop advanced computational models and to work with industrial partners to develop the requisite technologies, including



An addition to the FXR, the Contained Firing Facility, at Livermore's Site 300, will permit fully contained high-explosive tests with up to 60 kilograms of energetic explosives. This upgrade is desirable in light of increasingly restrictive environmental regulations.

Stockpile Stewardship: Advanced Experimental Facilities Needed by the program

A number of current and proposed experimental facilities are needed by the DOE-wide program to support assessments about weapon safety and reliability in the absence of nuclear testing. These include:

Laser Facilities

- *Nova Laser.* The Nova laser, located at Livermore, is used for weapon physics and weapon effects experiments in addition to research on inertial confinement fusion (ICF).
- *National Ignition Facility (NIF).* NIF, a 192-beam laser facility planned for Livermore, will simulate on a small but diagnosable scale conditions of pressure, temperature, and energy density close to those that occur during a nuclear explosion. It will also serve ICF researchers.

High-Explosives Facilities

- *Contained Firing Facility (CFF).* The CFF, an addition to the Flash X-Ray (FXR) facility at Livermore, will provide for well-diagnosed, fully contained high-explosives testing of up to 60 kilograms of energetic explosives.
- *Dual-Axis Radiographic Hydrodynamic Test (DARHT) Facility.* The DARHT Facility at Los Alamos will provide enhanced radiography of the high-explosive implosion, including data on implosion symmetry as a function of time.
- *Sub-Critical Experimental Facility (SCSS).* This facility at the Nevada Test Site will provide capability to gather data on fissile materials in explosive-driven experimental geometries.
- *Advanced Hydrotest Facility (AHF).* An AHF would provide three-dimensional time-radiography of high-explosive implosions. Its location is not yet determined.

Accelerator and Pulsed-Power Facilities

- *Los Alamos Neutron Science Center (LANSCE).* LANSCE provides an accelerator-based neutron science capability for materials science studies of weapon components and for development of the technology for accelerator production of tritium.
- *Atlas Facility.* The Atlas pulsed-power facility at Los Alamos will provide implosions of cylindrical assemblies to obtain physics information that apply to weapons.
- *High-Explosive Pulsed-Power Facility (HEPPF).* HEPPF will be used to study weapon physics issues of shock pressures and velocities close to actual weapon conditions.
- *Advanced Radiation Source (ARS).* An ARS facility would provide high-energy, high-temperature, x-ray pulses for experiments in weapon physics, radiation effects, ICF, and pulsed power technology.

processors, software, and data storage to implement them.

Enhancing Stockpile Surveillance and Maintenance

The standard surveillance effort of the SSMP is focusing on the real-time status of weapon components in the stockpile through inspections and testing. Scientists also need a better understanding of how materials change and interact over time and how such changes affect weapon reliability and safety. An improved understanding of aging and material compatibility will help experts predict which parts need to be replaced or refurbished long before they severely impact weapon performance.

Stockpile weapons will be disassembled, examined, and evaluated. Some components will be remanufactured in order to fix problems that will inevitably arise. In past years a large weapon production complex provided the means to rapidly fix any problems with new stockpile weapons. Today significant elements of the production complex have been shut down, and manufacturing capabilities are being consolidated at fewer sites because it is not practical or cost effective to meet manufacturing needs by keeping many of the old processes or facilities on standby. These new practices differ considerably from those in the past.

Clearly, investment is needed to develop manufacturing processes that are flexible, that minimize the production of hazardous waste, and that do not require extensive facilities and infrastructure. Concurrent engineering, in which the development of advanced manufacturing and material processing proceeds apace with the development of weapon components, is under active study. Where warranted, some production responsibilities are being

reconfigured to rely on the laboratories' capabilities in manufacturing technology and their facilities for handling nuclear materials.

The Challenges for LLNL

For LLNL, says Associate Director for Defense and Nuclear Technologies Michael Anastasio, the job of stockpile stewardship will be "as challenging as anything we have done." The work at Lawrence Livermore centers on seven major efforts: extension of weapon lifetimes, enhanced stockpile surveillance, revalidation of existing weapon systems, flexible manufacturing, high-explosives experiments, the NIF, and supercomputers (including ASCI).

Extending Weapon Lifetimes

The Department of Defense (DoD) typically has expected weapons to be fielded in the stockpile for 20 years. Now weapons will remain there longer, and more importantly, many will soon reach an age that exceeds our operating experience. At the same time, substantive reductions in the size and redundancy of the nuclear weapon complex are occurring. These substantial changes throughout the complex led to the need to integrate support for sustaining all weapon types in the stockpile. The Stockpile Life Extension Program meets this need by integrating programs and activities across the DOE complex.

The W87 life extension program, begun in September 1994, works to enhance and refurbish the structural integrity of the warhead to extend its lifetime. In 1995, with the DoD, LLNL conducted a successful flight test of a W87 test unit on a Peacekeeper missile launched from Vandenburg Air Force Base. Livermore also conducted ground tests to evaluate the performance of refurbished design options when exposed to environmental extremes. Physics analysis of the refurbished design options is continuing, and information has been transferred to Los Alamos for their independent technical review.

Enhancing Stockpile Surveillance

Surveillance and evaluation of the safety and reliability of U.S. nuclear weapons have been essential Lawrence Livermore responsibilities ever since the first LLNL-designed weapon entered the stockpile. A major current focus for LLNL weapon scientists is on surveillance responsibilities for the B83 bomb, the W84 cruise missile warhead, and the W62 and W87 ICBM warheads. Livermore weapon experts are developing comprehensive plans to extend the life of these systems through an expanded program of surveillance, maintenance, and refurbishment.

LLNL experts are working to increase knowledge in the science of surveillance to better understand and predict the effects of age on metals, high explosives, polymers, and other materials under realistic service environments. The program is developing new surveillance technologies, such as new sensors that will allow extensive self-diagnosis of weapon components.

Other nondestructive evaluation and imaging techniques involve tools like scanning tunneling microscopes to examine, on an atomic level, the effects of corrosion on critical weapon parts.

Enhanced stockpile surveillance requires more detailed computer models of materials, from the atomic level to the systems level. Advanced models will help experts anticipate the onset of potential safety or reliability problems as well as reveal the likely effects of substituting different materials or manufacturing processes. This ambitious modeling effort, one of the keys to stockpile stewardship success, involves researchers in Livermore's Chemistry and Materials Science, Physics and Space Technology, and Engineering Directorates, as well as colleagues at several universities (see the June 1996 *S&TR,* pp.6–13).

Assessing with Dual Revalidation

Resolving stockpile issues without nuclear testing requires a much better understanding of the physical processes that determine the safety, reliability, and performance of weapon systems. Part of the SSMP will include dual revalidation, in which two independent teams will assess a weapon system to revalidate its ability to meet its current military characteristics and stockpile-to-target-sequence requirements. The two independent teams, working with the coordination of the DoD/DOE Project Officers Group, are the original design team (made up of the weapons laboratories that were involved with the original weapon development) and the independent review team (laboratories not involved with original development).

The assessments will include analysis of historical development and nuclear and high explosives test data, surveillance data, and recent test data. Where new experimental and computational capabilities have become available since development, they will be applied to the weapon system being evaluated. The first weapon system to undergo such an assessment will be the W76, a Los Alamos system. Because the W76 is deployed on both the C4 and the D5 missiles, it will be assessed for both delivery systems.

Flexible, Affordable Manufacturing

An allied effort is providing the flexible, affordable manufacturing capabilities needed to replace and refurbish aging and defective weapon components. This streamlined

manufacturing capability will use modern commercial methods whenever possible to build a systematic refurbishment and preventive maintenance program for stockpile weapons. Much of this work is being done as part of the DOE-wide Advanced Design and Production Technologies (ADaPT) program aimed at developing innovative manufacturing processes that reduce cost and waste, improve efficiency, and are environmentally friendly.

LLNL researchers are testing several new fabrication technologies that generate less hazardous waste and are less costly than previous methods. One example is precision casting of plutonium, which requires little or no subsequent machining and thus significantly reduces cost, waste, and personnel exposure to radiation. Another innovative concept is reusing certain old components that already contain plutonium, instead of manufacturing new parts.

Lawrence Livermore experts are developing precision casting, spinforming, and machining techniques to replace the current methods of rebuilding uranium parts destroyed in the surveillance program. For example, a project is under way to demonstrate the feasibility of using lasers to cut uranium parts with very little waste and almost no damage to the remaining material. The process uses laser expertise developed in LLNL's Inertial Confinement Fusion program and Atomic Vapor Laser Isotope Separation program.

Remanufacturing of critical parts requires a process of recertification, based on detailed tracking of the remanufacturing process as well as experimental and computational tools. Even more important, recertification requires expert judgment to provide confidence that the remanufactured component or weapon will perform as designed. Such judgment is essential because it is impossible to exactly duplicate past processes and practices. Researchers must reconsider how to remanufacture many of the old components and weapons because they are considered unacceptable today for environmental, safety, and health reasons.

High-Explosives Tests Critical

High-explosives testing is the only currently available way of experimentally testing part of the operation of a nuclear weapon's primary stage. In the test units, the nuclear materials are replaced by inert, surrogate materials. LLNL's Flash X-Ray (FXR) facility, located at Site 300, is a part of the most capable high-explosives test facility in the world. The facility uses powerful x rays to penetrate deeply into dense materials and record the configuration of these materials at a chosen time during the operation of the test device.

A three-year upgrade of FXR is in progress. The upgrade is expected to increase x-ray output by 50% and decrease x-ray spot size by 50%, allowing examination of implosion phenomena in much greater detail. The replacement of film by a digital gamma-ray camera has also provided images of greater resolution. The camera paves the way for an upgrade that will provide two images of an imploding device a few millionths of a second apart during a high-explosives test.

An addition to the FXR, the Contained Firing Facility, will permit fully contained high-explosives tests with up to 60 kilograms of energetic explosives. This facility is desirable in light of increasingly restrictive environmental regulations.

Lawrence Livermore researchers also are working with colleagues from other national labs, Bechtel Nevada, and Britain's nuclear weapon community to develop plans for an Advanced Hydrotest Facility, which would yield three-dimensional movies and data of the interior of an imploding device. (The site of this new facility is not yet determined, but it is not expected to be at Lawrence Livermore.)

NIF for Critical Physics Data

When operational in 2002, the NIF will permit experiments with conditions of pressure, temperature, and density closer to those that occur during the detonation of a nuclear weapon. By addressing the high-energy-density and fusion aspects of stockpile weapons, researchers will obtain critical, fundamental physics data that are essential for refining advanced computer simulation codes. We will need these codes to assess potential stockpile problems, certify fixes to stockpile systems, and continue certifying LLNL-designed warheads. Also, by using NIF-heated targets, scientists will sharpen their ability to predict the effects of radiation on weapon components.

Last year LLNL began the detailed design work for the NIF, identified by DOE's Reis as "the most important new facility" in the Defense Programs' budget request for Fiscal Year 1996. Lawrence Livermore has been designated the preferred site for this $1-billion project because of resident technical expertise and infrastructure.

Until the NIF comes on line, Lawrence Livermore's Nova laser will provide essential data on many aspects of weapon physics. In 1995, more than 200 ICF experiments were conducted with Nova by weapon scientists from Livermore and Los Alamos. (See Dec. 1994 *Energy & Technology Review,* pp. 23–32 for an in-depth look at the national security aspects of research using NIF.)

Moving to New Supercomputers

Lawrence Livermore weapon scientists emphasize that greatly enhanced modeling and simulation capabilities are critical to their ability to

Lawrence Livermore computational scientists are using three massively parallel supercomputers—two Meiko CS-2s (one is pictured here) and a Cray T3D—to develop codes that will represent three-dimensional simulations of nonlinear high-explosive and plasma-physics phenomena present in a nuclear detonation. However, in the future, the equivalent of thousands of these machines will be required.

assess the status of nuclear stockpile weapons, predict weapon performance, analyze refurbishment options, and evaluate potential accident scenarios. Major improvements are needed in the fineness of detail, especially in three-dimensional calculations and in the physics incorporated into the codes. These codes must replicate existing nuclear test data before we can confidently use them for assessing stockpile problems.

Meeting these challenges requires computers with thousands of processors working together to rapidly solve a single problem. At Livermore, there are three of these so-called massively parallel supercomputers—two Meiko CS-2s and a Cray T3D. In these efforts, LLNL experts are using these computers to develop three-dimensional simulations that include the wide range of nonlinear high-explosive, nuclear, and plasma-physics phenomena present in a nuclear detonation. These efforts also require development of new numerical algorithms and programming techniques.

At the same time, Livermore computational experts are incorporating improved data from non-nuclear tests, developing a secure high-speed network to interconnect Livermore and Los Alamos supercomputer resources, and collaborating with universities and supercomputer companies to hasten the arrival of new generations of machines.

"Sustaining confidence in the stockpile in the post-Cold War world will be extremely difficult," says Associate Director Anastasio. "It's going to require us to adapt our skills to different approaches and different teaming across the Laboratory and throughout the DOE complex. That's the changing culture we face. There is plenty for everyone to do. We need the whole Laboratory working together to help pull it off. But this is something the Laboratory is very good at."

Key Words: Accelerated Strategic Computing Initiative (ASCI), Advanced Design and Production Technologies (ADaPT), Advanced Hydrotest Facility (AHF), Comprehensive Test Ban Treaty, (CTBT), flash x-ray (FXR), National Ignition Facility (NIF), Nova, Stockpile Stewardship and Management Program (SSMP), stockpile surveillance.

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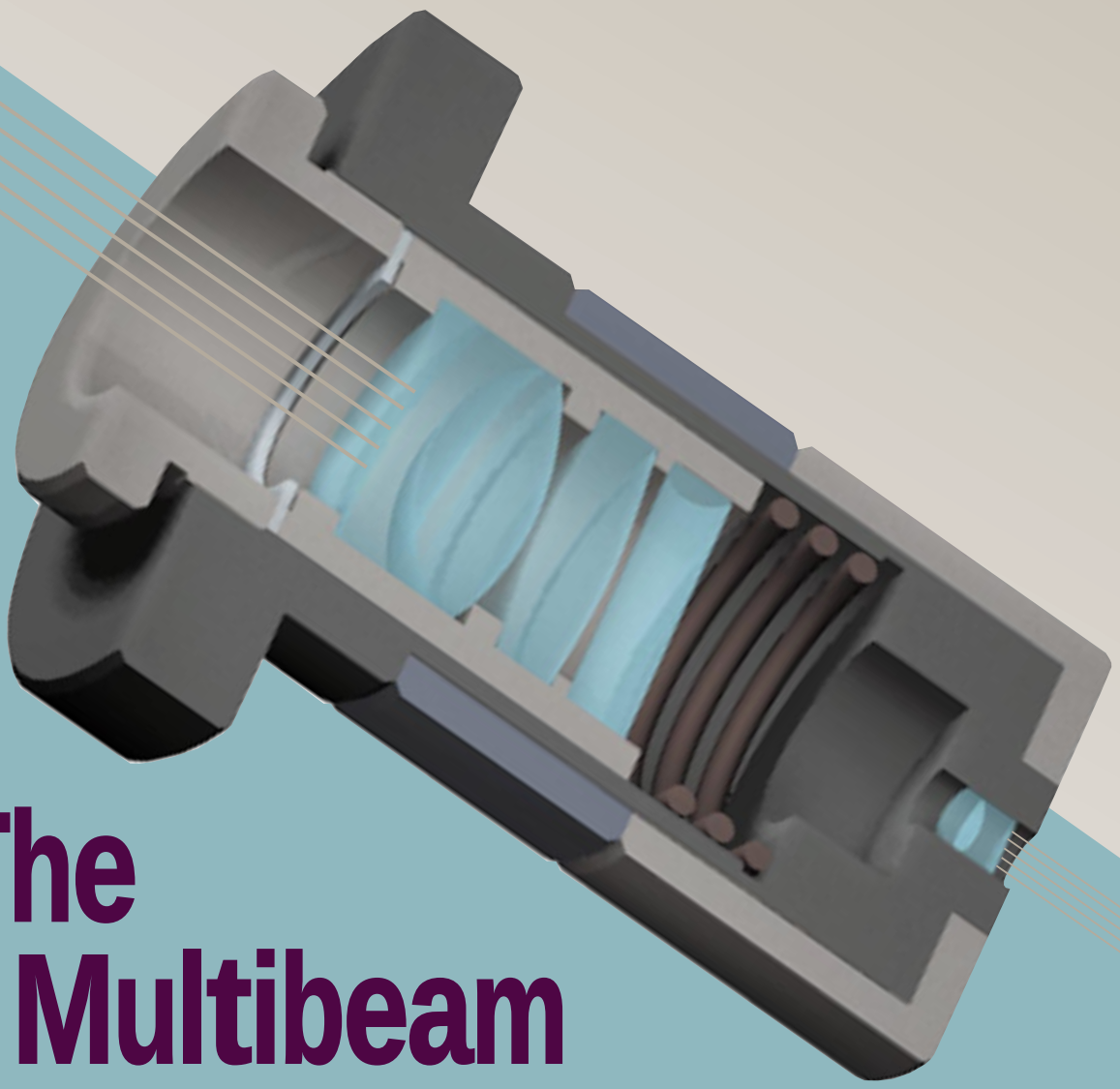


The Multibeam Fabry–Perot Velocimeter:

Efficient Measurement of High Velocities

Reprinted from July 1996 *Science & Technology Review*

THE standard method for measuring speed that we all learned in school is to divide distance by time. If we measure velocity rather than just speed, we can obtain information on direction. But how do we measure velocities of as much as 3,000 meters per second over distances as short as 2 or 3 millimeters? And why would we want to take such measurements?

As part of our responsibilities for scientific stewardship of our nation's nuclear weapons stockpile, Lawrence Livermore National Laboratory performs a variety of experiments to study the velocity and other motions of materials accelerated by explosives, gas guns, and electrically accelerated plates. We use a number of diagnostic tools, including a Fabry–Perot velocimeter, to analyze these experiments. These experimental data are then used to certify the safety and reliability of our nuclear stockpile without the validation provided by underground tests.

In our studies, we seek information on the equations of state of various materials, the behavior of materials subjected to strong shock waves and other hydrodynamic phenomena, the explosion process, and the behavior of projectiles and targets upon and immediately after impact. For example, we may look at how materials respond to various hypothetical scenarios. Our ability to measure continually changing velocities is important because shock waves, for instance, cause objects to have velocities that are not constant—the object may accelerate, then decelerate, and then accelerate again, all within a few microseconds.

A typical experiment might involve testing the behavior of a high-explosive material that has been shaped into a disk and coated with a half-millimeter-thickness of copper. Several diagnostic tools would be used to study the high explosive, one being a Fabry–Perot velocimeter to measure the velocity of the copper after the high explosive is detonated from the back. Depending on the experiment, we have from only 1 to 100 millionths of a second to obtain information, from detonation to the point where dust and debris from the explosion get in the way of data collection.

We compare the results from tests such as these to the predictions from our hydrodynamic computer modeling codes to determine whether the codes make adequate predictions. If the codes do not match test results, such data as material strengths can be changed in the codes. In the absence of a nuclear test program, this validation process must continue until we have full confidence in our modeling codes.

Obtaining accurate measurements is thus of critical importance. But efficient use of budgeted funds is equally important. For example, we could do one experiment five times to collect five comparable data sets for validation purposes. But then we would have the cost of the experiment times five plus the problem of replicating the experiment precisely, which is extremely difficult. We might or might not in fact collect five comparable data sets from those five experiments (the perennial apples and oranges problem). It would be better to obtain all five data sets at the same time, saving time and money and ensuring that we are comparing apples with apples when we study the data. But a traditional Fabry–Perot system, one of the best instruments available for obtaining continuous data on high-speed velocities, was able to

Livermore scientists have designed a multibeam Fabry–Perot velocimeter that is proving invaluable to the Laboratory's science-based stockpile stewardship mission. It provides high-resolution, continuous data records about the behavior of weapons materials accelerated to velocities as high as 3,000 meters per second.

take only one or sometimes two sets of measurements at a time. We could use five velocimeters to obtain five simultaneous data sets, but their cost would be very high, and the equipment would take up much space and be difficult to maintain and operate.

Scientists at Lawrence Livermore's High Explosives Applications Facility have been working for over 15 years to improve our capability to gather accurate information about high velocities. Building on that experience, we recently combined several newly developed devices with a high-power laser, a Fabry–Perot interferometer, and five streak cameras to create a multibeam Fabry–Perot velocimeter (Figure 1). We have split the laser light into five individual beams with very high efficiency and have devised the technology for keeping the five light beams distinct. Collecting five data sets simultaneously from a single experiment using one interferometer is now a reality.

Single-Beam Velocimetry

For many years Lawrence Livermore National Laboratory has been using laser interferometry to make high-speed velocity measurements. Interferometry operates on the principle of the Doppler effect, which is the apparent difference between the frequency at which sound or light waves leave a source and the frequency at which they reach an observer, caused by the relative motion of the observer and the wave source. It is the Doppler effect that causes the apparent pitch of a passing train to rise as the train approaches (creating shorter wavelengths or higher frequency) and to drop as the train moves away (creating longer wavelengths or lower frequency).

This same principle may be applied to the experiment described on p.85. We can shine laser light on the copper as it is being accelerated toward the light and collect some of the light that reflects off the copper. The velocity of the copper as it accelerates but before it disintegrates after detonation can be inferred by measuring the slight changes

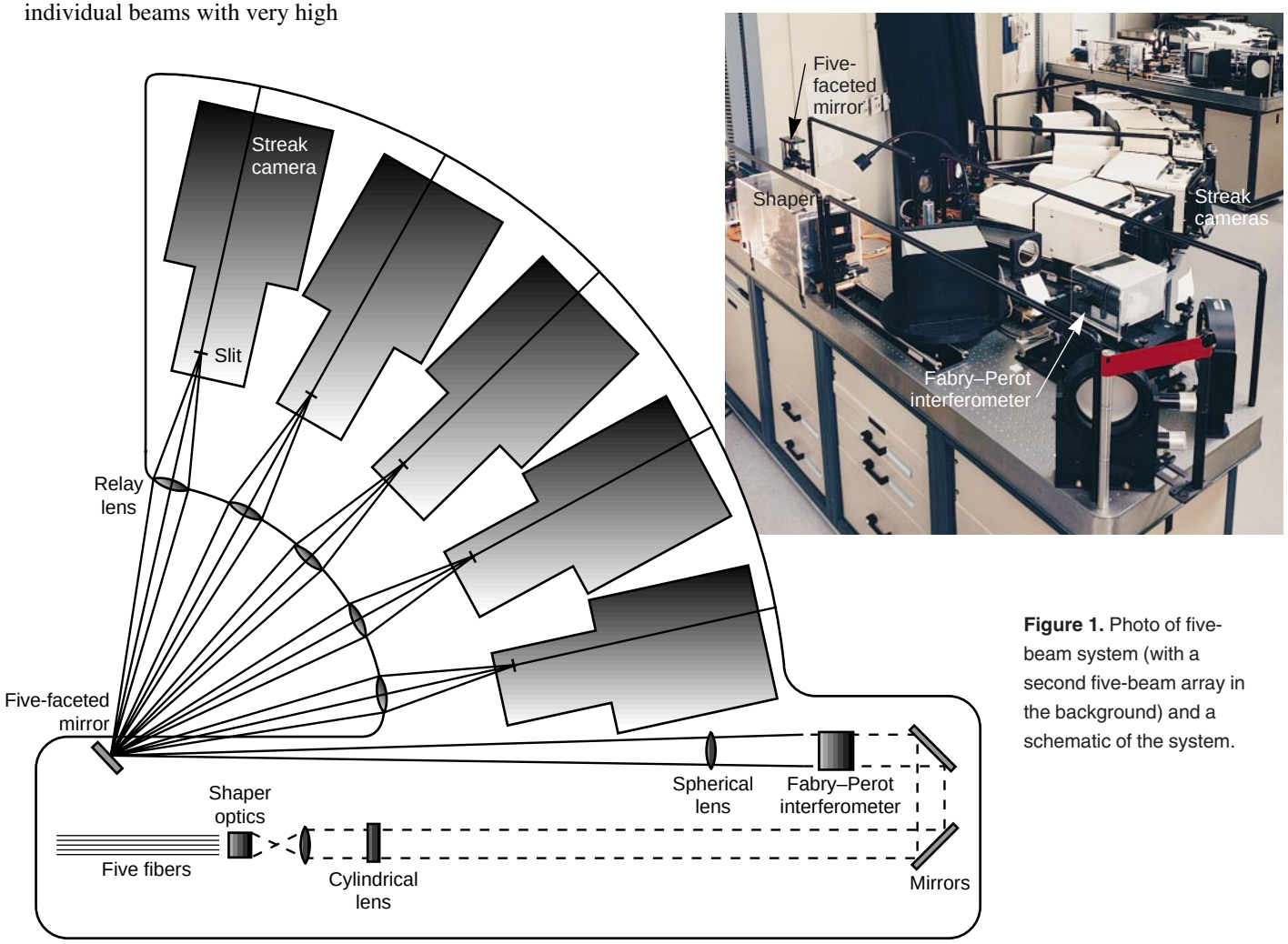


Figure 1. Photo of five-beam system (with a second five-beam array in the background) and a schematic of the system.

in the wavelength of the reflected light as the copper moves toward the unmoving light source. Because light waves are so small (about 2,000 wavelengths per millimeter), using them as a measuring device provides extremely high sensitivity. The laser's frequency is 6×10^{14}, or 600 trillion oscillations per second. Fifteen billion oscillations will occur in an experiment as brief as 25 microseconds.

The reflected light is sent through an interferometer, which splits the light source into several beams, sends them along different paths, and then combines them in an "interference" pattern. (In physics, interference refers to the increased amplitude of a wave that results from superimposing two or more waves of the same or nearly the same frequency.) Very precise velocity measurements may be made from this interference pattern.

The Fabry–Perot interferometer is almost 100 years old. Today, the Laboratory's version consists of a pair of round slabs of special glass, about 2 centimeters thick and about 7 centimeters or more in diameter. They are ground and polished flat to approximately one two-hundredth of a wavelength of light (or about three-millionths of a millimeter). The glass is made highly reflective by about 20 coatings of dielectric material evaporated onto its surface. The separation between these precisely parallel mirrors depends on the demands of the particular experiment and can range from a few millimeters for some applications to as much as 15 centimeters.

Before entering the Fabry–Perot, the reflected light passes through a cylindrical lens (see Figure 2), which converges the light vertically while maintaining the beam's horizontal dimension. Concentrating the light in this manner results in more usable light inside the interferometer.

The Fabry–Perot's first mirror is almost perfectly reflective (99.5%) and has a 0.75-millimeter-wide stripe of the dielectric coating removed from across its middle. The second mirror is typically about 93% reflective. Light enters the Fabry–Perot through the stripe in the first mirror and bounces back and forth between the mirrors about 50 to 100 times, creating the same number of weak transmitted beamlets parallel to each other and staggered in time. Because of the almost perfect reflectivity of the first mirror, virtually no light is lost back out the front mirror, except for a small amount that goes back through the stripe. The reduced reflectivity of the second mirror allows the beamlets to pass through it.

Each set of 50 to 100 beamlets travels a path from the first mirror, through the second mirror, and through a spherical lens to that lens's focal plane. Figure 2 shows that the first of the beamlets travels the shortest path, the second bounces once on the striped mirror before passing through the second mirror, the third bounces twice, etc. If the difference in the lengths of the paths of the successive beamlets is an integer number of wavelengths (e.g., 10,002 or 300,000), then the beamlets are all in phase and will interfere with (that is, reinforce) each other when they reach the spherical lens's focal plane. The interference pattern of each set of beamlets creates a bright dot.

Only certain combinations of the reflected light's wavelength and angle of reflection and the distance between the Fabry–Perot mirrors create resonant angles, which cause the beamlets from a

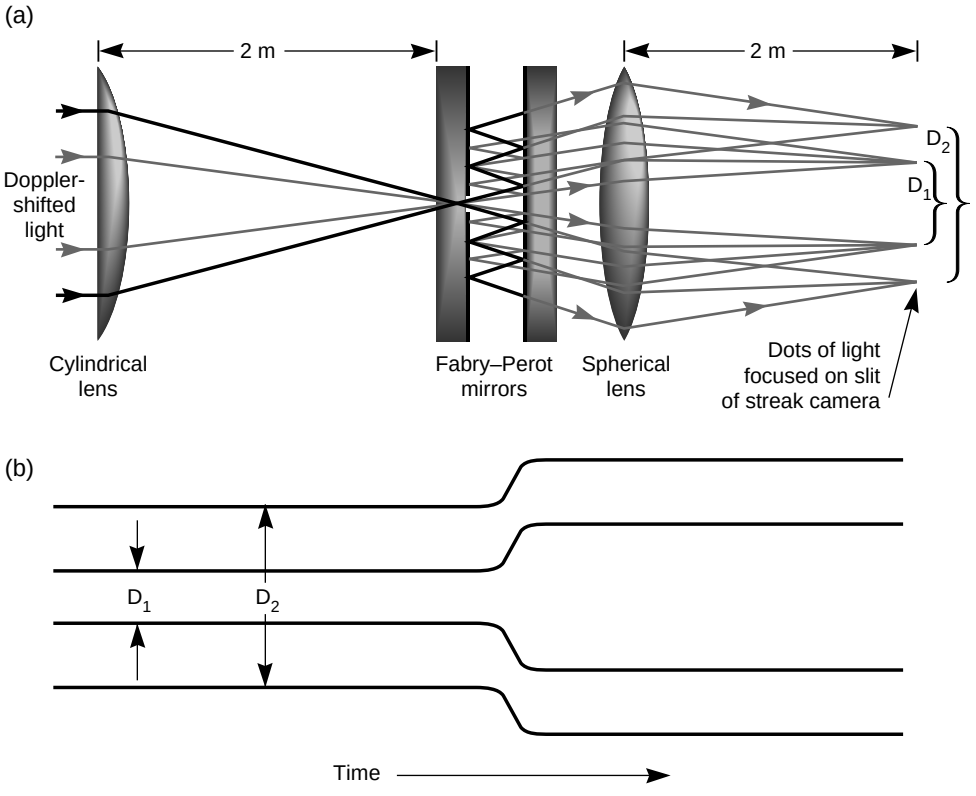


Figure 2. (a) A top view of the Fabry–Perot velocimeter system from the cylindrical lens to the slit in the streak camera. The interference pattern of bright dots—D_1 and D_2—is recorded on the streak camera. (b) A hypothetical streak camera record shows what happens to D_1 and D_2 when acceleration occurs. Velocities are determined using a formula based on measurements of the separation between the dots.

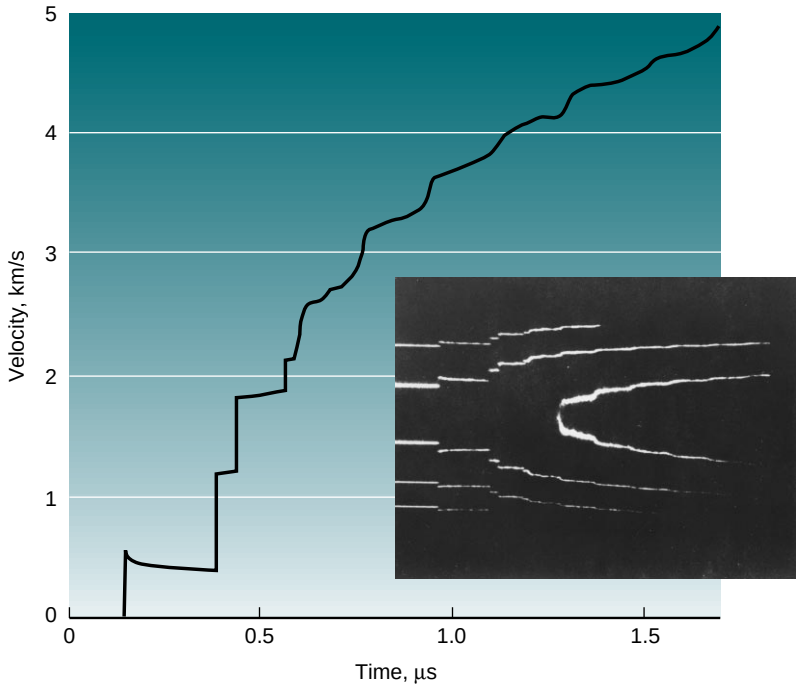


Figure 3. A time sweep as recorded by a streak camera (inset) translates into the velocity vs time record shown on the graph.

given beam to have the same phase and to interfere constructively with one another. The combination of the cylindrical lens and the narrow stripe in the first mirror assures that virtually all of the light entering the Fabry–Perot is at vertical angles, creating enough resonant angles to create six or eight bright dots.

As the copper accelerates, the reflected light's wavelength decreases, the resonant angles therefore increase, and the separation between the bright dots increases. This image of dots, known as an interference fringe, enters an electronic streak camera through a narrow vertical slit. In the streak camera, the image is swept across a piece of film (see Figure 3).

From the width and number of the fringes, extremely sensitive measurements can be made of the velocity history of the copper as a function of time, starting before acceleration began and continuing as long as conditions permit. The record of velocity versus time can be inferred using a formula that is based on measurements of the separation between the dots. Simple measurements of dot separation can be done with a magnifier and scale, and more precise analysis is done by digitizing the record.

Our Multibeam System

To collect five simultaneous sets of data, we cannot simply run five beams through a Fabry–Perot interferometer. Whereas the one-beam output is a series of bright dots with high velocity resolution, five beams would produce smeared records with low resolution. To obtain the high resolution required for precise velocity measurements, special optics are required to shape the five beams and keep them distinct.

There also needs to be a good way to split the laser light into five beams and to get the five reflected beams back to the instrumentation. The old method of shining the laser beam through a tilted mirror with a small hole in it works for one beam but would be unwieldy for more. There is also the problem of directing multiple outputs from the Fabry–Perot interferometer to several streak cameras.

The Laser

We use a frequency-doubled, neodymium-doped yttrium–aluminum–garnet (Nd:YAG) laser that produces a very pure green light for 80 microseconds. "Pure" color means that there is no change in the light's wavelength or frequency even over a distance of more than 10 meters and that the frequency is stable to 50 parts per billion for the duration of the experiment. Precise velocity measurements require that the light remain in phase across a distance equal to the total number of roundtrip "bounces" between the Fabry–Perot mirrors, or 5 to 20 meters depending on the separation between the mirrors.

A beam splitter divides the laser beam into five individual beams, which are carried to the experiment on fiber-optic lines. We have designed special probes, each of which holds two fiber-optic lines—one to carry light to the experiment and another to carry reflected light back to the instrumentation.

Figure 4 is a series of photographs of the experiment described on page 83. The five beams are visible as the disk begins to explode.

Keeping Five Beams Separate

As the 1- to 100-microsecond experiment takes place, the reflected light travels into the instrument room and through the "shaper," which is the heart of our multibeam system. The shaper is a complex of lenses of Laboratory design that compresses the fiber images horizontally by a

factor of 4 (from 100 micrometers to 25 micrometers) while maintaining the vertical dimension of 100 micrometers (see Figure 5). Even with this compression, we can preserve the same angular divergence of the light at the image as it had at the experiment. Now the five sets of dots are well separated relative to their width, and no light that could be used is wasted. (In single-beam as well as multibeam velocimetry, some light is wasted because the light comes in on a larger fiber than the instrumentation can use.) The shaper sends the light from the separate fibers into the velocimeter at slightly different horizontal angles, so that any given horizontal angle corresponds to only one fiber. The five beams can thus be distinguished from one another later when the streak camera results are analyzed.

The shaper can actually handle ten beams, although to date it has handled just five because of space limitations for streak cameras.

Getting Beams to Cameras

Our five-beam system creates five columns of six to eight bright dots. The columns, each of which comes from a specific incoming fiber, are only 0.9 millimeters apart horizontally at the focal plane of our spherical lens. We have designed and constructed a five-faceted mirror about 3 centimeters high, with the center of the three middle facets just 0.9 millimeters apart. The five facets are separated in angle by 7.5 degrees, allowing the five streak cameras to be placed 15 degrees apart. Each streak camera views one column of the faceted mirror through a large relay lens.

"Foolproofing" the System

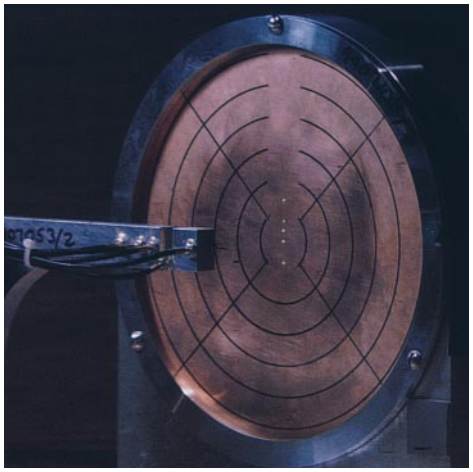
Our work on the Fabry–Perot velocimeter system has not been limited to pushing five beams through a single interferometer. We have made other improvements that make it an even more useful diagnostic tool whose records are now virtually foolproof to analyze.

A Referee to Verify Results

When a shock wave arrives at an object, the object's velocity can increase very rapidly, often too fast for our system to follow. Every time the velocity increases by a fixed amount (for example, by 0.6 millimeters per microsecond, a value that will vary depending on the distance between the Fabry–Perot

Figure 4. In photos of the experiment described on p. 13, the five laser beams are visible on the copper, but the probes themselves are out of the field of view. The visible bracket holds timing pins that short out when the copper material hits them. That timing information tells scientists the shape of the experiment as it explodes. Photo (a) was taken before detonation and (b) was taken 8 microseconds after detonation as the shock waves have reached the fourth ring. In (c), taken 14 microseconds after detonation, the dark material near the edge is the copper coming apart. The white glow around the edge of the disk is gas from the high explosives.

(a)



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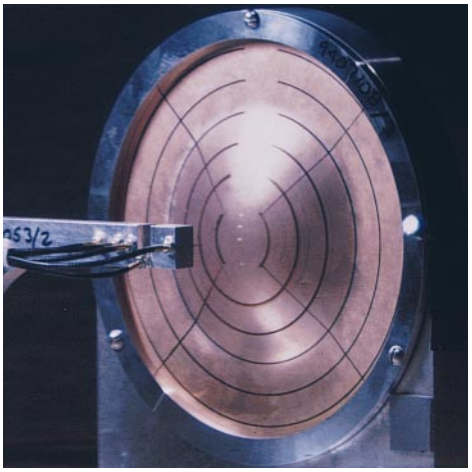

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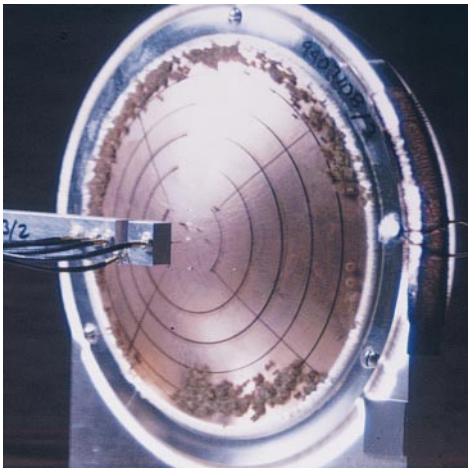


mirrors), the dot pattern repeats itself. This means that if the increase is too rapid to follow continuously, not one but several possible velocities can be inferred. Often common sense and experience allow us to infer the correct velocity. But in unusual experiments, this easy inference is not possible, and we therefore devised the dual-cavity interferometer, which has two mirror distances within the same unit.

With some of the light inside the interferometer traveling one distance and some a smaller distance, we obtain two sets of interference fringes for each beam coming from the cylindrical lens. Each streak camera thus records two sets of fringes (see Figure 6). This second, "referee" set of fringes is a significant aid in resolving the uncertainty in reading rapid acceleration data. Analysis of the fringe overlap shows that there is always, at any velocity, an adequate set of separated fringes to correctly interpret the experimental data.

In our latest version of the dual-cavity interferometer, we create the second cavity by suspending a piece of very-high-quality glass, about 2.5 centimeters square and 7.5 centimeters high, between the Fabry– Perot mirrors. It is relatively inexpensive and can be inserted or removed as experimentation needs demand.

Customized Streak Cameras

A relay lens images the dots from the faceted mirror to the vertical slit of the streak camera, which sweeps and intensifies the image across a piece of film, providing the record of velocity versus time. The electronics and housings for the cameras were custom made at the Laboratory to obtain special features not available commercially. For example, our cameras can be made to sweep the dot image at one speed for part of the record and then at another speed during the remainder of the record. This feature allows better time resolution for particular parts of the record. We have also installed a special time fiducial system, which provides both bright and dim marks in the field of view to allow absolute timing references between cameras.

Using the Incoming Beam Twice

For some experiments, we want the streak cameras to operate at very fast sweep rates to obtain fine velocity details but also to sweep more slowly to record the entire motion. With the dual sweep-speed streak cameras described above, we can do this using as many beams as there are cameras. However, by using ten cameras for five beams, we can get more detailed information.

We can have two cameras recording an experiment at two different speeds by making use of the fact that light comes into our multibeam system from a larger fiber size than the interferometer and streak cameras can use. After the reflected light goes through the shaper, the excess light enters a system of mirrors that carries it up, over, and down to another table set up with a second interferometer and five more streak cameras. This way, the first camera on the second table records slowly the same velocity history that the first camera on the first table is recording more rapidly. We have found that this method makes a far more efficient use of available light than a beam splitter would, and it has been successfully used on dynamic experiments.

The Power of Velocimetry

Fabry–Perot velocimetry provides unambiguous records of very complex situations. For example, in some experiments rather like the one described on p. 13, evaporated gold layers are applied to surfaces for higher reflectivity. After the shock wave arrives, the surface often decelerates, and

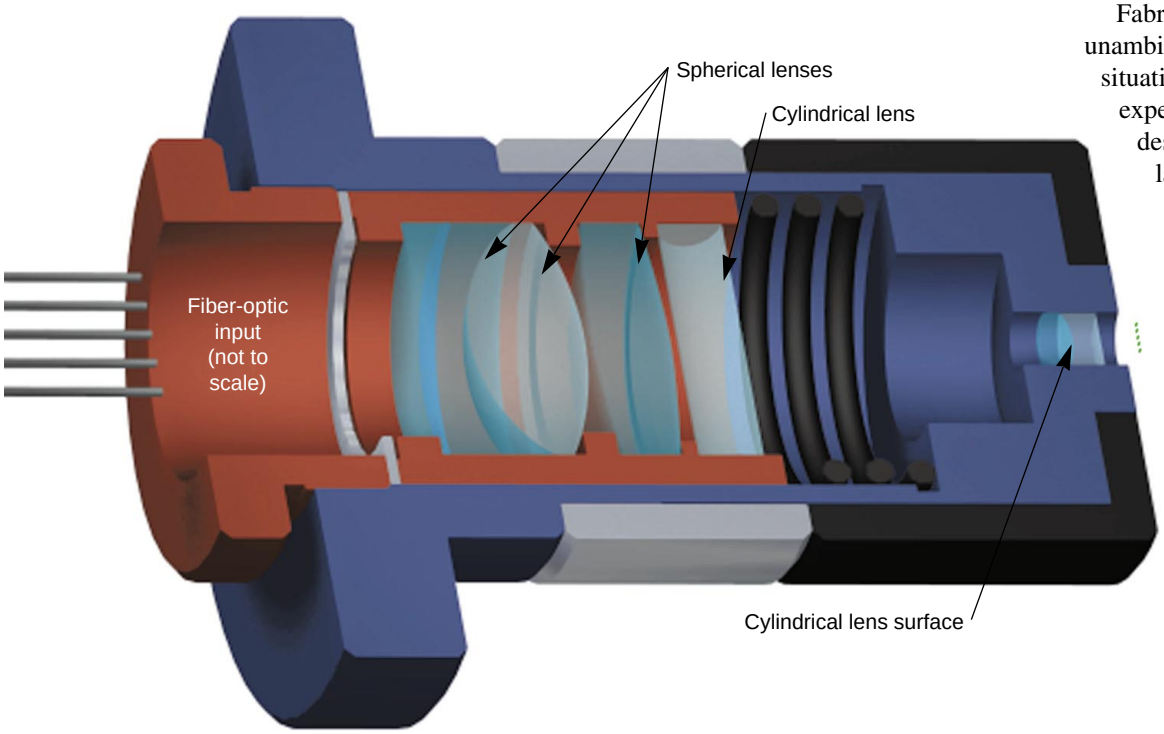


Figure 5. The shaper is the device that allows us to use five light beams simultaneously.

sometimes part of the gold pulls away from the surface, a process known as spallation. If illumination by the probe covers areas of the surface where gold has spalled and areas where it has not, we get two different velocity histories on the same camera. There may also be unshifted (no change in wavelength) light from non-moving surfaces such as a vacuum window, dust, or uncoated glass, in addition to shifted light from moving surfaces. Fabry–Perot interferometry can handle all of these situations on a single, easily read record.

The Fabry–Perot velocimeter is unique in providing information on continuous velocity from both simple and complex experiments. The multibeam Fabry–Perot velocimetry system is a powerful, practical diagnostic tool whose results can be quickly and easily verified. The value of the multibeam system has been recognized beyond the boundaries of the Laboratory: two five-beam arrays will soon be installed at the Nevada Test Site for non-nuclear testing.

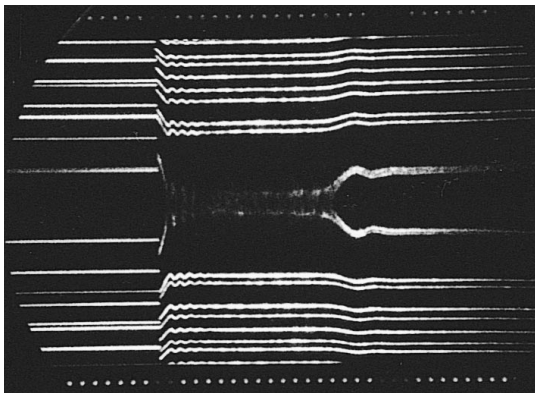
We presently have a ten-beam capability, with two five-beam arrays. We are in the process of expanding to four five-beam arrays, which will give us 20 simultaneous sets of measurements, at approximately half the cost of 20 single-beam Fabry–Perot velocimeters. As the system is further developed and expanded, it will become an ever more useful tool, with improved time and velocity precision.

With the multibeam system producing more meaningful data than has been available to us in the past, we can make our modeling codes increasingly accurate—a necessity for effective stewardship of our nuclear stockpile.

Key Words: Fabry–Perot interferometry, optical velocimetry, optics, streak cameras.

For further information, contact David Goosman (925) 422-1630.

(a)



(b)

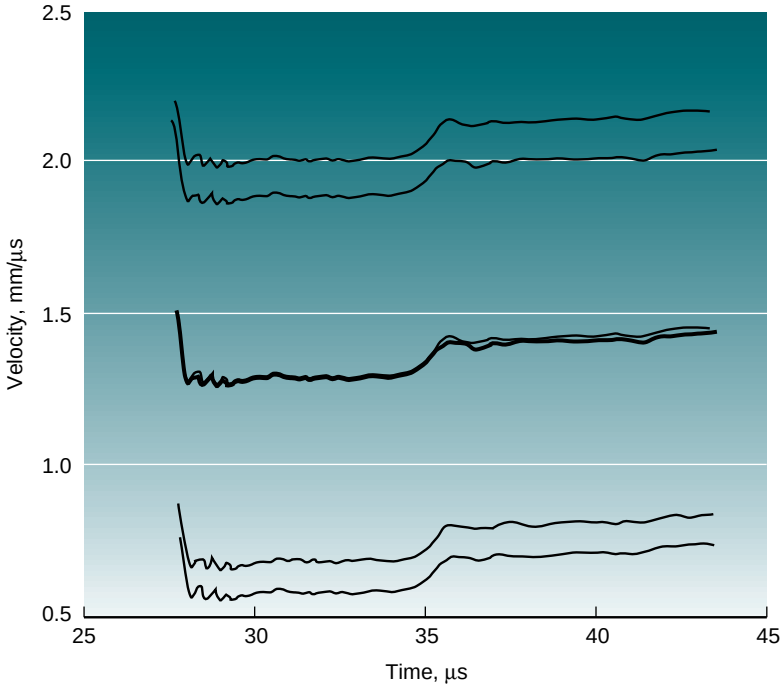
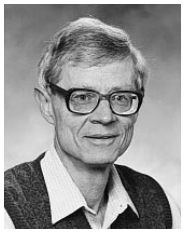


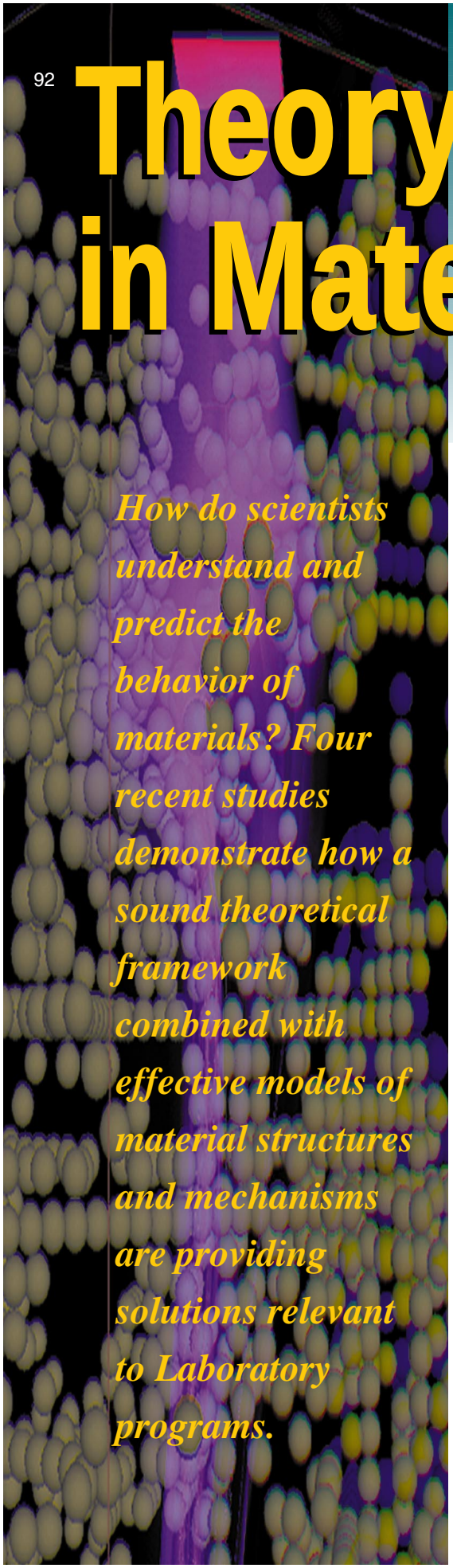
Figure 6. (a) An example of a streak camera record from an earlier version of our dual-cavity Fabry–Perot interferometer. (b) An example of data analysis using three different estimates of the "jump" in the dot pattern when rapid acceleration occurs. Without the second set of fringes, the scientists would not know which is correct. The overlap of the center two curves shows it to be the correctly estimated velocity.

About the Scientist



DAVID R. GOOSMAN joined the Laboratory in 1974 and has been Group Leader for Advanced Experiments Projects since 1980. He received a Ph.D. in Nuclear Physics from California Institute of Technology in 1967, and from 1967 to 1969, he was a post-doctoral fellow there. From 1969 to 1974, he carried out nuclear physics experiments at Brookhaven National Laboratory. He has published more than 60 articles on nuclear physics, radiography, and optical velocimetry.

Theory and Modeling in Materials Science



How do scientists understand and predict the behavior of materials? Four recent studies demonstrate how a sound theoretical framework combined with effective models of material structures and mechanisms are providing solutions relevant to Laboratory programs.

EVER since our ancestors first used tools to make tasks easier, understanding the properties of materials has been a practical concern. The challenge of explaining how modern materials behave is driven by the vast range of new materials and processing methods that are available and by the demands placed on performance, sometimes in harsh or unusual environments.

The cessation of nuclear testing and the advent of science-based stockpile stewardship as a primary Laboratory mission increase the challenge. Today, we need to predict changes in the structure and properties of materials in stockpiled warheads and the effects of these changes on how weapons perform. Success in fulfilling the stockpile stewardship mission will also provide far-reaching benefits to other Laboratory programs and the commercial sector.

One way scientists study material properties is by applying fundamental physical and mathematical principles to form the basis of models. By combining models with spectacular advances in computational technology, we can often shed light on the mechanisms that determine how a material behaves. Furthermore, theory and modeling in materials science are often directed toward predicting, not just describing, the properties of materials. Models have progressed to a point that they can often tell us not only what happens, but how or why it happens.

Lawrence Livermore scientists have an arsenal of tools and devices to model the behavior of materials without always resorting to experiments that can be expensive. On the other hand, experiments are usually used to validate models, so theorists and experimenters often work together.

Today in the Chemistry and Materials Science Directorate we are addressing increasingly complex phenomena and a broad range of problems in materials science relevant to Laboratory programs. Examples of our current modeling capabilities include:

- The evolution of microstructures, such as the formation and growth of voids produced by radioactive decay or irradiation of materials.
- The performance and degradation of high explosives and polymers.
- Alloy properties, such as phase diagrams.
- Analysis of spectroscopic scattering data.
- Metals processing.
- Corrosion damage.

These topics and many others also have important applications in defense, industry, and other sectors. The diverse materials we model include aerogels, alloys, ceramics, high explosives, metals, and polymers, to name only a few. The breadth of our modeling capabilities means that we cover length scales starting from atoms and electrons at the submicroscopic level, to grains and grain boundaries at intermediate

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These materials scientists use a variety of approaches to solve materials problems described in this article. (Left to right) Standing: Daniel Calef, modeling of aerogels; Lloyd Chase, division leader; and William Gourdin, physically based models of tantalum deformation. Sitting: Larry Fried, molecular dynamics and phenomenological modeling of high explosives; and Tomas de la Rubia, kinetic Monte Carlo modeling of ion implantation and defects in silicon.

lengths, to finished components at the opposite end of the spectrum.

About Length Scales

The concept of modeling on all relevant length and time scales is fundamental in our research; Table 1 illustrates the concept. Materials generally have a wide range of internal structures that determine their behavior and performance. Our objective is to predict, explain, and sometimes control properties across the full range of material structures, which span spatial dimensions from a fraction of a nanometer to meters. (A nanometer is one billionth of a meter; a typical atom is about 0.3 nm in diameter.)

At the shortest lengths and times relevant to materials properties, atoms and electrons determine characteristics such as a material's hardness, conductivity, and optical properties. Sometimes we are able to calculate the behavior of a material based on quantum-mechanical theory alone. In that case, we call the process a "first-principles" calculation because we essentially do not use or need any experimental input. About all we need to know is the atomic numbers of the atoms involved and sometimes their positions. First-principles calculations increase our understanding of materials by allowing us to make predictions, reveal trends, test hypotheses, and analyze experimental data.

First-principles calculations form the basis for many of our modeling activities at Livermore.[1] Examples include the properties of metals and alloys, the behavior of surfaces and interfaces, and the modeling of experimental measurements. Because first-principles theory and modeling were discussed extensively in the August/September 1994 issue of *Energy & Technology Review*,[2] this article emphasizes the other approaches.

At increasing length scales in Table 1, we study the properties associated with larger structures by using approaches such as molecular dynamics (MD), kinetic Monte Carlo, or phenomenological models. Models associated with greater lengths are increasingly based on the empirical or measured responses of materials to stress, deformation, temperature, and other factors. By combining several approaches, we can deal with the wide variety of physical properties we need to assess. Illustrating diverse approaches to modeling across a range of material structures and properties, the following four examples of recent accomplishments are only a few of our many modeling efforts in progress.

Defects in Silicon

Over the last 30 years, exponential growth of the semiconductor industry has been driven toward denser packing of smaller components that make up a silicon chip. To develop the silicon chips required for microelectronics components in the 21st century, we need to understand more about how defects are produced and how dopants diffuse in silicon.

Dopant atoms are required to make silicon usable for manufacturing

semiconductor devices. During manufacturing, dopants are routinely implanted (using ion accelerators) into very precise regions of a silicon wafer. This process damages the silicon wafer by introducing defects that must be removed. At the high temperatures used for the removal process, the defects and dopant atoms interact and diffuse over long distances. Dopants therefore can end up at destinations different from their intended location in a wafer. When that happens, the defective devices are not suitable for the marketplace.

We are creating a "virtual laboratory" to study this problem and to model other types of radiation effects in materials. Our strategy is to use an experimentally validated hierarchy of theoretical and computer simulation tools to span many length and time scales, from picoseconds to minutes. At the shortest lengths (at atom level) and times (up to about a nanosecond), we use MD simulations based on forces between atoms that accurately reproduce relevant properties of the material. Over time, defects in silicon can aggregate to form larger structures, like dislocations. To study how such structures evolve over longer times (minutes or hours), we use kinetic Monte Carlo simulations. In this work, we have a collaboration with scientists at AT&T Bell Laboratories, which allows us to develop a new capability to support other Laboratory programs.

Recent computer simulations based on our models are giving us a clear and consistent physical picture of the production and evolution of damage in silicon under energetic-beam bombardment. A typical simulation begins with a cube of silicon made of about one million atoms in a normal lattice arrangement. Then we simulate the bombardment of the top of the cube with high-energy ions to implant arsenic, boron, or other dopant atoms. Figure 1 shows the defects—that is, displaced atoms—in a silicon cube. We can simulate the full range of beam energies that are typically used to process silicon devices, from about one-tenth of an electron volt to several thousand electron volts. As the energy increases, the amount of total damage increases, as expected, but we also find that the size of the largest defect clusters increases.

Our simulations produce images that look as though they come from a high-resolution microscope. We validate the simulations by comparing them with damage observed in actual materials, as shown in Figure 2. Comparisons like this confirm that our computer-aided design package accurately predicts experimental results.

Our work on semiconductor devices also applies to a range of other problems. For example, the walls in nuclear power plants undergo radiation damage from neutron bombardment. Similar processes may occur in nuclear weapons components. Our simulations can help predict the performance of materials used in weapons, existing fission power plants, and fusion plants that may be developed in the future. Because void formation is also seen in

Table 1. Theory and modeling activities at Livermore cover all of the length scales associated with material structures.

Material structure	Length scale	Primary theory or model used
Atomic or electronic	Angstroms ($1\ \text{Å} = 10^{-10}$ m)	QM
Simple defects (vacancies, point defects, interstitials)	Angstroms to nanometers ($1\ \text{nm} = 10^{-9}$ m)	QM MD KMC
Extended defects (dislocation, cores, small voids, clusters, and precipitates)	10 to 100 nm	QM MD PM
Nanoscale to microscale structures (grain boundaries, grains, precipitates)	10 nm to 100 μm ($1\ \mu\text{m} = 10^{-6}$ m)	QM MD PM Phen
Polycrystallines, composites, and interfaces	Micrometers to meters	PM Phen
Continuum (i.e., auto or bridge)	Varies	CM

Quantum mechanics (QM) forms the rigorous theoretical basis for studies of electrons and atoms, chemical bonds, molecular structures, interfaces, and defects—the smallest structures that determine how a material behaves.
Molecular dynamics (MD) calculates the motions of atoms or molecules combining Newton's laws of motion with quantum-mechanical understanding, e.g., modeling the collisions of high-energy particles with the atoms of a solid undergoing radiation damage.
Kinetic Monte Carlo (KMC) models are used to study how atoms and defects in a material diffuse spatially by discrete jumps. The probability of a jump is determined by temperature and energy barriers for the movement.
Physically based models (PM) are based on physical concepts that emulate the behavior of material structures, e.g., dislocation movement, grain-boundary sliding, crystallographic twinning, and material movement.
Phenomenological models (Phen) use mathematical relations without any known physical basis to describe experimental observations.
Continuum models (CM) treat structures, such as a car frame or beams of a bridge, as a continuous or homogeneous material, e.g., the process of forging an automobile bumper.

metallic nuclear fuel rods and other structures, the modeling of defects and voids has applications to these problems as well.

Deformation in Tantalum

Anyone who has attempted household plumbing knows that copper tubing becomes more difficult to work by hand after repeated bends. This phenomenon, known as work hardening, occurs in many metals. The increase in strength is caused by interactions between lattice defects called dislocations.

Dislocations consist of extra or unequal planes of atoms, like an extra sheet of paper slipped part way into a stack of sheets. Another handy way to imagine dislocations is to think of them as "wrinkles" in the regular arrangement of atoms in a metal crystal—much like wrinkles in a rug. Imagine creating a small wrinkle at one end of a rug and then pushing the wrinkle along to the other end. In a similar manner, atoms in a metal lattice can be moved relative to each other by creating a dislocation and then moving it through the crystal. Like a wrinkle in a rug, dislocations are long, string-like defects. When many are present, they tangle like spaghetti. In metal, the more dense the tangles, the more energy is needed to deform it.

Copper belongs to a class of common metals with a simple structure known as face-centered cubic—a cube of atoms with an additional atom on each face. Another group of metals, including iron and tantalum, has a body-centered cubic (bcc) structure with atoms at the corners of a cube and one atom in the center. Because these metals are technologically important, their mechanical behavior is of considerable interest.

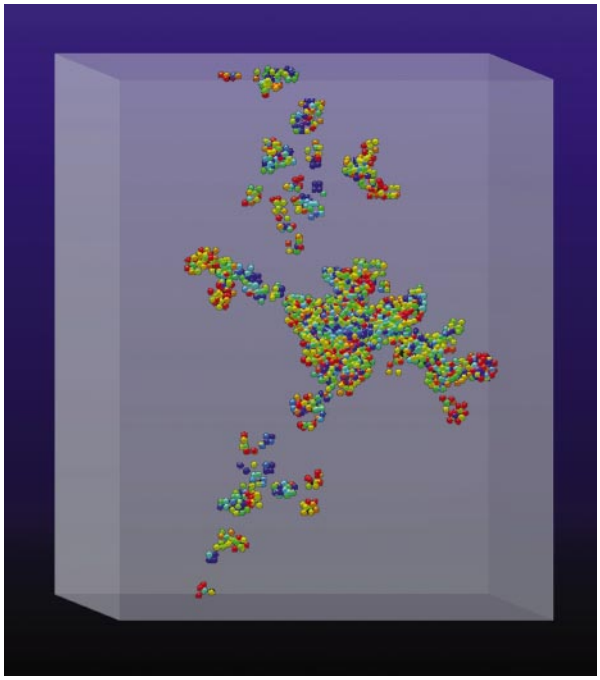

Figure 1. Monte Carlo computer simulation of displaced atoms in a cube of translucent silicon after implantation with 15-keV arsenic ions. The unaffected silicon atoms are not shown here. The atoms in blue are under tensile stress and represent areas with vacancies; the atoms in red are in compressive stress and indicate the presence of interstitials. The large mass in the middle is an amorphous zone; i.e., the crystalline order has been destroyed.

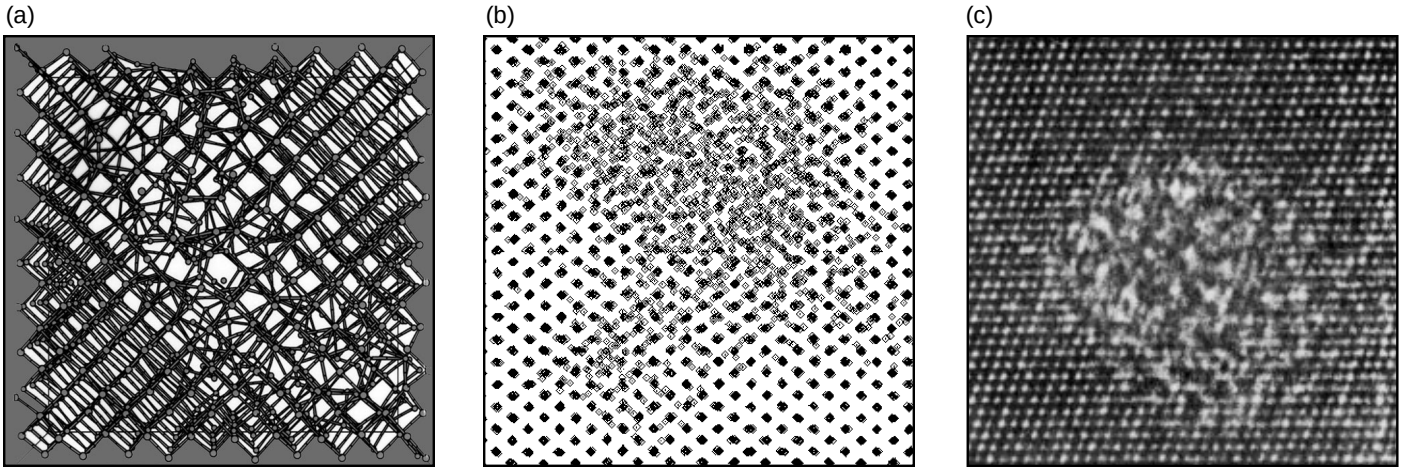

Figure 2. (a) Three-dimensional plot of damage created by a 25-keV platinum ion in silicon. A highly disordered, amorphous region is surrounded by crystalline material. (b) A two-dimensional projection of the atoms in (a). (c) An experimental high-resolution electron micrograph done elsewhere[3] of the impact of a 100-keV bismuth ion in silicon. Although the exact conditions of the simulation and experiment are not identical, this type of comparison helps us to validate the simulation and to interpret the experimental observation.

Our goal is to understand the mechanical behavior of bcc metals and to include enough physics concepts in the model so that calculations can be meaningfully extrapolated to new conditions. The problem is beyond the reach of quantum mechanical calculations. Instead, we are using physically based models that are realistic in representing the actual processes that control deformation. Tantalum is a good test case for this work because it is ductile, shows substantial work hardening, and has important defense applications.

Our model for tantalum accounts for both yield stress (force per unit area at which it begins to permanently deform) and work hardening. Previous explanations said nothing about work hardening and did not explain it for this class of materials. We suggest that there are two (or possibly more) barriers to moving a dislocation, as illustrated by the humps in Figure 3. At first, a dislocation in tantalum must move as if it were isolated, and enough force must be applied to overcome a series of small barriers. In the analogy of wrinkles in a rug, even if no other wrinkles block the path, some force is still required to move an isolated wrinkle. (The material in front of a wrinkle must be lifted as it moves forward.) After moving a certain distance, however, a dislocation may encounter a barrier produced by other dislocations. The force to overcome this barrier increases with deformation and accounts for work hardening in a natural way.

Our model combines the two mechanisms, yield stress and work hardening, and is able to describe which one dominates at different stages and under different conditions of deformation. Figure 4 shows how well the model can reproduce the observed mechanical behavior of tantalum at room temperature. We find similar agreement when temperature is varied.

What is the model good for? With the increased power of modern computers, companies like automobile manufacturers can now simulate the forming and performance of key structural components. However, computer simulations are only as good as the underlying models used to describe the behavior of materials under conditions that are often severe (for example, crashes). Physically based models more realistically describe material properties, yield more meaningful results, and can be reliably extended beyond the scope of experimental data. Whereas the current Livermore model for the deformation of tantalum was conceived for bcc metals, it provides a framework for face-centered cubic metals as well.

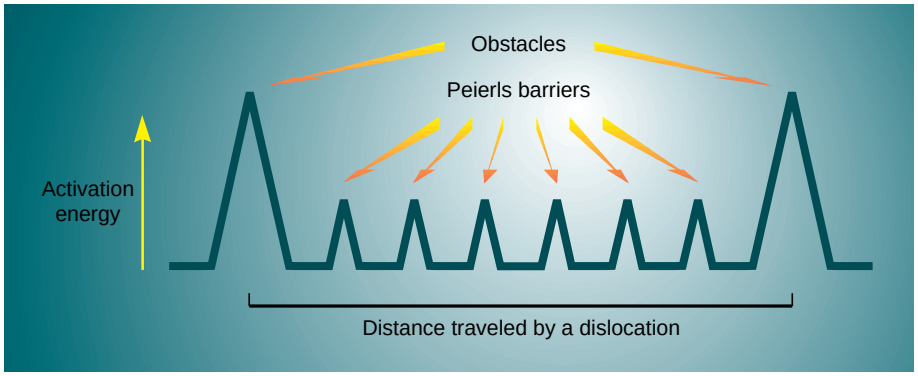

Figure 3. How to envision the two barriers to plastic flow in tantalum: The distance along the bottom refers to the distance traveled by a moving dislocation when a material is deformed. The Peierls barriers are associated with the motion of isolated dislocations (analogous to wrinkles in a rug). The larger obstacles occur where dislocations intersect.

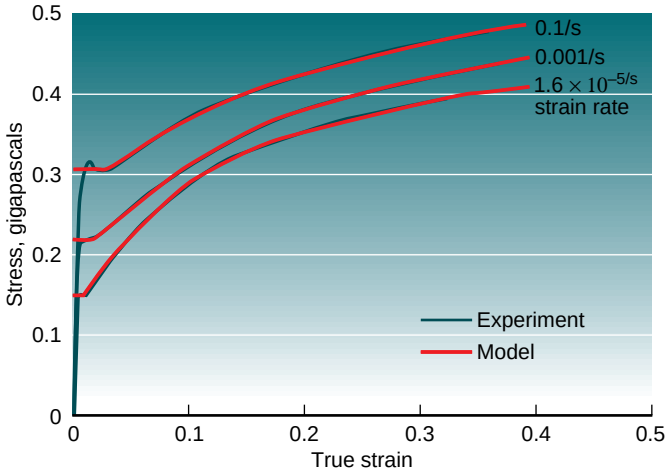

Figure 4. Our model accurately reproduces experimental values of stress (force applied per unit area) and strain (relative change in dimensions) for various strain rates (rates of deformation) in unalloyed tantalum at room temperature.

Modeling High Explosives

Energetic materials, which include high explosives, are widely used in both military and civilian applications. Livermore has studied high explosives for decades because they are crucial to the performance of nuclear weapons. In the area of stockpile stewardship, we studied how shock dynamics change in older, degraded materials. In another recent

project, we developed a candidate bunker-busting munition for the Air Force following their experiences in the Gulf War. In the civilian sector, the Bureau of Mines needs to evaluate explosives for mining operations. To better assess environmental concerns, we need to know what reaction products are generated following a detonation.

Typical energetic materials are made of large, floppy molecules with more than 20 atoms, and they can undergo a variety of chemical reactions. Over time, such molecules can degrade and the crystals become more porous, making them dangerous to handle. At the atomistic level, we are simulating how the propagation of a shock wave through high explosives is affected by the degree of degradation. On a macroscopic scale, we can model the performance of existing and novel energetic materials.

As one example of new work on the atomistic scale, we are applying MD simulations to study how the shock properties of the widely used explosive triaminotrinitrobenzene (TATB) change as a function of its degradation and increased porosity. By using this advanced capability, we can assess how an explosion is initiated on a molecular level in aged material found in weapons stockpiles.

As shown in Figure 5, we simulate crystals of about 10,000 TATB molecules and apply a shock wave (a simulated pressure impulse) to crystals with different degrees of defects. We found that the shock wave in degraded material travels much more slowly and spreads out over a much wider area than in pure TATB. At the molecular level, the collapse of voids leads to hot spots in degraded (porous) TATB, and the temperature behind the shock front becomes higher and much more nonuniform.

To understand how molecules like those in TATB react on a much larger scale, we have developed the CHEETAH computer code, a phenomenological thermochemical model to predict the performance of explosives.[4] In contrast to our MD simulations, this more mature modeling effort looks at macroscopic events at lengths of centimeters to meters. The code is empirically based and is derived from more than 40 years of experiments on high explosives at LLNL.

CHEETAH models the interactions (for example, the electrical potentials) of a mix of molecules between them to predict a variety of outcomes, such as those shown in Figure 6. If we think of explosives as a bucket of hot chemical soup, CHEETAH acts like a thermometer and pressure gauge. It predicts the reaction products and the detonation properties, such as pressure, velocity, and energy. The code allows us to vary the recipe (chemistry) and the starting conditions to optimize the properties we want, such as the best early- or late-time energy.

The value of CHEETAH is that it predicts the performance of a given amount of high explosives to within a few percent. With libraries of about

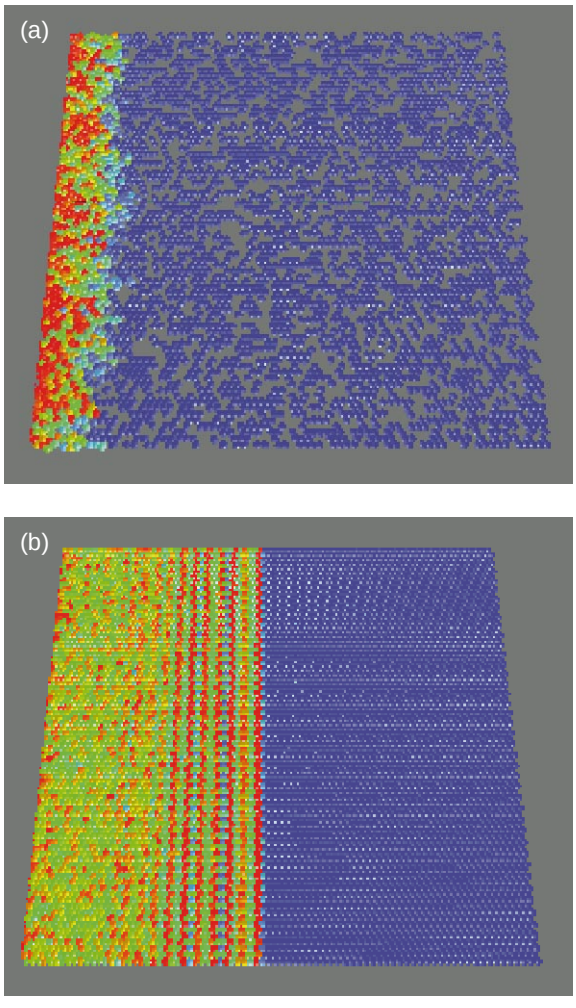

Figure 5. "Snapshots" of molecular dynamics simulations for (a) pure and (b) degraded TATB. The molecules are shaded according to their kinetic energy as a shock front passes through the lattice, with red corresponding to higher temperatures and black to lower temperatures. In contrast to a sharp, smooth shock front in pure material, porous TATB produces a broader and less uniform shock front with hot spots.

100 reactants and 6,000 products, the program is now used by more than 80 research teams in industry, academia, and the international scientific community, including England, Canada, Japan, Sweden, and France.

The code is both physically simple and user friendly, and it can guide applications ranging from rocket and gun propellants to the formulation of new explosives with improved performance.

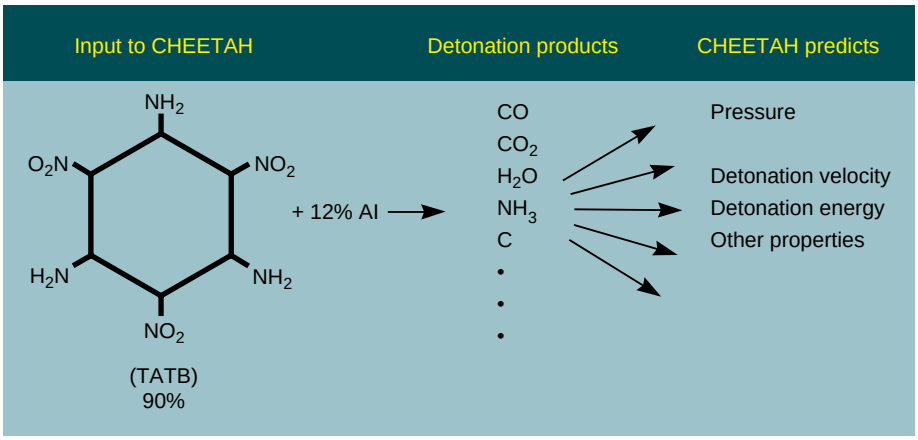

Figure 6. To predict the performance of explosives, CHEETAH starts with one or more base reactants, such as TATB and metallic aluminum. It then solves thermodynamic equations to predict the detonation products and their properties, such as temperature and volume. From these values, CHEETAH predicts the detonation properties, including pressure, velocity, and energy.

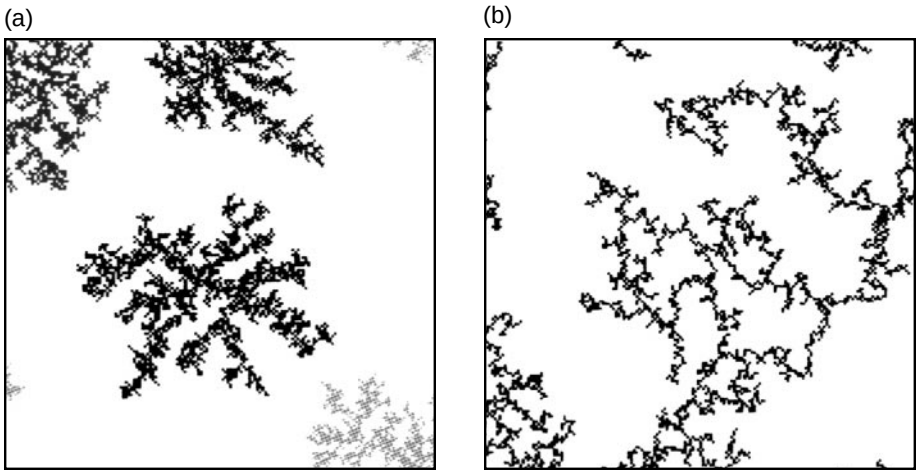

Figure 7. We model aerogel structures by varying the number of starting particles and the rules by which they move and adhere to one another. Compared to (a) clusters grown from fixed seeds, (b) cluster–cluster aggregates more accurately mimic real aerogels.

Transport Through Aerogels

Aerogels have exceptional strength and enormous surface area and are among the lightest solids known.[5] Some varieties are 100 times less dense than water. LLNL first studied aerogels for a national defense application, but their use is being proposed as electrical, thermal, and sound insulators; optics, space, and catalyst devices; capacitive deionization units for water purification; aerocapacitors for energy storage; and various novelties and toys. Many aerogel applications remain relevant to Laboratory programs focused on national defense, the environment, and energy. Their use as filters and catalyst supports take advantage of their tremendous surface area.

At the microscopic scale, these highly unconventional solids are made of "beads" that are some tens of nanometers in size. At an intermediate length scale (in the range of micrometers), groups of beads are clustered to form an open network with large and small voids or pores in the network. To understand how molecules flow through an aerogel, as they would in a filter, we need accurate structural models and flow codes for highly irregularly shaped networks.

Developing these models was a considerable challenge because the absence of any characteristic pore size in an aerogel complicates the treatment of fluid flow. We have replicated the structure of aerogels at the intermediate scale by simulating the growth of clusters.[6]

In the models, particles on the order of 10 nanometers wide represent the beads. These particles or "walkers" randomly move through a three-dimensional lattice and stick to each other. Both the number of walkers and the sticking rules are varied in different simulations. For example, if walkers only cluster around a set of fixed particles, then structures like

those in Figure 7a are created. Alternatively, if walkers adhere to each other and the clusters continue to diffuse, then we generate structures like those in Figure 7b, called cluster–cluster aggregates.

When we make the structures more like those in Figure 7b, they act more like a simple, random distribution of obstacles, and they more accurately mimic the structure and behavior of real aerogels. A commonly measured quantity for flow through porous materials is permeability. In comparisons of calculated permeabilities based on our models, the cluster–cluster aggregates closely match the observed experimental behavior for the flow of a gas through aerogels.

Figure 8 shows a puff of smoke flowing through one of our modeled aerogels. This visualization, developed by the Livermore Computer Center graphics laboratory, clearly shows that the flow patterns are dominated by the largest pores. Such results reinforce the view that our approach successfully models these highly irregular and unconventional solids.

Work to Come

What does the future hold for theory and modeling of materials properties at LLNL? To accomplish our stockpile stewardship mission, we must improve our ability to predict how the structures of metals, high explosives, and polymers change with time or vary with manufacturing methods. Then, we need to assess the effects of these changes under the extreme conditions relevant to weapons performance. For this purpose, we need robust models that can be used reliably. We are collaborating with Laboratory colleagues in the Physics and Space Technology and Engineering Directorates, as well as with researchers at many universities, to develop the required approaches.

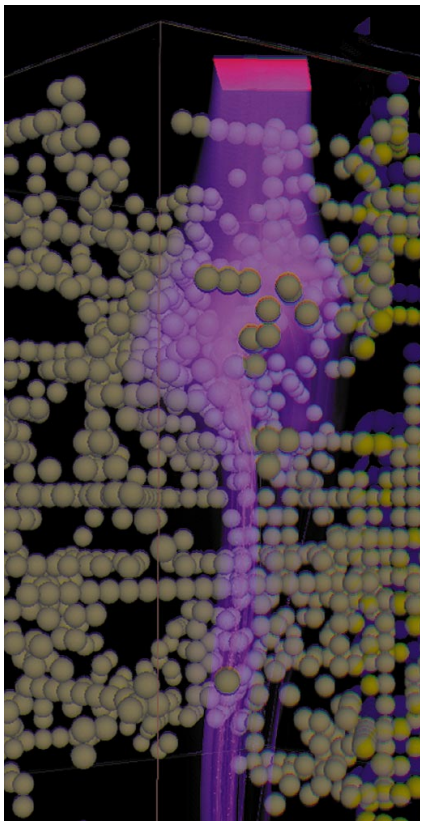

Figure 8. A puff of smoke flowing through an aerogel shows that the flow patterns are dominated by the largest pores.

Key Words: computer modeling, materials science, material structure, microstructures, molecular dynamics.

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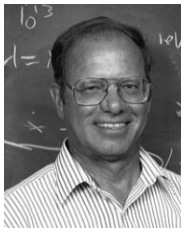
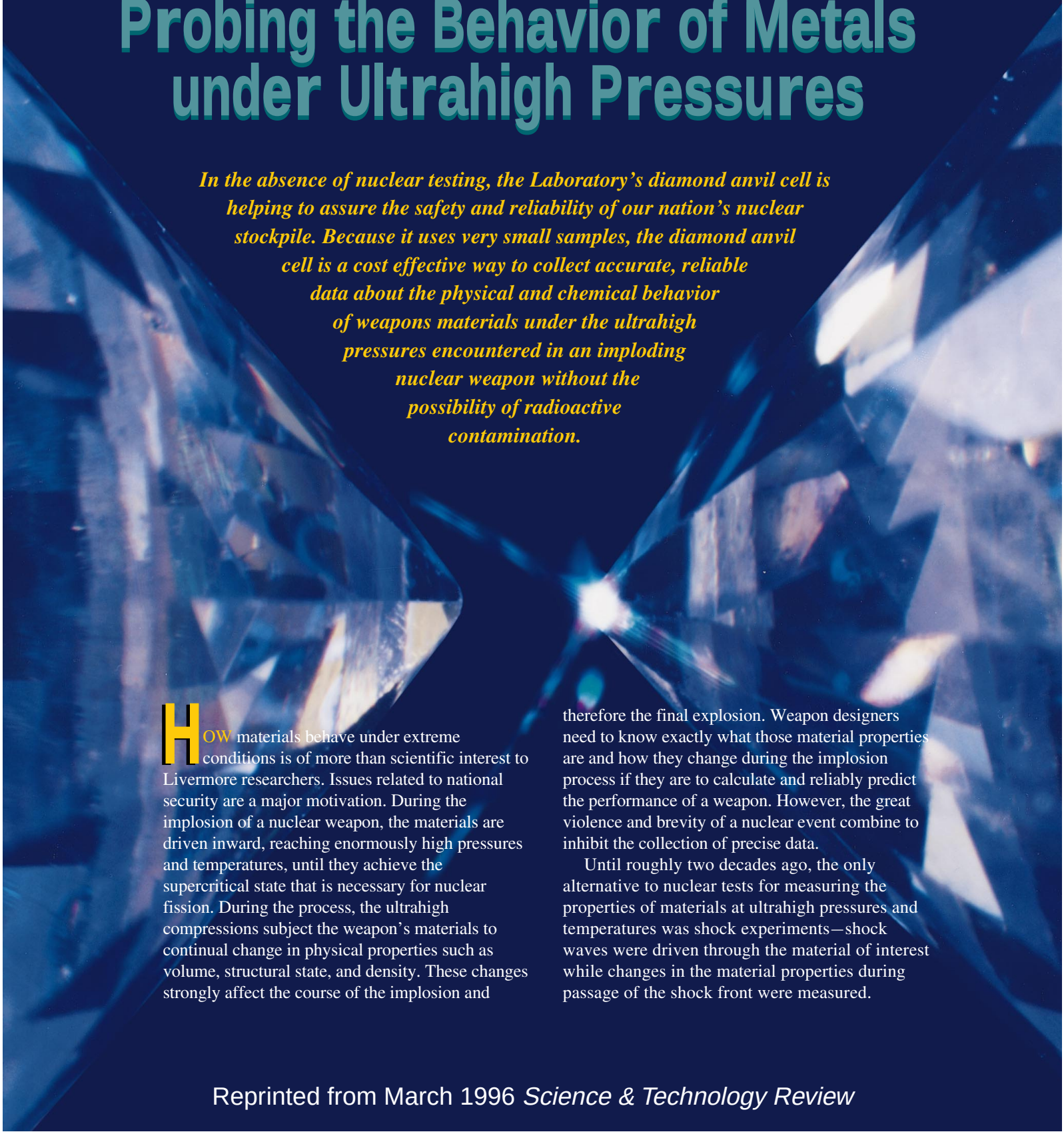
About the Scientist



LLOYD L. CHASE is the division leader for Materials Science and Technology in the Chemistry and Materials Science Directorate. He joined the Laser Program at LLNL in 1985, where he did optical materials research and development. He transferred to Chemistry in 1991. He received a B.S. in engineering mechanics in 1961 at the University of Illinois and a Ph.D. in physics at Cornell University in 1966. Before coming to the Laboratory, he was on the technical staff at Bell Telephone Laboratories and professor of physics at Indiana University. His areas of research have been in solid-state physics and materials science with an emphasis on development and characterization of optical materials. He has more than 130 publications in these fields and holds three patents.

The Diamond Anvil Cell:

Probing the Behavior of Metals under Ultrahigh Pressures



In the absence of nuclear testing, the Laboratory's diamond anvil cell is helping to assure the safety and reliability of our nation's nuclear stockpile. Because it uses very small samples, the diamond anvil cell is a cost effective way to collect accurate, reliable data about the physical and chemical behavior of weapons materials under the ultrahigh pressures encountered in an imploding nuclear weapon without the possibility of radioactive contamination.

HOW materials behave under extreme conditions is of more than scientific interest to Livermore researchers. Issues related to national security are a major motivation. During the implosion of a nuclear weapon, the materials are driven inward, reaching enormously high pressures and temperatures, until they achieve the supercritical state that is necessary for nuclear fission. During the process, the ultrahigh compressions subject the weapon's materials to continual change in physical properties such as volume, structural state, and density. These changes strongly affect the course of the implosion and therefore the final explosion. Weapon designers need to know exactly what those material properties are and how they change during the implosion process if they are to calculate and reliably predict the performance of a weapon. However, the great violence and brevity of a nuclear event combine to inhibit the collection of precise data.

Until roughly two decades ago, the only alternative to nuclear tests for measuring the properties of materials at ultrahigh pressures and temperatures was shock experiments—shock waves were driven through the material of interest while changes in the material properties during passage of the shock front were measured.

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However, because shock techniques are dynamic, precise material properties are difficult to measure directly. Instead, the diagnostics were focused on measurements that could be captured in such brief durations; then, using large-scale numerical simulations that incorporated data from the experiments, researchers inferred the properties of interest.

The Diamond Anvil Cell

The diamond anvil cell (DAC) has changed these circumstances because of the pressure and temperature regimes to which a sample can be subjected. It joined shock experiments and tests driven by high explosives as means of providing the experimental data that are important starting points for science-based stockpile stewardship. This apparatus enables Lawrence Livermore researchers to measure many of the properties of interest directly under static pressure conditions (instead of indirectly as in dynamic shock-wave experiments). The use of static pressure means that ultrahigh pressures can be maintained for significantly longer times than in shock experiments, allowing more accurate measurements to be taken directly. Pressures within the diamond anvil cell can approach 350 gigapascals (1 GPa = ~ 10,000 atmospheres*) and temperatures can approach 6,273 kelvin (10,832°F, 6,000°C)—that is, pressure and temperature equal to those at the center of the Earth.

The DAC is also more cost effective than shock-wave experiments. Instead of providing only one volume–density number at a given pressure per experiment, it provides a range of data across the pressure spectrum of the experiment and thus more information for fewer experiments. Another advantage of the DAC is the small sample size needed. Each experiment requires about a microgram of an element, significantly less than in a weapon. The small samples present minimal possibility of radioactive contamination, and containment of the small amount of radiation is assured.

The DAC's capabilities are particularly important for weapons physicists now that the United States is no longer conducting nuclear tests. The safety and reliability of nuclear weapons must now be maintained with indirect experimental techniques and large-scale computations. In particular, the DAC enables direct measurements of changes in volume and density, as a function of changes in the material's crystal structure and of melting under high pressure, that strongly influence the hydrodynamic stability of imploding systems. Fifty years ago, instability was an intractable problem for the designers of the first nuclear weapons. Despite major advances in science and technology, our understanding of instability remains limited because the actual physical state of the material experiencing these changes in volume and density often could not be measured. The DAC now changes this situation. It can provide *some* of the data required to accurately predict the yield and performance of nuclear weapons—and thus their safety and reliability—without nuclear weapons tests.

LLNL's physicists also use the DAC data to interpret the data collected from earlier shock-wave experiments. Shock waves passing through a material raise its pressure and temperature simultaneously, making it difficult for researchers to identify with certainty the separate effects of pressure and temperature alone from the data. By statically compressing the same type of material at room temperature in the DAC, we can isolate the effects of pressure on the changing pressure–density relationship (i.e., equation of state) of the material. Physicists then use these data to calculate the temperature component from the shock data and thus derive separate pressure and temperature values for those data. They thus deduce further information about the high-temperature equation of state and phase stabilities useful to weapons physicists in confirming or modifying the complex theoretical calculations upon which weapons computer codes are based.

Figure 1 shows a comparison of DAC data with data from shock experiments recalculated using a theoretical equation-of-state model for uranium. The slight discrepancy between the DAC and theoretical equations of state suggests that the parameters chosen for the theoretical calculations may need further minor modifications that could lead to more accurate predictions of weapon safety and yield. The DAC is thus an important tool that provides weapons physicists with the experimental data that allow them to improve the calculations upon which weapons codes are based without doing actual nuclear tests.

The Compressing Mechanism

The diamond anvil cell is a small mechanical press that forces the small, flat faces (the culets) of two flawless, brilliant-cut diamonds together on a microgram-size sample to create very high pressures in the sample (see Figure 2).[1] It uses diamonds because, as the hardest known solid, they do not break or deform under the intense pressures of the DAC and are transparent to light and x rays. The mechanism for applying the pressure is a stout lever with a mechanical advantage of 10:1. It is actuated by a

* 1 atmosphere = the ambient air pressure at sea level.

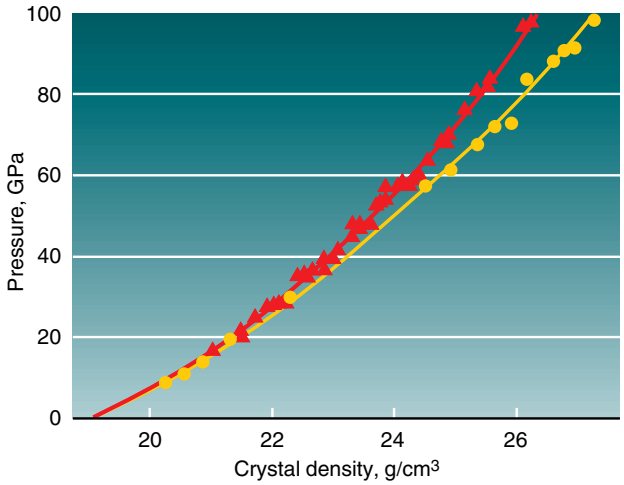


Figure 1. Comparison of diamond anvil cell data (●) with values calculated from a theoretical equation-of-state model for uranium using data from shock experiments (▲). The plot shows that the data derived from theory and shock experiments warrant correction by the data from the diamond anvil cell.

heavy screw and Belville springs at the long end. (Belville springs are cupped washers stacked back to back around the screw to apply a balanced pressure.) The diamonds, which range from one-eighth to one-third carat each, are in an opposed anvil configuration and mounted over zirconium pads on a pair of tungsten–carbide rockers. These rockers (hemicylinders with their axes at right angles) can be tilted to align the culet faces perfectly parallel. Apertures in the rockers permit x rays and other kinds of radiation to enter and exit

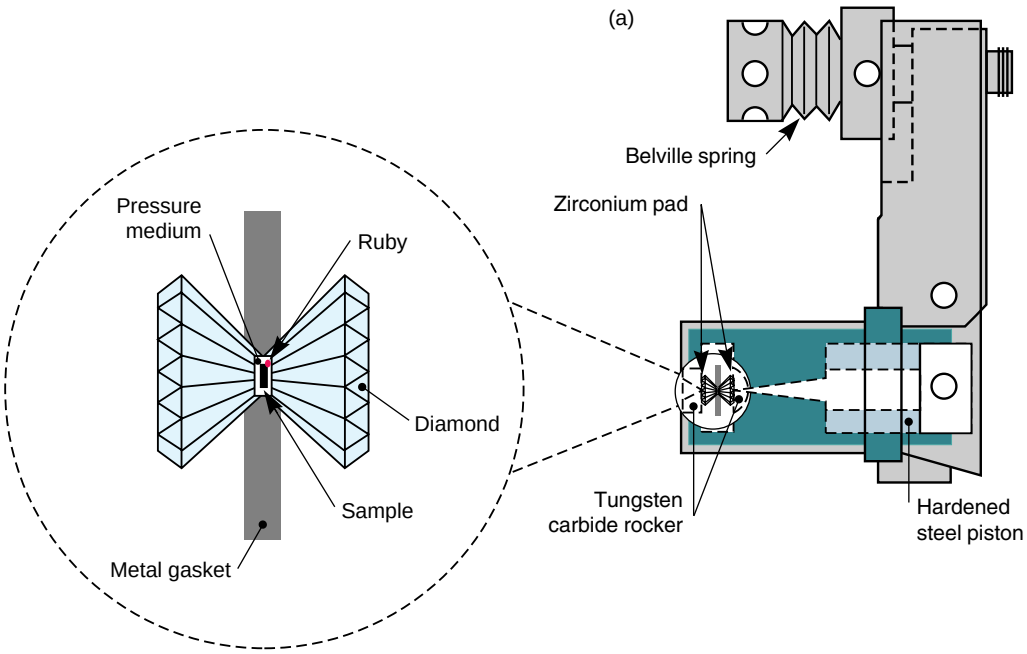
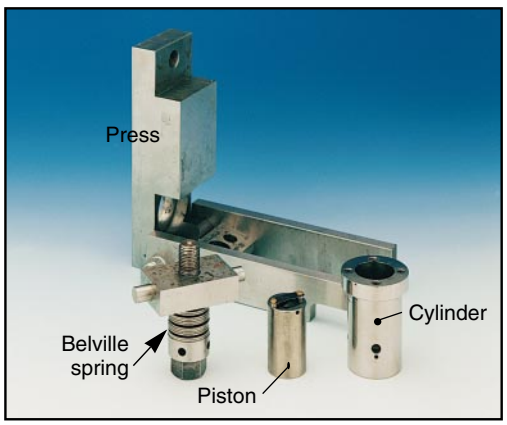
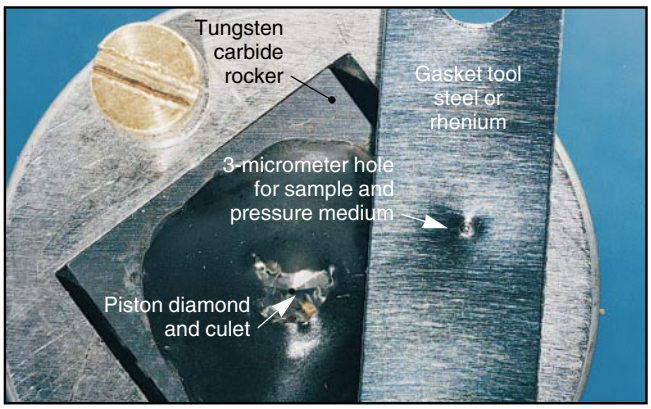


Figure 2. (a) Schematic of the diamond anvil cell. (b) The cell disassembled, showing the major optical and mechanical components. (c) Close-up of the apparatus for holding and compressing the sample.

(b)



(c)



Lawrence Livermore National Laboratory

through the diamond anvils, thus allowing for diagnostics and heating during experiments.

We customize the surface shapes of the diamonds for the pressures at which we perform experiments. For experiments at pressures below 500,000 atmospheres (50 GPa), each diamond is ground to have a flat face that ranges from 100 μm (micrometers) to 500 μm in diameter; for experiments at still higher pressures, we use beveled diamonds having a 7- to 8.5-degree bevel on a 300-μm culet with a 30- to 75-μm flat face. (As points of reference, a standard sheet of paper is about 50 μm thick and a human hair is about 100 μm in diameter.)

Once the diamonds are perfectly aligned, we remove the tight-fitting piston that holds one of the two diamonds in place. Between the culets of the anvils, we place a 250-μm thick gasket (a strip or circular metal disc of tool steel or rhenium) and apply a small force to indent or prepress its surface. Then we drill a hole that is 30 to 150 μm in diameter in the center of the indented area. Into that hole we place the sample with a pressure medium—liquid, gas, or solid—which helps to distribute the compressive force of the diamond faces.

To calibrate pressure during the experiment, we add a pressure marker, such as a small ruby chip or platinum powder. Under illumination of a helium–cadmium laser, the ruby chip emits fluorescent light at characteristic frequencies (spectral lines), the wavelengths of which are calibrated as a function of pressure against a known marker material. The volume of the platinum under pressure can be calculated from the x-ray lattice parameters and compared with the known pressure–volume relationship from shock-wave data in order to ascertain the sample pressure. (The pressure marker acts as a pressure sensor and also indicates when the applied stress becomes nonuniform.) When the pressure is no longer hydrostatic, because, say, a fluid pressure medium has become a solid or has become very viscous, the resulting nonuniform stress broadens the ruby fluorescent peaks.

The Diagnostics

A significant advantage of the DAC is that diamonds are transparent to x rays and visible light. We exploit this feature when we watch the changes in the material as the pressure and temperature are changed. To determine the sample material's crystal structure during an experiment, we collimate the x-ray beam, selecting rays nearly parallel to one another with a slit system.[2] We pass the well-collimated beam of monochromatic (single-energy) x rays from a rotating anode generator through the sample and both diamonds and record the resulting diffraction pattern on x-ray film (see Figure 3). Efficient computer programs interpret the resulting patterns, which consist of a complex series of concentric arcs or reflections in a spectrum. These x-ray

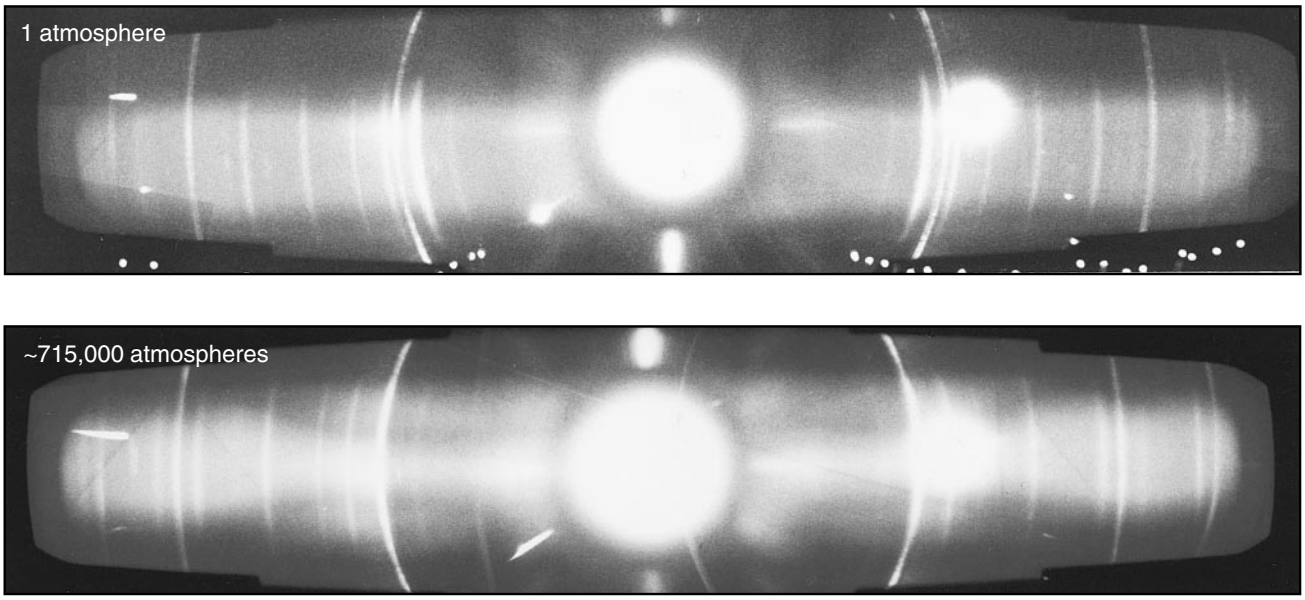


Figure 3. The experimentally interpreted structural sequence for uranium at increasing pressures recorded as an x-ray diffraction pattern by a collimated x-radiation experiment. It is x-ray diffraction patterns like these, but at much higher pressures, that provide the diamond anvil cell data of use to weapons physicists.

diffraction patterns thus become the means of "seeing" the changes in the crystal structure of the sample and collecting data about its changing equation of state under the intense pressure of the DAC.

Commonly, phase transformations are thought of as those from a solid to a liquid to a gas. However, there are transformations from one solid to another, and these are the structural transformations generally studied using the DAC. In solid-to-solid structural changes, the atoms of an element rearrange themselves in response to changing pressure, changing temperature, or both to new configurations. The shape of the atomic structural "cages" changes by the rearrangement of the atoms. Structural changes can be accompanied by a sudden volume change. However, the volume change can be small enough not to be recognized or to be able to be accounted for by a normal margin of experimental error. It can also be smooth and gradual and not exhibit the spikes associated with large, sudden changes. Whether subtle or sharply defined, these are the structural transformations of interest in DAC experiments.

The diagnostic x rays used to record these data in our DAC experiments at ultrahigh pressures are not like those from medical or conventional laboratory x-ray units, which are too weak to yield data in a reasonable time and cannot be collimated sufficiently to collect accurate data. Rather, we use the very bright, highly coherent x rays from a synchrotron source such as the one at the National Synchrotron Light Source at Brookhaven National Laboratory in New York State and collimate them to 5 to 10 μm in diameter. A combination of high beam intensity and excellent collimation is essential to reduce the time required for data collection (10 to 30 minutes at each pressure, rather than tens of days) as well as to reduce the effects that the pressure gradient across the sample has on the data.

When pressures exceed 40 gigapascals (GPa), we use the apparatus shown schematically in Figure 4 to record the diffraction pattern. First, we use a pair of adjustable slits to collimate the beam from the synchrotron x-ray source to a diameter of less than 10 μm. Then we clamp the DAC, with sample and ruby-chip pressure marker in place, to a four-circle goniometer* in order to align the DAC with respect to the x ray. Aided by the ion chamber, we align the DAC so the 10-μm-diameter x-ray beam probes the center of the sample (the area of greatest pressure and the least pressure gradient). The penta prism is essentially a microscope that directs light so that we can see the sample prior to experiments. The x-ray beam from the synchrotron source passes though the diamonds, diffracts from the sample, and passes through the pinhole collector in the upper part of the apparatus. It then enters the germanium–lithium detector, which records the energy diffraction pattern from the sample, data essential to identify the changing crystal structure. The optical multichannel analyzer in the lower part of the apparatus determines the pressure at which the crystal changes take place by measuring the laser-

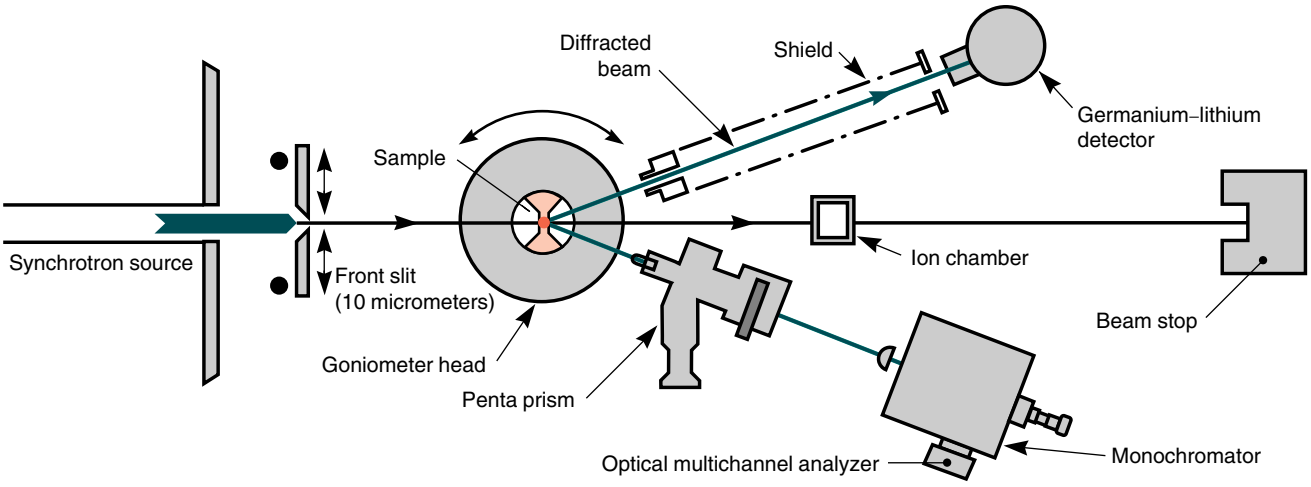


Figure 4. The configuration of our static high-pressure experiments using synchrotron radiation, the means of recording accurate diffraction patterns of materials in a reasonable time when pressures exceed 40 gigapascals.

* A goniometer is an instrument with a number of degrees of freedom to move a crystal in space and uses x-ray diffraction to measure the angular positions of the axes of a crystal.

induced fluorescent light from the ruby-chip pressure marker. Thus, the changing volume and density of the sample are measured as a function of pressure.

Heavy Metals Experiments

As part of our continuing investigation into the high-pressure properties of metals, we have used the diamond anvil cell to determine the pressure–volume relationship and any possible changes in the crystal structure for some actinide and lanthanide metals to approximately 325-GPa pressure at room temperature. Figure 5 shows the lanthanide and actinide series from the periodic table of the elements; shading highlights those elements we have studied in some depth. The Laboratory is the world leader in the study of lanthanides and actinides under extreme static pressure and temperature conditions.

One purpose of these investigations is to obtain consistent, thorough data of general scientific interest about the properties of these metals under pressure. Another is to study the behavior of the actinide weapons metals uranium and plutonium under pressures approaching those in imploding nuclear weapons. These purposes, however, are not separate. In theory and reality, there are connections between the high-pressure behavior of elements in both series that are of particular relevance to the high-pressure behavior of the actinide weapons metals uranium and plutonium.[3] Representative DAC findings about lanthanides and actinides illustrate how DAC research works in general and how it contributes to weapons safety in the absence of nuclear testing.

Our findings concerning the lanthanides and actinides to date fall into three categories: those concerning the lanthanides, those concerning the heavy actinides (americium through the end of the series), and those concerning the lighter actinides (thorium, uranium, neptunium, and plutonium).† In all three categories, we are in search of data about the stability—or lack of it—in each crystal structure and the equation of state under ultrahigh pressures. We are looking for structural changes as a function of pressure and temperature, changes in volume (density) due to the structural changes, the ultimate structural form that is stable for these elements, and the similarities between

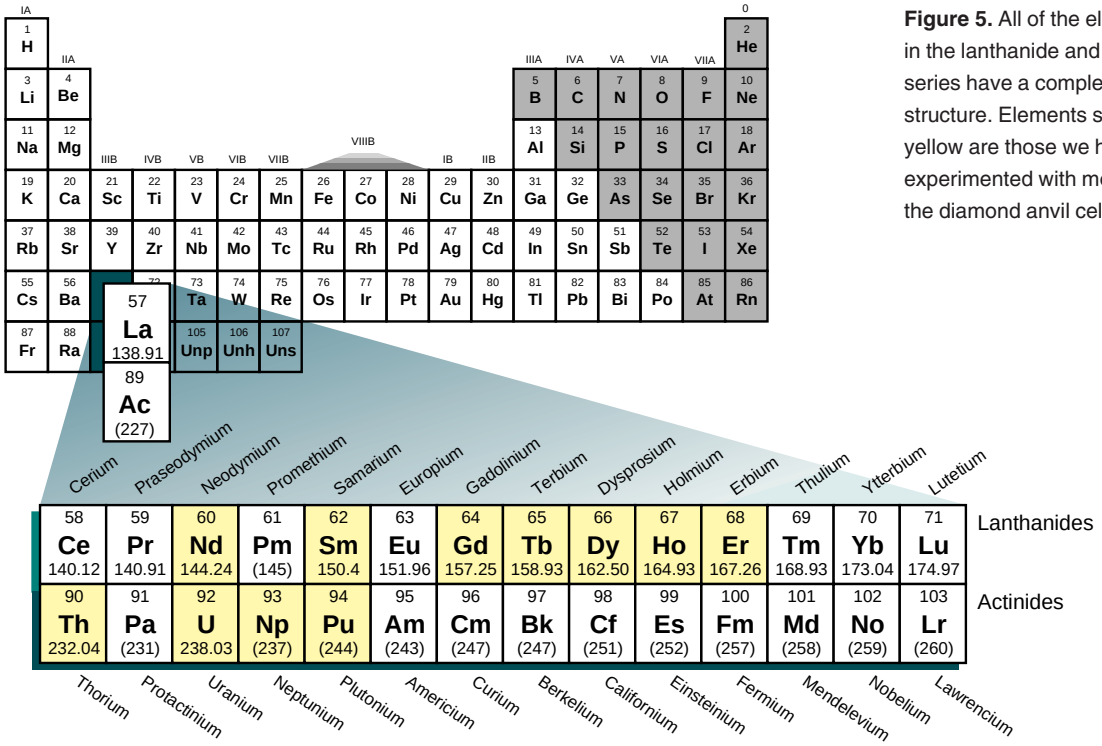


Figure 5. All of the elements in the lanthanide and actinide series have a complex atomic structure. Elements shaded yellow are those we have experimented with most using the diamond anvil cell.

† We have avoided DAC experiments with protactinium because it is too radioactive even in the small quantities needed for our work.

lanthanides and actinides. These are the data that physicists require in combination with shock-wave-derived data to confirm or modify the theory concerning the high pressure behavior of these metals upon which weapons code calculations for uranium and plutonium are based. These DAC data can improve the precision of the computer codes for the behavior of weapons materials and thereby improve the predictability of their structural behavior in the weapons regime.

The Lanthanides

The lanthanides, or rare-earth series of elements (elements 57 through 71 of the periodic table—lanthanum through lutetium), are nearly indistinguishable in their chemical behavior. Although they all have the same outer electronic shell configuration, each element has one more electron than its next lighter neighbor. This additional electron is located deep within the atom's electron structure. This configuration causes a smooth progression of physical properties across the series but has little effect on chemical properties. The normal (unpressurized) crystal structures of these elements (Figure 6a) show a regular progression across the series.

We studied the lanthanides in the DAC primarily to confirm experimentally the broadly related pattern of the elements' crystal structure across the series predicted by theoreticians.

Our detailed studies of some rare-earth elements have experimentally confirmed the existence of the structural sequence predicted by theoreticians. As pressure increased, the lanthanides transformed to face-centered cubic and a six-layered structure (Figure 6b). Under increasing pressure, the lanthanides follow the reverse of the normal, unpressured progression pictured in Figure 6a. When we increased the pressure beyond 100 GPa, we observed that the six-layered structure further transforms to a body-centered tetragonal structure. However, we did not see any big volume changes when the lanthanides transformed from one structure to another as the pressure increased. This behavior is contrary to what other experimenters have conjectured. Thus, our data suggest that the volume of these metals changes rather smoothly as a function of pressure without big, sudden changes.

The Actinides

In theory and in experiments, the actinides, especially the lighter ones early in the series, are less consistent in their behavior at high pressures than the lanthanides. The heavier actinides (americium through the end of the series) are predicted to behave under increasing pressures like trivalent lanthanides such as samarium and gadolinium. Our DAC experiments generally agree with theory for the heavier actinides. Thus at room temperature and pressures to 20 GPa, the trivalent lanthanides and heavy actinides studied exhibit similarities.

On the other hand, the light actinides, which include the weapons metals uranium and plutonium, are believed to behave less symmetrically and predictably under intense pressure than the lanthanides and heavy actinides. We are therefore studying them in the DAC in order to compare the electron behavior deep within them with similar behavior in the lanthanides and other actinides so that we can make critical conclusions about their high-pressure behavior.

Our findings concerning the other early actinides we have studied in depth (thorium and neptunium) illustrate the methodology and potential uses of DAC experiments for the study of uranium[4] and plutonium.

At room pressure and temperature, thorium has a face-centered cubic structure. In previous experimental studies to pressures below 100 GPa, we studied thorium with gold as a pressure marker. Because of the interference of the thorium and the gold diffraction lines, we did not identify phase changes in these experiments. However, our detailed investigation of thorium to 300 GPa with platinum as an internal pressure marker showed that indeed thorium goes through a structural change from face-centered cubic to a body-centered tetragonal at about 72.6 GPa with no further transformations even up to the highest pressure. Our studies also suggested significant transfer of electrons from outer shells to those deep within the atoms as the pressure increased.

Because thorium has a stable body-centered tetragonal structure even at 300 GPa and similar body-centered tetragonal structures are stable, as we have seen, for some lanthanides, LLNL researchers have asked whether the body-centered tetragonal phase is the ultimate high-pressure stable structure at room temperature for these metals. Answers to such questions are essential if theoreticians are to fine-tune their computer-generated models and code calculations.

Recent studies on the next actinide metal, neptunium, have, provided answers to the question. As pressure is increased, the orthorhombic crystal structure of neptunium at ambient conditions transforms to a body-centered tetragonal structure and then to a body-centered cubic structure that is stable to the highest pressure (see Figure 7).[5] This suggests that we might

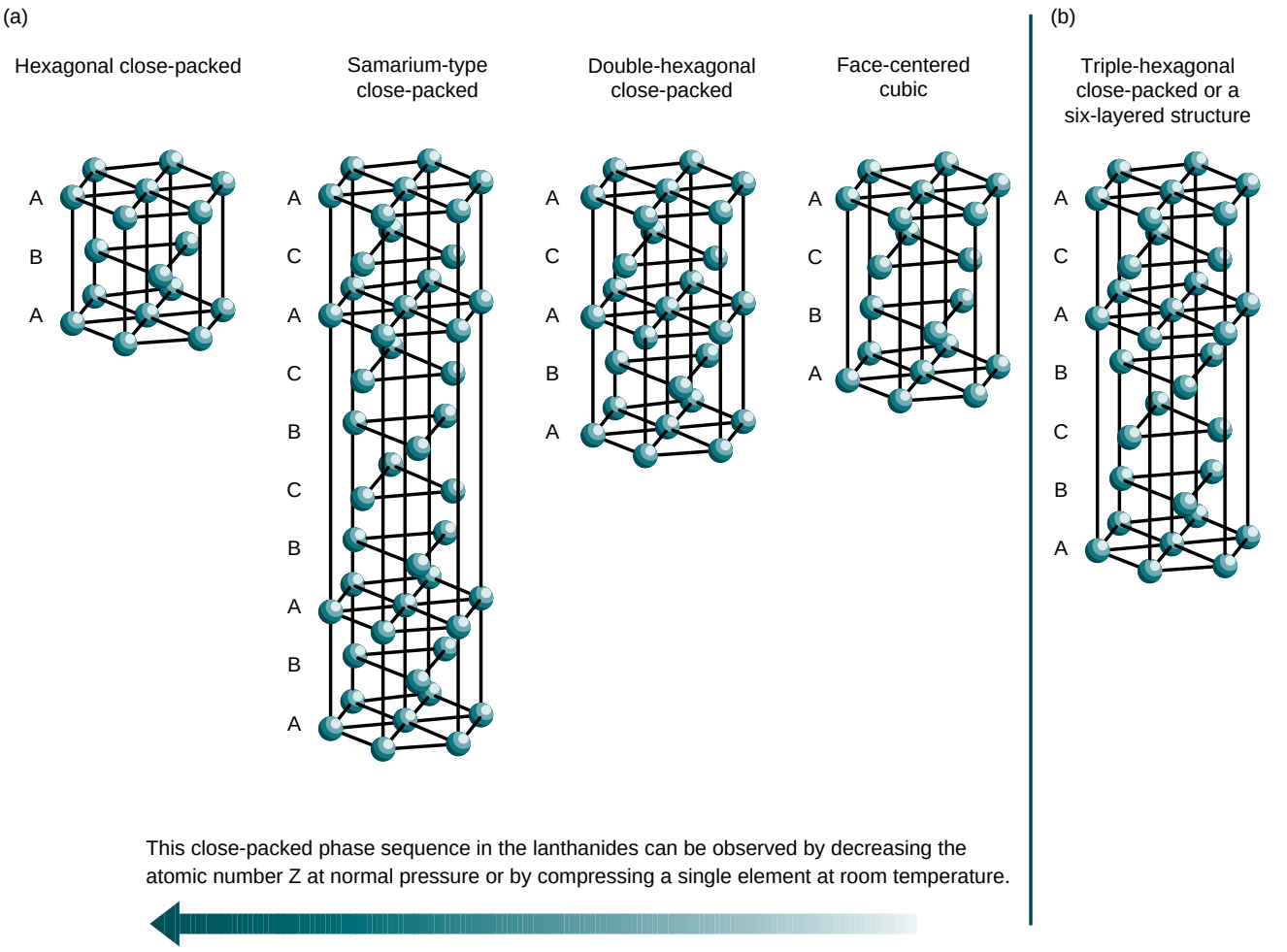


Figure 6. (a) The basic crystal structures found in lanthanide solids at room temperature and normal pressure across the series beginning with the lightest elements and moving to the heaviest. Our diamond anvil cell experiments have confirmed theoretical predictions that under increasing pressures approaching 100 gigapascals (GPa), the crystal lattice structure of the lanthanides follows the reverse of this sequence. In recent experiments, we saw a further transformation to a six-layered structure (b), which transforms to a body-centered tetragonal structure at pressures beyond 100 GPa but without the major volume changes predicted by some researchers.The crystal structures in (a) were first drawn by C. J. Alstetter, *Metals Transactions*, **4**, 2723 (1973).

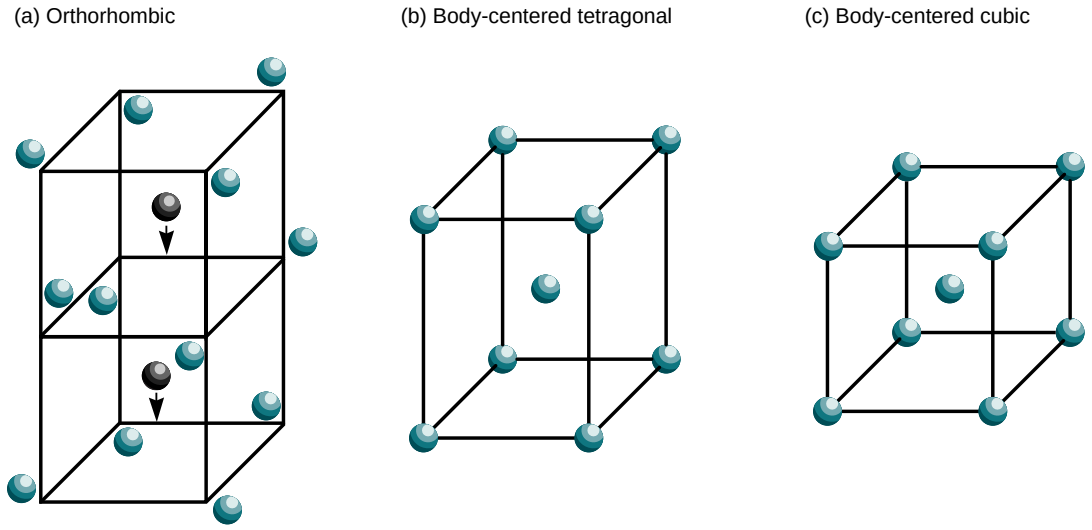


Figure 7. Schematic of the transformation of (a) orthorhombic neptunium at ambient temperature and pressure to (b) body-centered tetragonal to (c) body-centered cubic. The green circles in (a) represent one type of neptunium atoms, located near the corners of an orthorhombic subcell; the gray circles represent another type located near the centers of two subcells (the arrows indicate they are offset from the centers). Applying pressure moves the atoms to their nearest corner and the center of each subcell and results in (c) a smaller, more symmetric body-centered cubic form.

see similar body-centered tetragonal to body-centered cubic structural transformation in the other actinides and rare-earth metals. Thus, the ultimate stable structure of the trivalent lanthanides, the heavy actinides, and some light actinides may be body-centered cubic, not body-centered tetragonal. We also hypothesized from these studies that neptunium should have two body-centered cubic structures, one at low pressures and high temperatures before melting and another at high pressures and low temperatures. Both hypotheses provide new input to theory that can improve the precision of computer weapons code calculations.

Our classified DAC research on the light actinides uranium and plutonium has provided vital information that allows us to revise the computer modeling of the behavior of plutonium during nuclear explosions. In the absence of testing, this data is vital in assuring weapon safety, reliability, and predictability. To a lesser but equally vital extent, our DAC work on the lanthanides and other actinides related to weapons materials has contributed to those refined codes. It allows confirmation or revision of calculations derived from theory and dynamic experiments with accurate data that we can "see" from a high-pressure spectrum captured in static DAC experiments.

Future Directions

The DAC has enabled us to obtain phase stability information that dynamic techniques such as shock-wave methods could not supply and to incorporate that information into our theoretical models. Our scientists constantly endeavor to improve DAC experimental techniques in order to obtain better data and to obtain further information about the physical properties of any material, including weapons-related materials. With the addition of a laser or a resistance heater or with cryogenic cooling, we can also use the DAC to explore the pressure–volume–temperature relationship and the resulting structural changes of any material—its equation of state and phase diagram. Higher pressure and increased temperature may force further structural changes, until the material loses its crystal structure entirely—that is, it melts.

An area of new technology for obtaining high pressure and temperature data using x-ray diagnostics is electrical transport experiments such as ohmic heating based on resistance to the current. So far, these experiments have been among the most difficult to perform with diamond anvil cells. Special preparation of the sample, anvils, and cell is required, and electrical connections fail easily under the high stresses present in the diamond anvil cell. Consequently, electrical transport experiments have been very difficult to

perform beyond several tens of gigapascals. Our scientists have developed techniques to overcome these problems and will embark on further studies of the weapons materials to still higher pressures and temperatures.

In any nuclear weapon, high explosives play a pivotal role at the time of detonation. These energetic materials generally have complex crystal structures with low symmetry and are poor x-ray diffractors. Consequently, properties that are crucial to performance—such as how the behavior of high explosives depends on increased pressure and thus on changes in crystal structure—have not been thoroughly investigated at elevated pressures and temperatures. The DAC should allow researchers to collect such critical data under static conditions. We recently embarked on an exploratory study of equations of state and structural changes in high explosives using the DAC and synchrotron radiation. These studies will also inform us whether crystal structural changes in a high explosive such as triaminotrinitrobenzene (TATB) under pressure could cause changes in burn rates.

Key Words: actinides, diamond anvil cell, equations of state, lanthanides, science-based stockpile stewardship, shock-wave experiments, x-ray diffraction.

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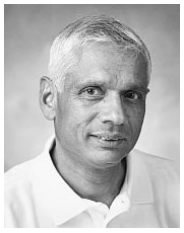
About the Scientist



JAGANNADHAM (JAGAN) AKELLA, who holds a Ph.D. in geochemistry, is the principal investigator of a Lawrence Livermore project that uses the diamond anvil cell (DAC) to study the *f*-electron metals and related weapons materials under ultrahigh pressures and temperatures.

Akella has successfully used DAC technology in conjunction with synchrotron x-radiation to investigate under controlled laboratory conditions the physical and chemical behavior of highly toxic radioactive samples under ultrahigh pressures and temperatures. These investigations have improved understanding of the fission triggers in nuclear weapons. Akella is also interested in developing new DAC techniques to investigate a wide array of nuclear and nonnuclear materials. Such work is relevant to a better scientific understanding of science-based stockpile stewardship issues as well as geological phenomena.

Akella joined the Laboratory in 1977 and has published more than 80 papers covering geological sciences, condensed matter physics, and materials science. He is an elected fellow of the Mineralogical Society of America and the Indian Mineralogical Association and is one of the recipients of the Department of Energy's 1994 Weapons Recognition of Excellence awards of the nuclear weapons program.

Gamma-Ray Imaging Spectrometry

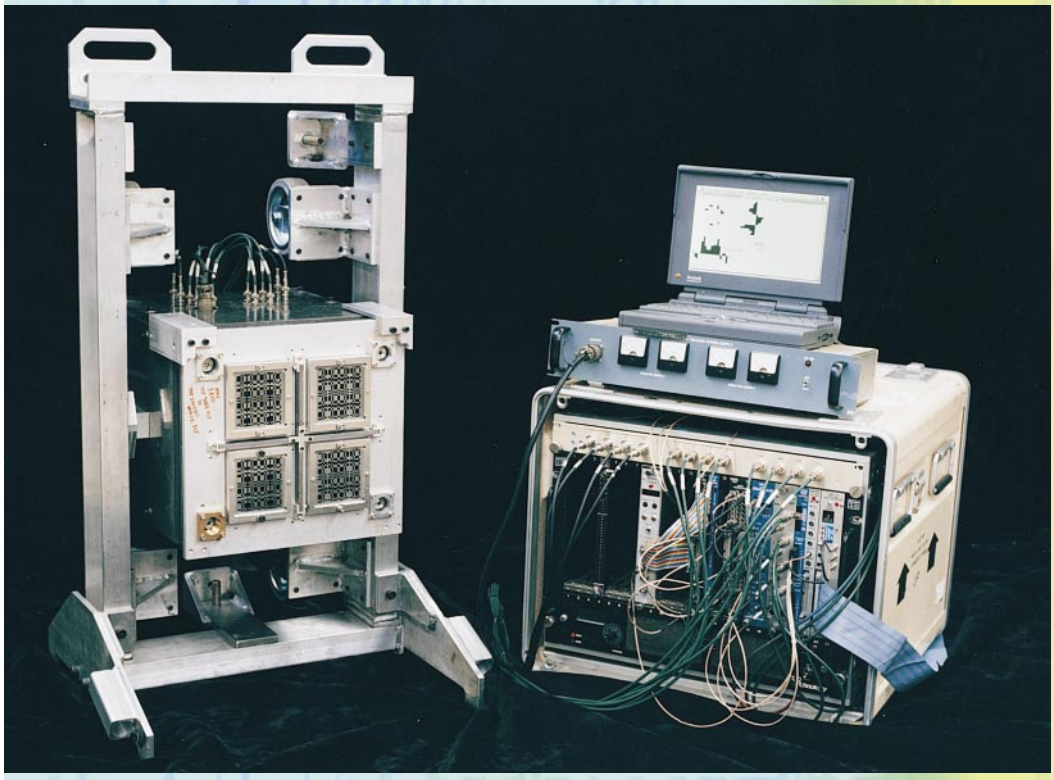


Figure 1. A Gamma-ray imaging spectrometer (GRIS) configured for work in gaseous diffusion plants. On the left, the GRIS imager head has four independent gamma-ray imagers. On the right is its data-acquisition system.

ONE of the challenges facing today's world is to keep track of the nuclear material generated during the Cold War. Some of the materials are radioactive isotopes that fuel nuclear weapons; others are used in the nuclear power industry. At Lawrence Livermore National Laboratory, we have developed an instrument that can help locate and identify these materials.

One of the characteristics of many nuclear materials, including those used in weapons, is that they emit gamma radiation. Each isotope emits a unique spectrum of gamma rays that can penetrate substantial amounts of ordinary matter without being scattered or absorbed like visible light. This radiation is imagable and can be used to indicate the presence and specific type of nuclear material.

Although nonimaging, nondirectional gamma-ray radiation detectors have long been used to monitor the presence and general location of nuclear materials, gamma rays have been poorly exploited to provide information about the precise location of the nuclear material. Recent

Lawrence Livermore National Laboratory

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Laboratory scientists have developed an imaging instrument for locating and identifying nuclear materials by taking "photographs" of the gamma rays emitted by these materials. This instrument, the gamma-ray imaging spectrometer, has many potential applications as wide ranging as treaty verification, environmental cleanup investigations, gamma-ray astronomy, and nuclear medicine.

advances in position-sensitive detector technology, coupled with advances from gamma-ray astronomy, have allowed researchers to design and build a gamma-ray camera capable of taking gamma-ray "photographs" that quickly characterize radiating materials. When these images made with invisible radiation are combined with visible-light images, they clearly show the exact location of the gamma-ray emitting materials.

Looking at Gamma Rays

The gamma-ray imaging spectrometer (GRIS) we have assembled comprises four coaligned, independent imagers, each with its own detector and coded-aperture mask (Figure 1). Each detector "sees" incoming gamma rays only through its mask, which serves as the imaging optic for the gamma rays (see box, pp. 114–115). This mask is mounted on a movable mask plate in front of the detector plane; moving the plate provides different levels of zoom for the gamma-ray images.

At the back of the housing are the electronics that take the relatively weak signals from the detectors and amplify them before they are sent to the data-acquisition system, which can be located remotely. Our system currently consists of a commercial electronics module, whose data are read out by a notebook computer (Figure 1). Coaligned with the gamma-ray imagers is a video camera. Images from this provide both a visual aim point and visible light images that can be overlaid with the gamma-ray images to pinpoint the location of the radioactive material.

Applications and Results

Although the spectrometer was developed to control the special nuclear material (SNM) associated with nuclear weapons, there are a myriad of applications in other areas, including environmental cleanup, astronomy, medicine, the nuclear power industry, and any other enterprise where radioactive sources are used.

Arms Inspection

GRIS was initially designed for use in arms inspections called for by the Strategic Arms Reduction Treaty (START)—specifically, to count the number of warheads on board a missile without requiring either close access to the missile or its disassembly. Inspections would be conducted remotely, based on the premise that the gamma-ray signature from the on-board warheads, although weak, is strong enough to be detected through the top of the missile. GRIS was constructed with four detectors to decrease the time it takes to obtain a good image approximately 10 m from the source. Figure 2 shows GRIS being used to inspect a Peacekeeper missile in its silo; the missile's ten warheads in the GRIS image are easily seen in Figure 3.

Confidence through Transparency

As the U.S. and Russia strive to reduce their respective nuclear stockpiles, each must have the ability to identify and verify the location of the other's weapons components throughout the demolition process. Each

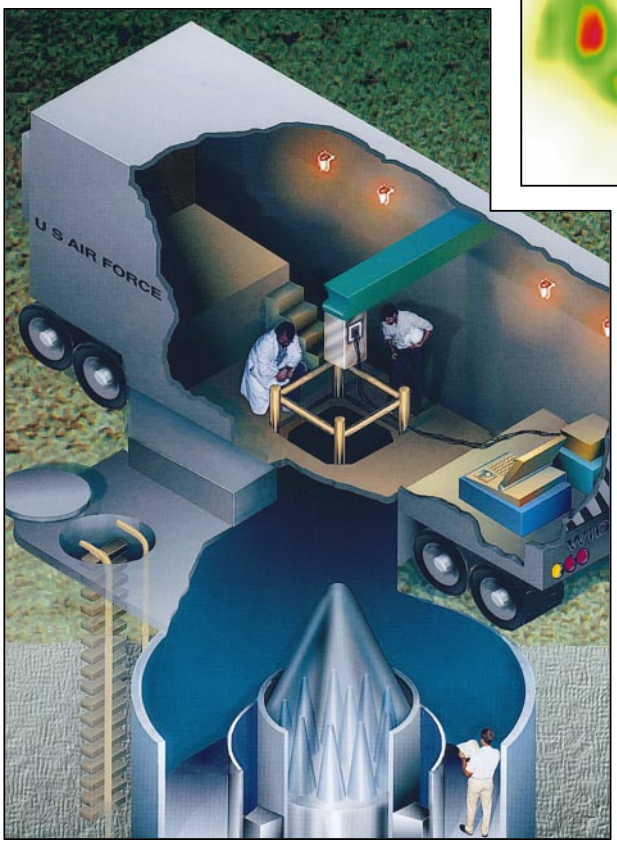


Figure 2. Rendering of the configuration used for gamma-ray imaging of a Peacekeeper missile. The GRIS imaging module is suspended above the open silo door and generates an image from the radiation given off by the warheads at the top of the missile.

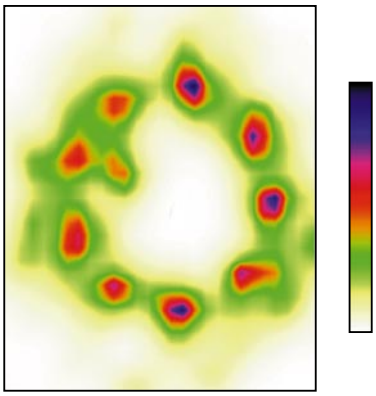


Figure 3. This enhanced gamma-ray image is from an emplaced Peacekeeper missile. The warheads are shown in a ring of nine, with the tenth inside the ring at the 10 o'clock position. The colors represent radiation intensity contours.

must have confidence that the SNM in the other's storage vessels is associated with nuclear weapons components but must be able to develop that confidence without performing an inspection that is sufficiently detailed to raise classification issues. This ability, or confidence, is called transparency.

In a recent joint U.S.–Russian demonstration at LLNL, we obtained data with a conventional, nonimaging gamma-ray detector and with GRIS. The data were collected from a radioactive source hidden inside a typical weapons component storage container. Both detectors possessed similar energy resolutions and could identify the type of material present. However, in a single measurement, the non-imaging detector could not verify the quantity of SNM present or the likelihood that the material was a weapons component. Such information could only be obtained from the nonimaging detector by scanning it across the storage vessel in small steps. Although this generated a crude image of the object that allowed identification, it also required most of a morning to complete. By comparison, the inspection with GRIS took half an hour—a time which could be easily reduced to a few minutes. The GRIS images taken from two directions 90 degrees apart (Figure 4) clearly show that a disk of plutonium and not a weapons component is in the storage container.

Related applications that take advantage of GRIS's ability to "see" behind shielding occur in nuclear waste disposal and in the characterization of nuclear weapons. Figure 5 illustrates such an application. Here, we placed a rectangular shape made from plutonium

rods inside a storage drum. To simulate shielding, we placed a depleted uranium plate about 3 mm thick outside the drum. The uranium serves as shielding, as a source of confusing radiation, and as a different radioactive isotope.

Figure 5 indicates both the energy resolution of the system and how images using data from different spectral regions can show the locations of different materials. The image obtained using only the data in the region of the spectrum shaded blue is on the left. This image represents emission from uranium and shows only the large uranium plate. On the right is the image obtained using data in the region of the spectrum shaded pink. These data are characteristic of plutonium and reveal the rectangular figure behind the uranium inside the container.

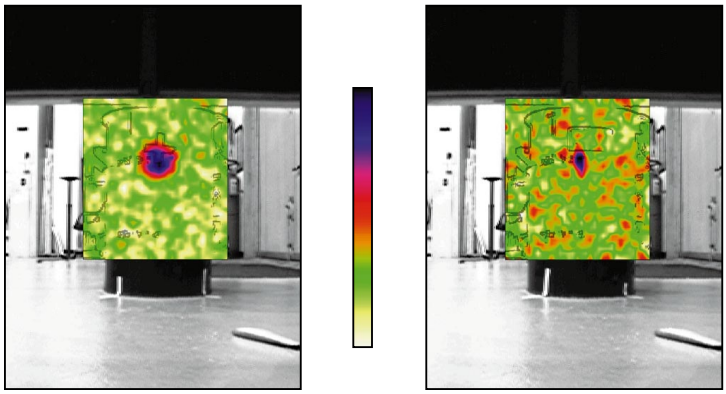


Figure 4. Overlaid on a video picture, a color gamma-ray image shows the difference between a face-on (left) and an edge-on (right) image of a plutonium disk. The images were obtained at a distance of 1.8 m and a position resolution at the source of 3.8 cm. Black represents the highest radiation intensity.

Safeguarding Weapons

When nuclear arms and their components are secured and stored, the primary concern is to verify that no material is removed from a storage area. In addition to armed guards, an inventory control system that constantly

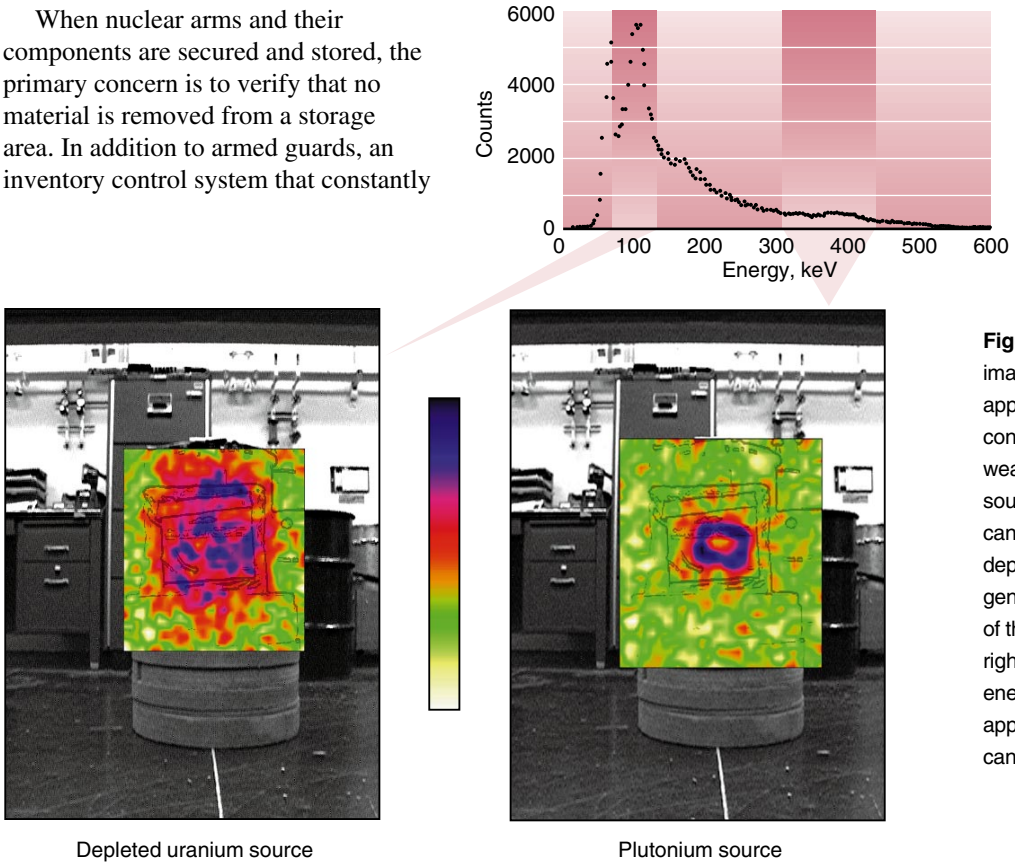


Figure 5. Demonstration of gamma-ray imaging and energy discrimination in applications for arms control transparency, contaminated waste identification, and weapons forensics. That the plutonium source is distributed inside a storage drum can be clearly seen, even through 3 mm of depleted uranium. The image at left is generated from 100-keV gamma radiation of the depleted uranium; the image on the right is generated from the plutonium energy band at about 400 keV. With the appropriate energy selection, the plutonium can be seen through the uranium.

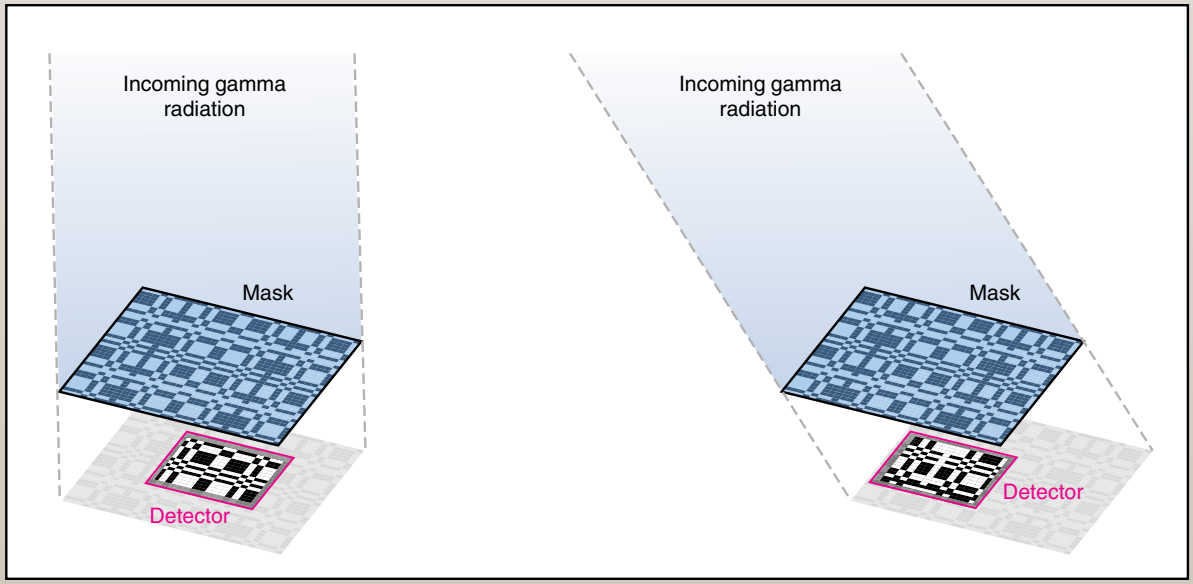
How the Gamma-Ray Imaging Detector Works

Astronomers have worked on the problem of imaging gamma rays for about 30 years. Although cosmic sources of gamma rays are extremely bright, they are also exceedingly far away, so the problem is how to image dim sources in a relatively large background. In principle, a pinhole camera could be used, but only a small fraction of the available radiation would reach the film or detector. In the late 1960s, it was recognized that one could improve the pinhole camera by punching more holes in the blocking sheet. Each hole projects its own image on the detector, and the different images overlap. If the hole pattern is known, one can mathematically recreate a faithful reproduction of the scene.

Although initial attempts showed that the technique worked, they also showed that the pattern had to be selected carefully, or false sources would appear in the image. The research on pattern effects was largely completed in the 1970s when a class of patterns called uniformly redundant arrays was created. These patterns possess a unique property: the information present in the shadow pattern from any one source in the image is not affected by the presence of gamma-ray sources in other parts of the image.

In the schematic of the imager (see the illustration below), we assume that radiation is coming from a very distant source. The light rays from this source are parallel, so a shadow of the mask is projected on the detector much the way it would be projected by the sun. Each pixel (the smallest picture element) in the image is represented by parallel gamma rays incident from one direction that project a detector-sized portion of the mask pattern onto the detector. The pattern is selected such that each projection is unique and independent of all other projections.

The image is recreated by a cross-correlation technique: the complete detector pattern is summed against each unique mask position by adding counts to the sum if the mask is open at this position and subtracting them if it is closed. Physically, counts are added if they could have come from that direction and subtracted if they could not. If no source is present, any detector-sized portion of the mask pattern has the same fraction of open



Uniformly redundant-array coded apertures produce an image by having each source pixel cast a unique mask shadow pattern on the detector. The mask is four times the area of the detector. On the left is the system response for a source in the center of the field of view. On the right, is a response for a source near the left edge of the field of view.

and closed area relative to all other portions of the mask of that same size, so the sum is zero (except for statistical fluctuations). If a source exists at the particular location being summed, then every time there is an opening there will be counts, and the sum will recreate the true flux (amount of signal per unit time) from the source.

The advantage of this technique is that half the detector area is exposed to each of the sources in the field of view. The rest is behind closed mask elements. Compare this with a pinhole camera, in which the open area is only one pixel's worth. For a point source, the signal-to-noise ratio increases as the square root of N, where N is the number of open holes. For our system, N is approximately 200, meaning a 14-times-greater signal strength and significantly reduced data-acquisition time.

Unfortunately, because all the counts in the detector are used at each image location, the more sources there are in the field of view, the less one gains from this technique. It reverts to one with the same sensitivity as a pinhole camera if the whole field of view glows at the same intensity.

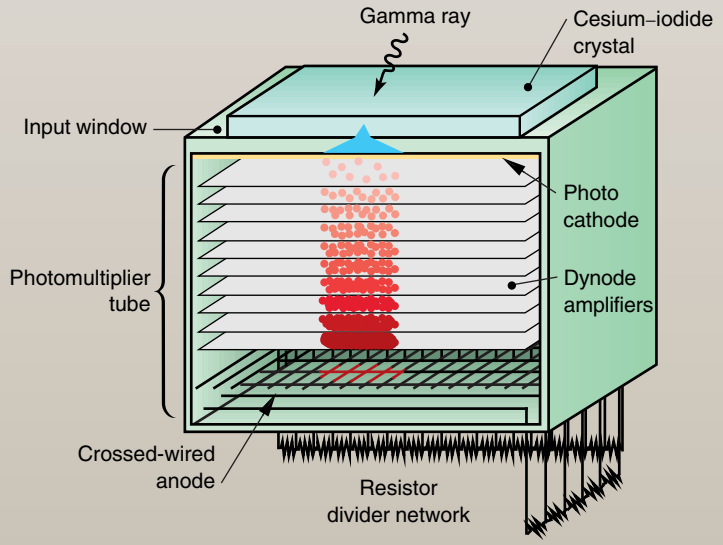
The resolution of a coded-aperture camera is just what it would be for a pinhole camera. For each pixel, the angular offset in incoming radiation is the basic hole size divided by the focal length (detector-to-mask spacing). To obtain the resolution at the source, one must multiply this angle by the distance to the source.

Position-Sensitive Detector

Converting the signal to a visual image requires a position-sensitive detector. Moreover, the position resolution must be comparable to the mask hole size; otherwise the pattern washes out. Because typical position-sensitive detectors (known as Anger cameras) for gamma rays of energies from 20 kiloelectron volts to greater than 1 megaelectron volt have position resolutions of the order of 1 cm, an imager must be quite large to have a reasonable number of pixels across the detector. An imager made with such a detector must also have a long focal length to achieve even modest position resolutions at the source

Our development of a gamma-ray detector with a position resolution of about 1 mm allowed the full exploitation of the coded-aperture technique in a compact system. In the schematic of the detector at the left, a position-sensitive photomultiplier tube is combined with a thin cesium–iodide crystal. When a gamma ray hits the crystal, it causes a brief flash of light, which is converted to an electronic signal by the photomultiplier tube. The tube is unique in that it allows the position of the light flash to be determined from its four output signals. The amount of light is proportional to the energy of the gamma ray and is also measured by the photomultiplier tube. The 4- × 5-cm active area of the detector yields about 40 pixels across its face, allowing for a mask pattern about 20 × 20 pixels (ideally, one oversamples by a factor of two.)

This schematic of the GRIS detector shows how it locates gamma radiation. A sodium-doped cesium–iodide crystal emits a flash of light when struck by a gamma ray. This light is converted to electrons and amplified by the photomultiplier tube on which the crystal is mounted. The tube uses a unique mesh dynode structure and a crossed-wire anode to determine the location of each event over the face of the tube.



monitors the radiation from each radioactive component is desirable. However, such a level of security is not always possible. Particularly in establishing an interim storage area, the costs and time required to make individual security monitors for each location can be prohibitive. However, the need for such facilities will be particularly important as U.S. and states of the former Soviet Union dismantle nuclear warheads. In this case, a GRIS-type imager can be a relatively inexpensive and very rapid way to establish inventory control.

Although we have not fielded such an application, the implementation is straightforward. The gamma-ray imager is installed so that it can "see" all sources, and a baseline image is taken. Then, the imager is set on a timer to take that image over and over again. A mathematical comparison of each successive image to the original can be used to sound an alarm should something be moved; we developed suitable algorithms to do this in the course of analyzing the Peacekeeper data. The advantages of using an imager in this case are that it can be set up very quickly, personnel need not leave the room, and visible light is not required.

Locating SNM in Process Plants

GRIS has been demonstrated at two U.S. gaseous diffusion, uranium-enrichment plants—K-25 at Oak Ridge, Tennessee, and the Portsmouth plant near Portsmouth, Ohio. The images we obtained from these plants demonstrate the utility of gamma-ray imaging in a number of complex situations.

Gaseous diffusion is used to separate the useful uranium-235 isotope from the predominant uranium-238 isotope present in natural uranium. Uranium-235 is the fissionable material used both as nuclear fuel in reactors and as weapons components. In the gaseous diffusion process, uranium metal is combined with fluorine to make uranium hexafluoride (UF_6), which is a

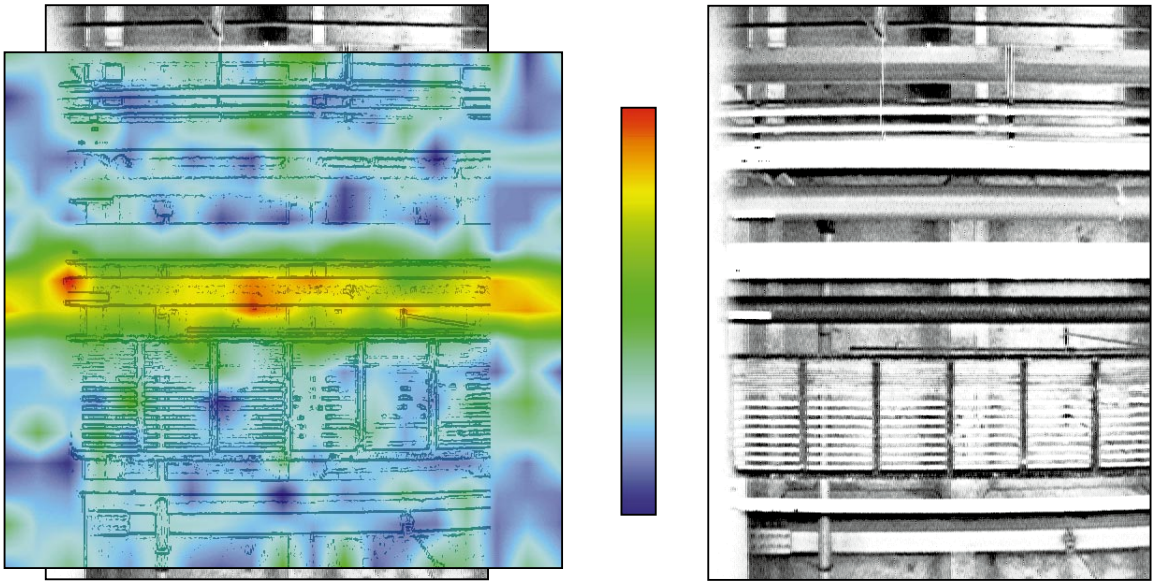


Figure 6. Video (right) and composite gamma-ray/video overlay (left) of a contaminated pipe at the K-25 gaseous diffusion plant at Oak Ridge. The gamma-ray image clearly shows which of the pipes overhead is contaminated.

gas at elevated temperatures. Separation takes advantage of the fact that the gas, composed of the lighter uranium-235 isotope, diffuses at a slightly higher rate than the gas containing heavier uranium-238. The UF_6 is enriched in heated equipment and piping contained within insulated housings.

Occasionally, because of leakage of wet air or environmental changes in the housing, solid UF_6 deposits develop. Such deposits routinely occur in an operational plant and must be located and identified. This task is not trivial. Many different pipes share the same heat shielding in the miles of pipe galleries. To enter these enclosures, workers must don protective gear to avoid radioactive contamination from possible residual leaks from more than 30 years of operation. In addition, some facilities—including those going through decontamination and decommissioning—contain highly enriched uranium, which could cause a criticality accident if a deposit of uranium-235 becomes too large.

Current characterization of the uranium deposits in these plants is performed primarily using sodium-iodide-based radiation detectors. These are carried through the plant, and readings are taken at fixed intervals to map the radiation fields. If a "hot" region is found, workers must either enter the heat-shield-enclosed area or take many measurements with a collimated version of the detectors to try to locate the deposit. Both are time-consuming, expensive, and potentially hazardous tasks. GRIS avoids these problems by generating images from outside the heat shielding that definitively locate the hot material.

Our first use of GRIS in this environment was at the idled K-25 plant. GRIS was mounted on a cart to look up some 4 m at the pipe galleries overhead that range in width from a few meters to more than 12 m across. Each gallery, enclosed in heat shielding, contains pipes ranging in size from a few centimeters to more than a meter in diameter. The building had been entirely scanned by K-25 personnel walking under and on top of the galleries using an uncollimated radiation detector; the results from this survey were used to select sites of interest for application of the GRIS imager. The first image was a pipe used to exhaust the building's many vacuum pumps. We selected this pipe because the lack of heat shielding allowed us to verify that the gamma-ray and video images identified the hot pipe (Figure 6).

A second exposure was taken of a more representative location where an isolated deposit of material was known to exist. After an initial wide-field image was taken to see the complete deposit, we moved the imager under the hot spot and zoomed in on this region. Figure 7 shows a deposit in a 1.2-m-diameter pipe, where an expansion joint exists. The deposit is probably uranium oxide, formed when a leak developed in the expansion joint.

The images from the next location, although they are nearly featureless, clearly demonstrate the power of the technique. We took GRIS to a location where we expected to find a series of radioactive pipes running the length of the area covered in the image. Two exposures were needed to cover the full width of the 12-m-wide pipe gallery. The resulting images (Figure 8) revealed only a few hot spots, not the contamination expected from the standard analysis.

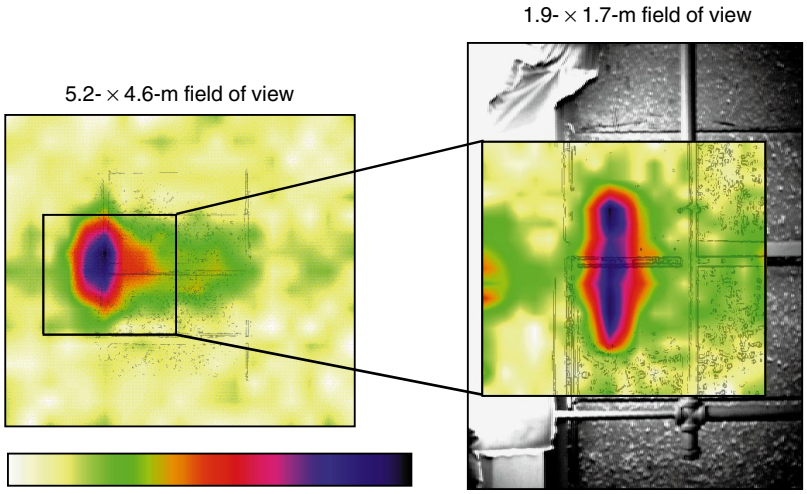


Figure 7. Overlay of gamma-ray intensity as a function of position for wide-field (left) and zoom views (right). The gamma-ray image on the right, which is overlaid on a video image, was taken after the imager was moved under the hot spot initially identified from the image on the left. The radiation is emitted by a uranium deposit inside a 1.2-m-diameter steel pipe hidden behind heat shielding.

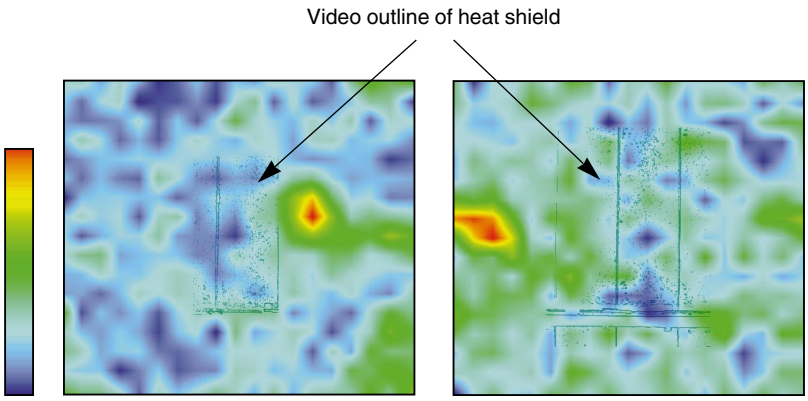


Figure 8. A powerful example of the advantages of gamma-ray imaging, this image shows little contamination within the heat shield. Instead, the image shows that the contamination is in a nearby area.

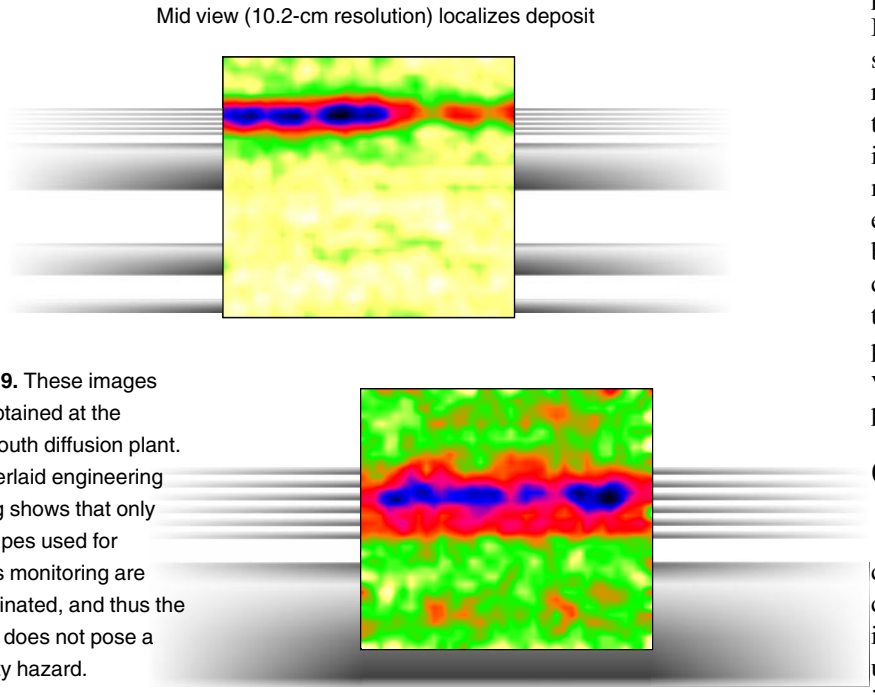


Figure 9. These images were obtained at the Portsmouth diffusion plant. The overlaid engineering drawing shows that only small pipes used for process monitoring are contaminated, and thus the deposit does not pose a criticality hazard.

Following the K-25 visit, we took GRIS to the diffusion plant at Portsmouth. There we made two measurements of note. The first was taken to determine the exact location of a known deposit of highly enriched uranium. There were concerns that a criticality accident was possible if the deposit was in the main 20- or 30-cm-diameter pipes of the gallery. One image (Figure 9) shows that this was not the case and that the deposit was in much smaller instrumentation pipes. The second image (Figure 10) shows a deposit in a diffuser cell, a large heat-shield-enshrouded area about 25 m × 6 m. The image, overlaid onto a plant blueprint, clearly shows plant personnel where the deposit is located before someone enters a cell.

In addition to its usefulness to personnel who operate and clean up these facilities, gamma-ray imaging also promises to be very useful to the International Atomic Energy Agency's safeguards programs for monitoring reactor fuel production facilities around the world. One of the major uncertainties in inspecting such plants is the nuclear material remaining in the process equipment. The ability to take images of both deposits and gas in the equipment can significantly increase the accuracy of the estimates of the quantity of material present. In addition, the settings of valves and the flow of gas through a plant can be independently verified.

Other Applications

Other GRIS applications are being considered. For example, a private company working for the nuclear power industry is studying the feasibility of using the gamma-ray/video overlay imagery to direct workers away from areas of particularly intense radiation.

In a similar application, GRIS could be used to find "lost" radioactive sources. Intense radioactive sources are sometimes used for materials characterization in construction and maintenance. If these sources are lost from their holders, they present a significant radiation hazard.

Finally, nuclear medicine could potentially benefit from application of a gamma-ray imager with capabilities similar to those of GRIS. The gamma emissions of several well-known radionuclides used in medicine fall within the range of energies GRIS exploits.

Spectrometry and the Stars

In addition to the programmatic imaging work described so far, we have collaborated with the University of California at Berkeley and at Santa Barbara to combine our unique detectors with a novel implementation of coded-aperture imaging to build the world's highest angular-resolution, gamma-ray telescope (Figure 11). Constructed with Laboratory Directed Research and Development funding, GRATIS (gamma-ray arc-minute telescope imaging spectrometer) comprises 36 individual imagers specifically tailored to work in the astronomical energy band from 20 to 200 keV. Our high-position-resolution detectors combined with a 4-m focal length allow GRATIS to achieve an unprecedented angular resolution of 2 arc-minutes (arc-min). By providing each of the 36 detectors with its own one-dimensional coded-aperture mask (Figure 12), we provide better overall performance at lower manufacturing cost than a more conventional telescope of similar size. Every one of these telescopes produces a one-dimensional

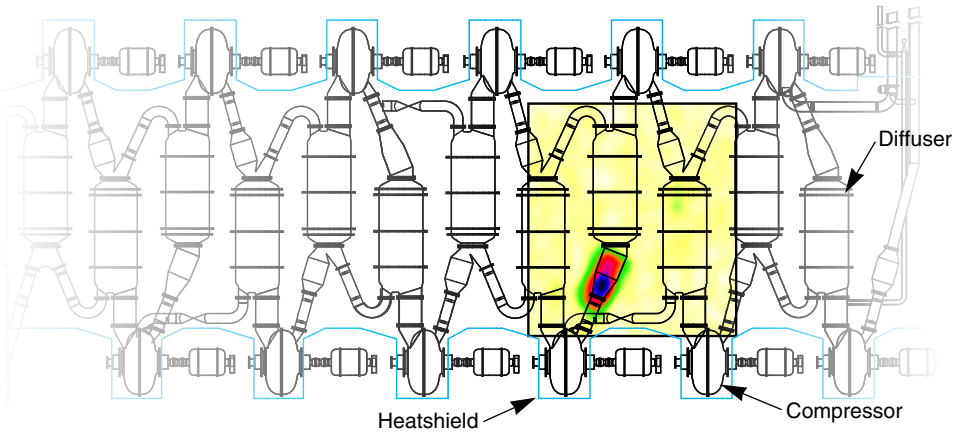


Figure 10. Overhead view of process equipment at the Portsmouth, Ohio, facility overlaid on engineering drawings of the area. The gamma-ray image clearly localizes the deposit to one length of pipe. The cylindrical diffusers are spaced about 2 m apart.

Figure 11. GRATIS is held by the launch vehicle as it is transported to the launch site at Palestine, Texas. Although significantly larger in size, the telescope is operationally very similar to the GRIS system developed for LLNL programmatic work.

picture of the sky; the images are combined mathematically to give a full two-dimensional image.

GRATIS provided a special challenge because viewing radiation from the cosmos requires that the telescope be above all but the most tenuous portions of the atmosphere. Thus, GRATIS is hung from a helium balloon, and the pointing system is operated by remote control. To keep a source in the center of the field of view requires that the pointing system be stable to 1 arc-min. To reconstruct the images properly requires that we know where the telescope is pointing to an even higher accuracy, which is obtained by using a coaligned star camera and a gyroscope system that allow us to reconstruct the pointing after the flight to approximately 20 arc-seconds.

GRATIS was first flown successfully in spring 1994 from Palestine, Texas. During its 11-hour flight, we observed three scientific targets: Cygnus X-1, Cygnus X-3, and Her X-1; we are in the process of analyzing the data. Meanwhile, GRATIS is on the ground in Alice Springs, Australia, ready for its next flight this fall, when we will observe the center of our galaxy.

Continuing Development

Our ongoing efforts in gamma-ray imaging include improvements in the detectors and in image-generation techniques. We are building a new detector that takes advantage of the rotated one-dimensional imaging used in GRATIS to extend the useful energy range of this work and to significantly lower the cost per unit area of detector. Called the Gamma-Ray Bar Imaging Telescope (Figure 13), GRABIT achieves these advances by separating the energy- and position-resolving functions of the detector.

A series of scintillator bars is mounted on a nonimaging photomultiplier tube. Most of the scintillation light from a gamma-ray event is collected by this tube, the signal from which is used to determine the energy of the gamma ray. To determine where the gamma ray hits, we pick off a small fraction of the light with a fiber-optic bundle and transmit it to an imaging device such as the photomultiplier tube used in GRIS. By observing which fiber end glows and knowing its arrangement on the imager, we can determine which bar is hit by the gamma ray.

To understand how this feature improves the system performance, note that the GRIS detectors determine an event's position by finding the center of the light footprint at the input to the photomultiplier tube. However, as one makes the crystal thicker, the average event size will increase because the light spreads out more before it reaches the tube, thus decreasing the ability to find the flash location. By dividing the crystal into bars, we remove this problem: the position resolution is limited only by the width of the bar. The costs are lower because the unit area of nonimaging tubes is only about one-tenth that of imaging tubes. By reading out a bar with a fiber optic, we effectively increase the expensive imager area some 40 times. We are currently assembling a laboratory prototype of this detector system.

Our previous imaging work clearly demonstrates the advantage of generating images using different parts of the energy spectrum. Unfortunately, the energy resolution of the cesium iodide currently used is only about 10%, not enough to distinguish commercial (reactor-grade) plutonium from weapons-grade plutonium. Higher energy resolution makes this distinction possible because it separates the different gamma-ray energy lines of the various plutonium isotopes.

Another advantage of improved energy resolution is the ability to obtain information from a strong source that lies behind a significant thickness of other material. In such a case, the overlying material acts much like the diffuser in front of a light, scattering the radiation and blurring the image.

Figure 12. Close-up view of the GRATIS mask plane. There are 36 individual one-dimensional masks, each rotated with respect to all the others. The resulting rotated individual images are combined mathematically to give a two-dimensional image.

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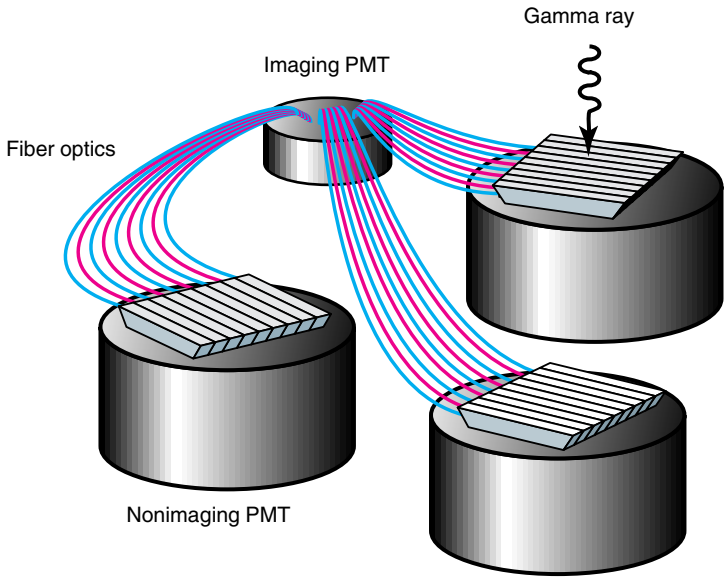

Figure 13. This schematic of the GRABIT detector shows how the position- and energy-resolving functions are separated. The light collected from the bottom of the bar arrays provides the energy information for an event. The small amount of light transported to the image tube by fiber optics allows one to determine which bar was struck.

However, unlike visible light, the scattered radiation at these higher energies is also shifted to a lower energy. By restricting the image to photons, which are in a known spectral line from the source, one can remove this type of blurring. With these advantages in mind, we plan to develop position-sensitive, solid-state detectors such as germanium- or zinc-doped cadmium telluride, both of which provide much better energy resolution.

Because it was developed for gamma-ray astronomy, the coded-aperture imaging technique as it has been applied by others assumes that the source is very far away. In the close imaging work we have described, this assumption does not hold. We have applied several techniques to compensate for this difference and are continuing to make improvements to the imaging techniques.

We are investigating the application of more advanced imaging algorithms to the coded-aperture data. These techniques rely on iterative approaches, based on Bayesian logic, that seek the best image on the basis of prior knowledge of the source and instrument. We are already applying one such technique, known as maximum entropy, to obtain the two-dimensional image from our set of one-dimensional images in GRATIS data. This technique selects the "flattest" image (the one with the least structure) commensurate with a statistical goodness-of-fit indicator based on the known instrument properties. In this case, we assume that the scene nature supplies will not have a lot of rapid variations in counts versus position.

Key Words: gamma rays—gamma-ray arc-minute telescope imaging spectrometer (GRATIS), gamma-ray astronomy, gamma-ray bar imaging telescope (GRABIT), gamma-ray camera, gamma-ray imaging spectrometer (GRIS); special nuclear material (SNM); Strategic Arms Reduction Treaty (START).

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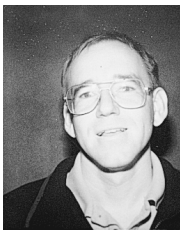
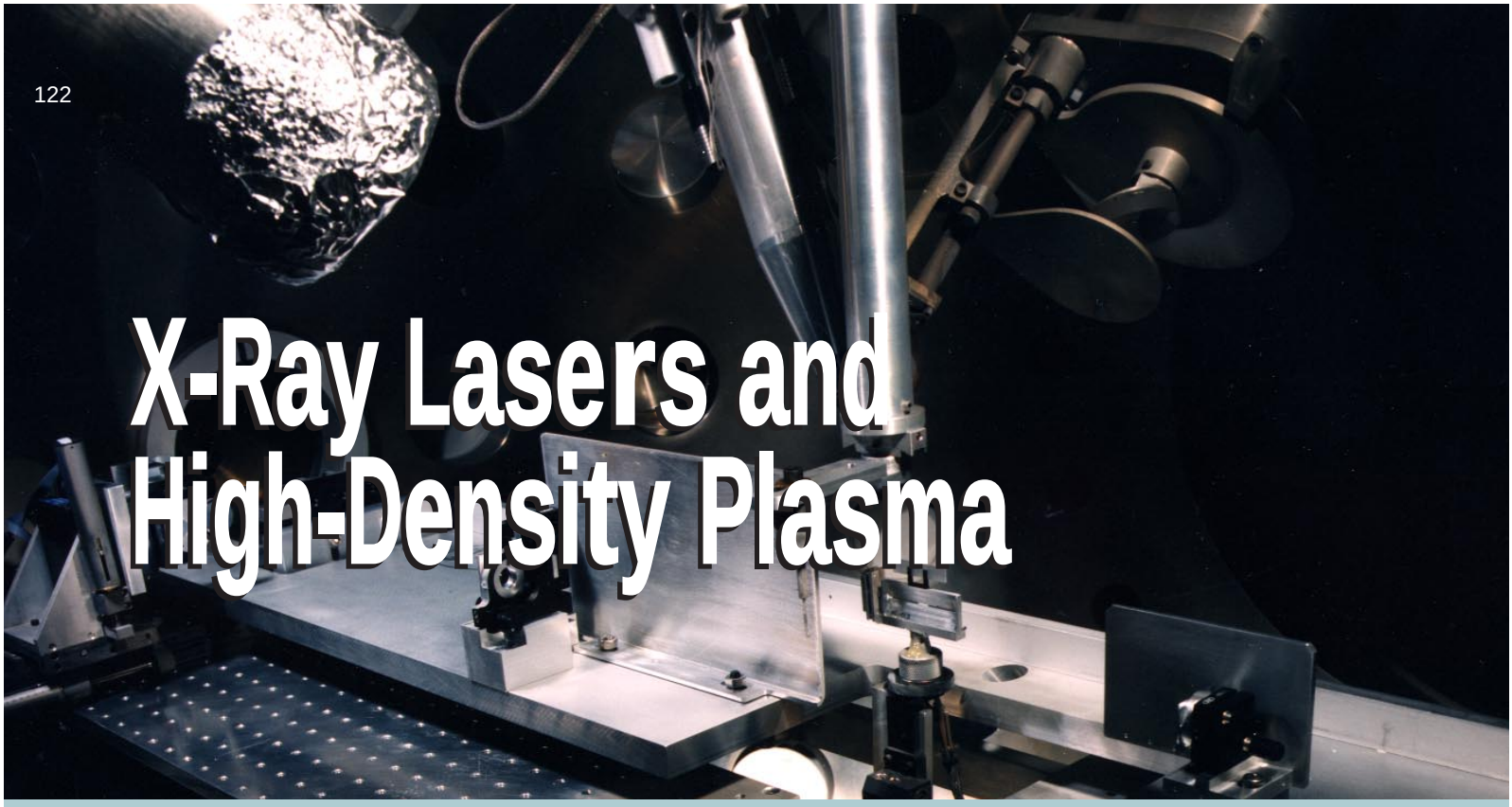
About the Scientist



KLAUS-PETER ZIOCK came to Lawrence Livermore National Laboratory 10 years ago as a post-doctoral scientists in V Division. Since 1988, he has been a staff scientist in V Division's Laboratory for Experimental Astrophysics. He received his Ph.D. in Physics from Stanford University in 1985 and his B.A. from the University of Virginia in Physics and Chemistry in 1978. His primary area of scientific research is low-energy gamma-ray astrophysics. He has been involved in the development of GRIS, GRABIT, GRATIS, GRB (a gamma-ray burst detector), and SXRP (an x-ray polarimeter).

His numerous publications to date (about 40) are in the area of atomic physics, including high-atomic-number systems, positronium spectroscopy, and instrumentation development for astrophysical research.



X-Ray Lasers and High-Density Plasma

X-ray lasers are ideal for studying high-density plasmas of the sort produced by the Nova laser. We have demonstrated single-micrometer resolution of plasma images and interferometric techniques for determining plasma density. Current work on developing shorter pulses of x-ray laser light will improve resolution in two dimensions.

OVER the course of only a few decades, lasers have become ubiquitous. In the future, x-ray lasers are likely to become widespread because of their growing range of uses. Among other promising developments, x-ray lasers are being applied in areas ranging from biological imaging to materials science. One of our most recent and sophisticated uses of the x-ray laser is as a probe for imaging and understanding high-density plasmas.

Optical probes have been historically important in studying and characterizing laser-produced plasmas. However, researchers have had to overcome many obstacles in their attempts to analyze large, high-density plasmas of the sort that can be created at LLNL by the Nova laser. The difficulties arise from several problems, including high absorption of the optical probe light, the adverse effects of refraction, and the impossibility of probing beyond critical densities in plasma. (Critical density, which is determined solely by the wavelength of the probe, is the electron density beyond which light of a given wavelength will not penetrate.)

Advances in high-energy, more reliable x-ray lasers together with improvements in mirror technology have made it possible to develop diagnostic techniques that are now suitable for evaluating the plasmas of interest. This article reviews the status of laboratory x-ray lasers and their clear advantages in plasma diagnostics. It describes our three principal techniques: high-resolution imaging of the fine structure in plasma, moiré deflectometry used to measure density gradients in plasma, and interferometry for directly measuring electron density. Our recent work in the area of interferometry is made possible as a result of new beam splitter technology developed at LLNL. Finally, we discuss future applications for this important tool, including the characterization of plasmas that will be created by the proposed National Ignition Facility (NIF).[1]

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About Plasmas

Researchers need detailed knowledge of the distribution of electron density in a laser-produced plasma for a wide range of endeavors. This type of information is essential for research in inertial confinement fusion, for laser–plasma interaction physics, and for interpreting high-temperature, high-density laboratory astrophysics experiments.

In laser-induced fusion, for example, a tiny capsule containing deuterium–tritium fuel (two heavy forms of hydrogen) is struck from all directions by radiant energy called the "drive." In one arrangement known as direct drive, many powerful laser beams are focused so they impinge on the capsule. The rapid, rocketlike expansion of the capsule shell drives the inner portions of the capsule inward, compressing and heating the fuel. At a density of more than 200 g/cm^3 (more than a thousand times the density of solid hydrogen) and a temperature of about 100 million K (kelvin) (comparable to temperatures deep in the sun), a fuel plasma forms, and nuclear fusion reactions occur. In the next several decades, fusion energy could become a clean and limitless alternative to our current reliance on fossil fuels.

On Earth, plasma is a short-lived, highly or completely ionized gas that can be produced using several different types of targets. When high-intensity laser light irradiates a solid target, such as a metal foil, the extent of the plasma is determined by the laser spot size; therefore, plasmas can range from hundreds of micrometers to several millimeters in diameter. The plasma is also relatively long in the direction parallel to the drive laser, so an irradiated foil can span orders of magnitude in density and temperature at a given time.

With each new laser system, we need increasingly sophisticated diagnostic instruments to "see" what is happening: as a function of the laser beam parameters (such as intensity and size), in targets of various types, and in the plasma. The central challenge in diagnosing such experiments is the ability to accommodate the spatial and time scales involved. The phenomena we are interested in occupy spatial scales from a single micrometer (about one-hundredth the diameter of a human hair) to a few millimeters, and time scales from several picoseconds (the time it takes light to move about a millimeter) to several nanoseconds. The plasma density can range from about 10^{20} to 10^{26} cm^{-3},* where solid density is about 10^{23} cm^{-3}. The electron densities we are interested in approach 10^{22} cm^{-3}.

We can obtain electron density information in many different ways. Examples include x-ray spectroscopy, absorption and scattering of incident laser light, and ultraviolet interferometry. However, each of these techniques has limitations, including the range of densities and scale sizes that can be measured. To overcome some of the limitations, we have developed several techniques based on a soft x-ray laser beam. Whereas the details of our techniques differ, they all have one central feature in common: they involve creating one plasma with one beam of Nova as a source of coherent x rays to image or diagnose a second plasma produced when a target is irradiated by another Nova beam.

What Is an X-Ray Laser?

The human eye sees only a small portion of the electromagnetic spectrum, namely, wavelengths extending from about 700 nm for red light to about 400 nm for violet light (a nanometer is one billionth of a meter). At shorter wavelengths beyond violet light is the ultraviolet region that is invisible to the unaided eye and associated with potentially skin-damaging rays of the sun. X rays are a form of penetrating electromagnetic radiation with even shorter wavelengths ranging from about 10^{-6} to 10^2 nm. The soft x rays various researchers are using as a probe lie just beyond the ultraviolet portion of the spectrum and have wavelengths of a few to tens of nanometers.

X rays can be generated by accelerating electrons to high velocities and then stopping them suddenly by collision with a solid body. This technique produces short-wavelength x rays that can be dominated by radiation from atomic inner-shell transitions. Electron bombardment is the technique used for generating medical x rays.

In recent years, researchers have developed many different schemes for producing a laser of x rays. The most successful of the schemes has been collisionally pumped x-ray lasers, which are produced in plasmas containing ions in a highly charged state. Within the ions, electrons move between the ground state and various higher energy levels so that the conditions are achieved for producing x rays. The box on p. 128 explains in more detail the principles behind lasers and collisional pumping schemes for generating a soft-x-ray laser.

In practical terms, collisionally pumped x-ray lasers are highly useful because they can operate over a wide range of pump conditions and with a variety of targets. Moreover, the range of wavelengths over which collisionally pumped soft-x-ray lasers operate (about 3.5 to 40 nm) make them good candidates for many different applications.

For our work in plasma diagnosis, we selected the neonlike yttrium x-ray laser.

* This is the conventional mathematical expression of electron density in a given volume. In this instance, it records how many electrons are contained in 1 cubic centimeter.

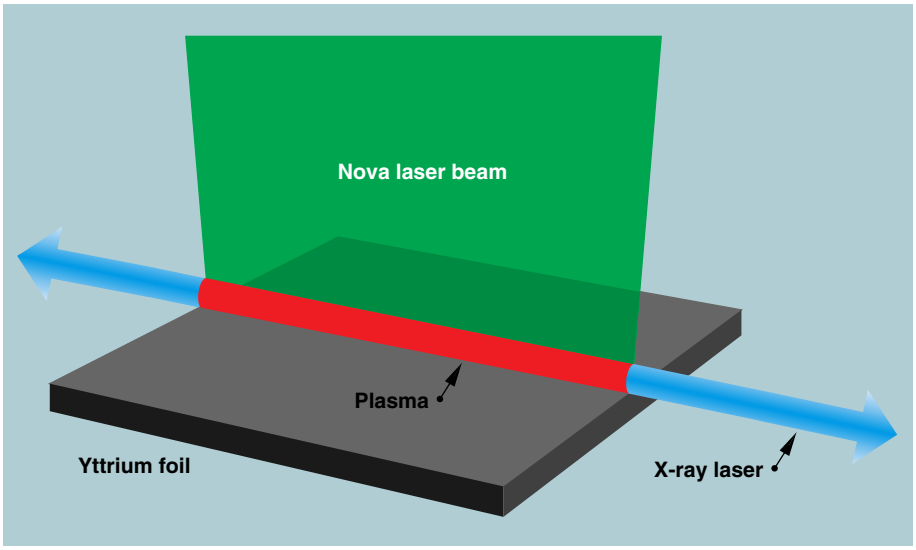


Figure 1. X rays are produced when a beam of high-intensity laser light from Nova bombards a plastic foil coated with a thin layer of yttrium. In our setup, the lasing medium we create is a very hot (approximately 10^7 K), uniform, and cylindrical plasma that is relatively long (3 cm) but only about 120 μm wide and 500 μm high. The lasing photons interact with enough other excited atoms only in the long direction (that is, along the 3-cm plasma line) to produce more photons, resulting in amplification. X-ray laser light emerges from both ends of this plasma line, but not in other directions.

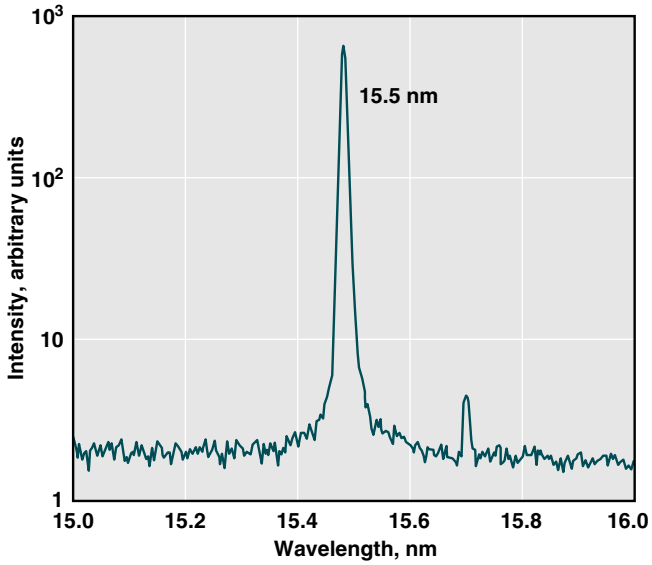


Figure 2. This curve shows that the output of our yttrium x-ray laser is dominated by a single line, or monochromatic spike, at a wavelength of 15.5 nm. Such monochromatic light from a neonlike yttrium laser makes it well suited for studies of laser-produced plasmas.

The name itself says a good deal about how the device functions. The atomic number of yttrium is 39, so it normally contains 39 protons and an equal number of electrons. In a neonlike yttrium laser, yttrium is stripped of 29 of its 39 electrons, leaving 10 electrons, like neon.

In our laser, the x rays are produced by using high-intensity optical laser light to irradiate a cold lasant material, as shown in Figure 1. Whereas the lasant material in various types of lasers can be a solid, liquid, or gas, the material we irradiate is either a 3-cm-long plastic foil coated with a thin layer of yttrium or a solid slab of yttrium. We irradiate the yttrium with one of the ten beams of the Nova laser. When the intense optical laser light interacts with the lasant material, a very hot (approximately 10^7 K) cylindrical plasma is produced. X-ray laser amplification takes place along this plasma column.

Notice in Figure 1 that the three-dimensional plasma we create is relatively long (3 cm) but not very wide (approximately 120 μm) or high (approximately 500 μm). It is only in the long direction—along the line of the plasma—that x-ray photons interact with enough other excited atoms to produce more photons, resulting in amplification. The result is that our x-ray laser emerges from both ends of the plasma line, but not in other directions. The x-ray laser is coherent because a stimulated photon is similar to (has the same phase as) the photon that stimulates it.

X-ray lasers have several features that make them ideal for studying dense plasmas. First, the short wavelength of such lasers provides decreased refraction and greater penetration, compared to other longer-wavelength optical probes. As shown in Figure 2, the operating wavelength of our neonlike yttrium laser is dominated by a single line, or monochromatic spike, at

15.5 nm. We have produced multilayer mirrors for use in our experiments that are highly reflective at this wavelength.

A second advantage has to do with brightness. In imaging systems, brightness is one of the most important factors, and yttrium x-ray lasers are unequaled in this regard.[2] The high brightness of x-ray lasers makes them particularly well suited for imaging bright sources, such a laser-produced plasmas.

A third advantage arises from the fact that our x-ray probe is, indeed, a laser. This means that we can exploit the coherence properties of the x-ray laser, in particular, as a density diagnostic.

A potential limitation of collisionally pumped x-ray laser systems has to do with their output pulse lengths. When the pulse is relatively long, a few hundred picoseconds, considerable motion can take place in the plasmas we want to investigate. Such motion can cause blurring in an image. We have been developing ways to generate the short pulses (with durations of less than 50 ps) needed for extending diagnostic techniques. Our recent work on decreasing the pulse duration is described toward the end of this article.

Direct Imaging of Plasmas

Two fundamental issues in high-resolution imaging are the wavelength of the probe and refraction in the medium being imaged. In general, shorter-wavelength probes allow us to see an object better, with ideal optical systems achieving resolutions comparable to the wavelength of the probe. At present with our imaging system, we are imaging structures as small as 1 μm, but we can do better in the future.

As shown in Figure 3, refraction is a change in the direction of light that occurs when light passes through a density gradient, that is, through material in which the index of refraction changes. Refraction can be a substantial problem in imaging because the amount of refraction, or bending of light, increases directly with the magnitude of the density gradient and the length along the gradient. Conversely, the amount of refraction decreases with increasing critical density, which is solely determined by the wavelength of the light. The rule to remember is that shorter-wavelength light generally penetrates much farther into a plasma and is less affected by gradients.

Currently, we are using the neonlike yttrium x-ray laser to image high-density, large plasmas of interest to the laser-fusion and astrophysics communities. In the past, probing high-density or large plasmas was difficult. With the yttrium laser, a broader range of electron densities and plasma lengths is accessible to us, as shown in Figure 4. By using short-wavelength (15.5-nm) light, we can reduce the adverse effects of refraction and probe plasma densities up to 10^{23} cm^{-3}. Beyond this density, imaging is limited primarily by absorption.

Figure 5 shows our setup for high-resolution imaging experiments. To use an x-ray laser fully as a plasma diagnostic, we must include optical elements, such as mirrors. Notice that the setup in Figure 5 uses a sequence of two multilayer mirrors. The x-ray beam is first collected with a spherical multilayer mirror that collimates the beam so that it does not converge or diverge appreciably. This collimated beam backlights the laser-produced plasma formed when a target, such as a foil, is irradiated by another optical laser beam from Nova (the second beam is shown at the top of Figure 5). An image of the plasma is focused by a second spherical multilayer mirror onto a charge-coupled device (CCD) detector that has high sensitivity to x rays and high dynamic range.

One potentially serious problem in our type of imaging system is that multilayer mirrors can be damaged by

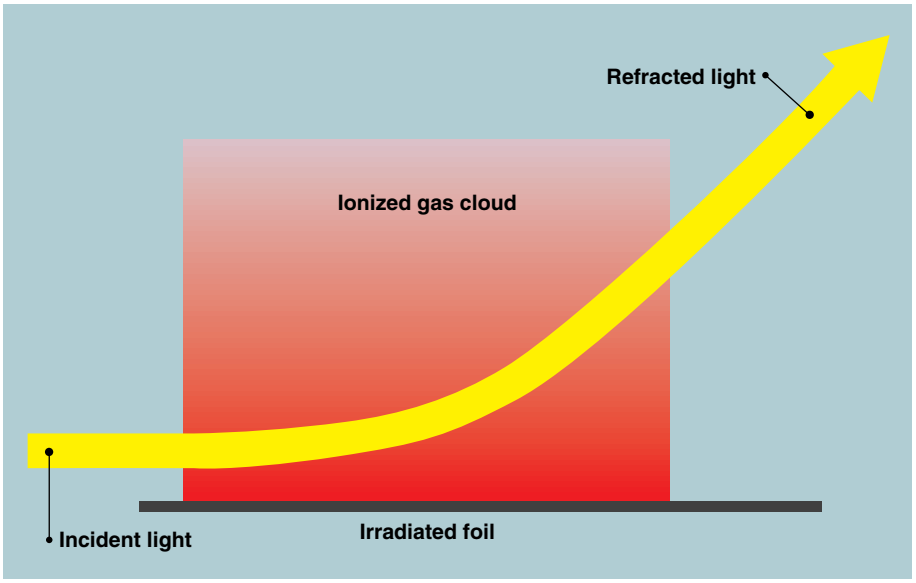


Figure 3. When light passes through material in which the index of refraction changes, the light changes direction. As shown here, the amount of refraction, or bending of light, increases directly with the magnitude of the density gradient and the length along the gradient. In our work, the density gradient is a "cloud" of highly ionized gas, that is, a plasma produced when we irradiate a target. In general, shorter-wavelength light penetrates much farther into such a plasma and is less refracted by gradients.

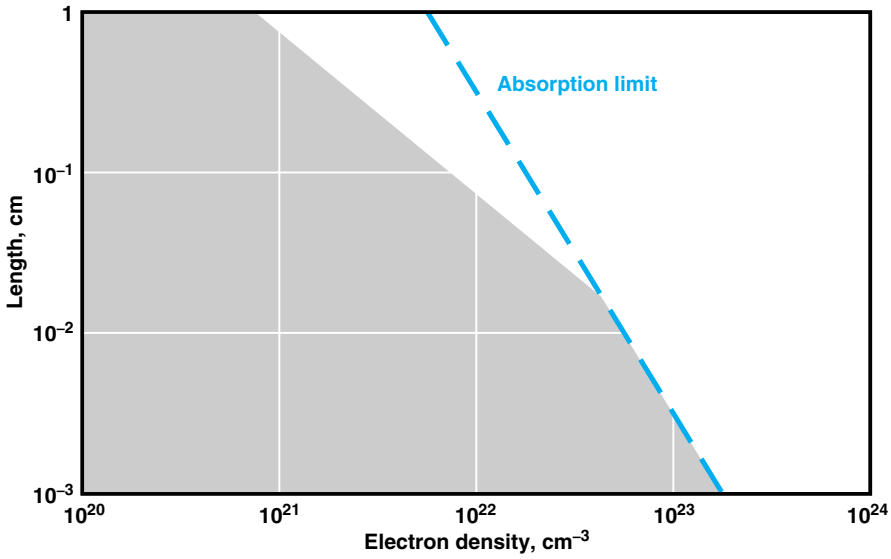


Figure 4. The shaded area shows the broad range of electron densities and plasma lengths that are accessible to us by using the yttrium x-ray laser. With its short-wavelength (15.5-nm) light, we can probe plasma densities up to 10^{23} cm^{-3}. Beyond this density, imaging is primarily limited by absorption. (At lower densities, the number of fringe shifts that can be resolved via interferometric techniques becomes the constraint.)

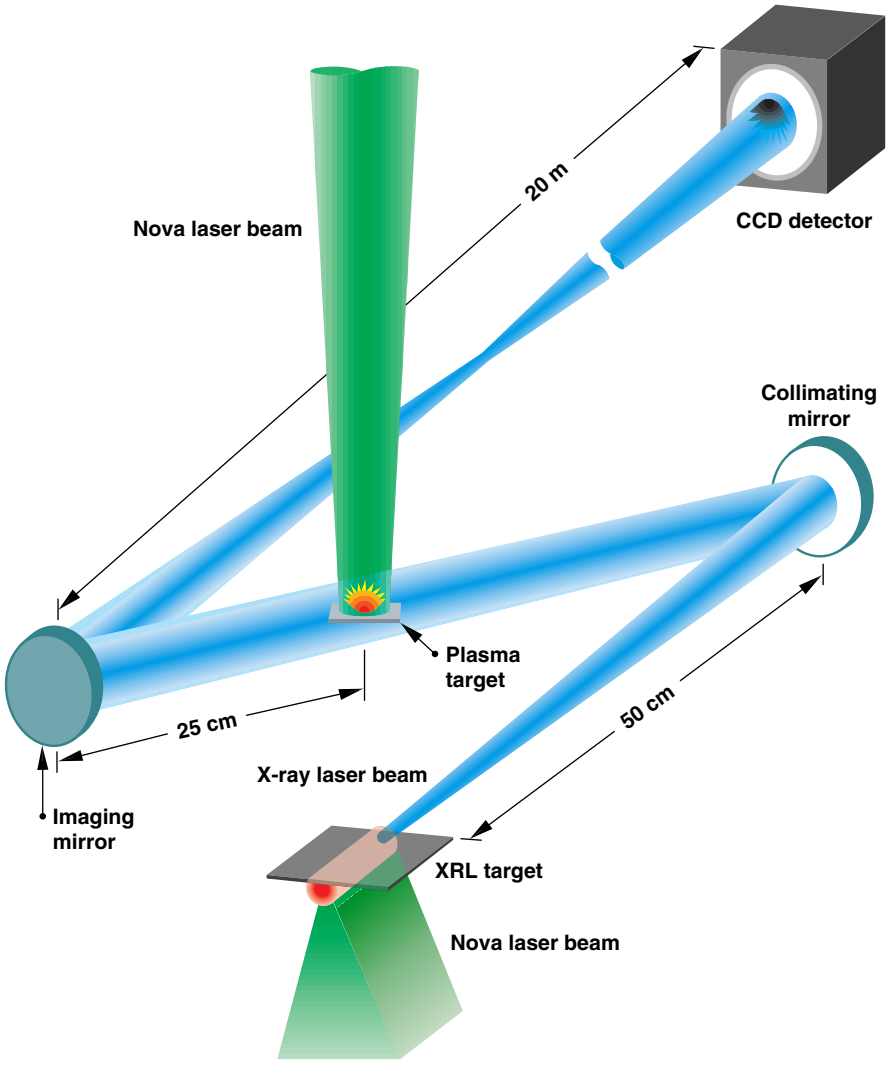


Figure 5. Experimental setup for directly imaging plasma. We use two beams of Nova, one to create the x-ray laser and another to produce a plasma. The yttrium x-ray laser beam (formed at the bottom) backlights the target. This beam is first collected and collimated by the multilayer mirror on the right. As the sample target is irradiated by another beam of the Nova laser (center), the backlit plasma image is formed by a second multilayer mirror (left) and is focused onto the backside of a highly sensitive charge-coupled device (CCD) detector (top right).

side-scattered laser light, especially when distances are short (less than 25 cm from mirror to plasma) and the laser light is intense. We have solved the problem by locating highly reflective mirrors 50 cm away from the plasma and by using only a small part of each mirror, shielding the remainder of the mirror. Multilayer mirrors are essentially crystals with layer spacings that are matched to the wavelengths being diagnosed. Our multilayer mirrors consist of 15 layer pairs of molybdenum and silicon, and they have a measured reflectivity at 15.5 nm of about 60% at normal incidence. High reflectivity is essential because the mirrors must be efficient in a complex optical system.

At our highest magnification (30×) the spatial resolution of our imaging system is better than 1 μm. The resolution is limited by the CCD detector and by spherical aberrations caused by the mirrors.

Figure 6 shows an image of a 10-μm-thick polyethylene (CH) foil overcoated with 3 μm of aluminum and irradiated with a 1-ns pulse of intense green light (10^{14} W/cm^2) from the Nova laser. The foil was illuminated on the polyethylene side, where the CH serves as an ablator, similar to the function of a fusion capsule. We backlit this foil with a 150-ps pulse from the yttrium x-ray laser. Figure 6 is what we call a side-on image of the foil and plasma where the top of the picture corresponds with the foil's exploding rear surface. In this view, the Nova laser pulse comes from the bottom of the picture, and the x-ray pulse comes from behind the plane of the object to serve as a backlighter.

This image of an "accelerated" foil shows density perturbations on the foil's rear surface. At first, we hypothesized that the fine 5- to 6-μm structures visible in the side-on image might be small plasma filaments, which are sometimes seen in other kinds of experiments. Our imaging system, with its approximately 1-μm spatial resolution (along the x axis in Figure 6) was clearly able to resolve the structures, but an important question remained: exactly what would account for such perturbations? Repeated shots gave similar results. It seemed possible that the structure could arise from nonuniformities of the target mass or from techniques used to smooth the Nova laser beam.

More recently, we have concluded that the foil itself is breaking up as a result of the Nova beam imprinting its near-field beam intensity pattern on the foil. This finding could have important implications for inertial fusion target development for direct-drive experiments. Shots performed with smoother Nova beams show reduced filamentation. We will soon begin to take face-on images of exploding foils (where the foil's front surface is essentially driven toward the detector) to get another perspective on what is happening.

Notice that in Figure 6, the spatial resolution along the flight path of the foil (that is, along the vertical axis) is limited by the duration of the x-ray laser pulse. For a pulse about 200 ps in duration,

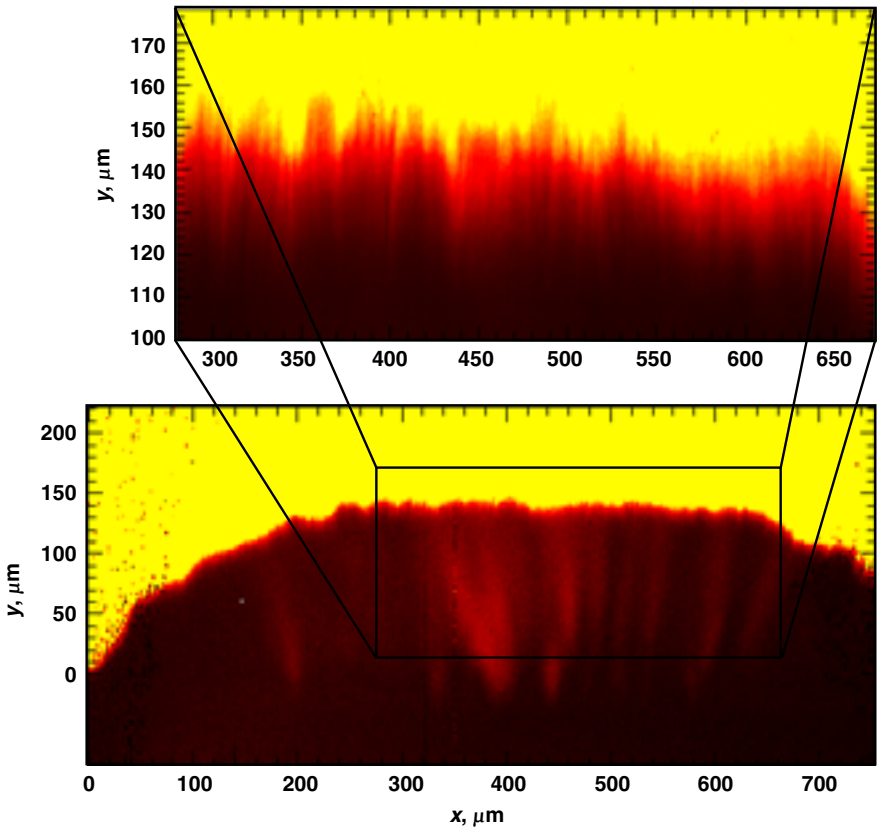


Figure 6. X-ray laser image of an exploding 10-μm foil overcoated with 3 μm of aluminum and irradiated with a 10^{14}-W/cm^2 beam of the Nova laser. The picture is a side-on view of the central region of the foil plasma, which is being driven upward. The foil was originally located at zero on the vertical scale. The resolution of the image is about 1 μm along the x axis. The plasma structure shows both large- and small-scale electron density perturbations, which may arise from breakup of the foil.

which is typical in our work, we obtain a longitudinal resolution ranging from a few to 20 μm. Obviously, it would be desirable to improve the resolution along the flight path. This desire is just one of the reasons why developing a shorter-pulse x-ray laser is important.

We have also used our imaging system to study x-ray-heated foils. In this work, we use one Nova beam to illuminate a thin gold foil from which high-energy x rays heat an aluminum target foil placed 1 mm away. The smooth expansion of the aluminum we have observed agrees well with earlier computer simulations.

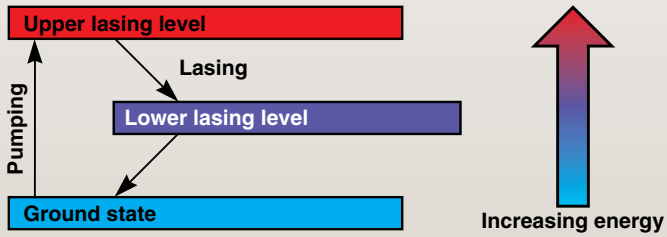
One drawback of direct plasma imaging is that we need an accurate estimate of opacity to determine the electron densities of plasmas. At the wavelengths of soft-x-ray lasers and with the metal targets we are using, such estimates can be difficult to make. Thus, we have developed two alternative techniques. Moiré deflectometry allows us to measure electron density gradients, and interferometry allows us to measure electron density itself directly.

Moiré Deflectometry

Moiré deflectometry is a relatively recent technique that has been widely used to measure many different physical phenomena. Deflectometry can be applied to characterize optical components, to study the dynamics of fluid flow, and to measure variations in plasma density.

What We Mean by a Collisionally Pumped X-Ray Laser

To produce a laser, the lasing material (lasant) must be put in the proper state; then the individual atoms (or ions) of the lasant must be properly prepared and then stimulated into emitting a photon at the laser wavelength. In each lasing atom, preparation is accomplished by adding energy to the atom so that an electron (usually the outermost electron in the atom) is excited to the upper lasing level, which is generally a metastable, or relatively long-lived, state. This is called pumping.



The excited atom can be induced to make a transition to the lower lasing level if the atom interacts with a photon possessing an energy equal to the energy difference between the two lasing levels. In the process of making the transition, the de-exciting atom emits a photon with this same energy. The emitted photons end up being in phase with each other; i.e., they are coherent. The emitted photon can induce the emission of additional photons (of energy and phase) in other already-pumped atoms. Additionally, each can be pumped again if the atom can be returned to its initial state, so the lower lasing level is usually very short-lived. This exponential increase in the number of photons in a given direction (called gain) gives rise to a large amount of coherent directed energy; this is a laser. In general, the more lasant atoms and the longer the laser, the brighter the resulting laser beam.

Most commercially available lasers use gases or lasing atoms suspended in a solid (such as glass) or a liquid. The pumping mechanism for these lasers is a bright light source (such as a flashlamp) that emits photons of the right wavelength to excite the lasing atoms to the upper lasing level. This is called photopumping. It is not a viable method of making an x-ray laser, however, because a very bright (and unavailable) source of x rays would be required to pump the atoms. Moreover, excitation produced in neutral atoms by x rays involve inner shell electrons (electrons interior of the outermost electron). In this situation, it is difficult to find a state to serve as an upper lasing level because the atom is very unstable.

The trick is to ionize the atoms first, removing many of the outer electrons so that excitation of the ions occurs in the remaining outer shell. These transitions can be at x-ray wavelengths. In our collisionally pumped x-ray laser, the ionization is accomplished by heating the lasant very quickly to high temperatures using one beam of the Nova laser focused to form a line, creating a long (a few centimeters), thin (a hundredth of a centimeter) plasma. This heating puts the lasant in the proper state to be pumped (for yttrium, 29 of the 39 electrons are removed). Pumping the ions is not performed by an outside x-ray source; it is done by the unbound electrons. The energetic electrons collide with the ions, thus creating a collisionally pumped x-ray laser. Lasing can then occur along the line of plasma. Finding the combination of material, ionization state, temperature, electron density, and lasing levels that will produce an x-ray is challenging.

Deflectometry measures the refraction of a collimated beam of light passing through a medium or subject of interest. In our case, the collimated probe beam is a set of intense x rays that are nearly parallel. As in our direct-imaging work, we use the yttrium x-ray laser beam to probe millimeter-scale, laser-produced plasmas.[3] Previous work using visible and ultraviolet probe beams has been limited by excessive refraction. Our soft-x-ray laser provides the desired short-wavelength probe beam to avoid the problem.

When a probe beam passes through a pair of evenly spaced stripes (gratings) that are offset and rotated slightly with respect to one another, a moiré pattern is created. The moiré pattern, as shown in Figure 7, is a set of dark regions, or fringes, corresponding to the stripe intersections and lighter regions that are the open areas in between the stripes. In everyday experience, we see moiré patterns if we look through a double-screen door or window. Normally, we don't see all the details of such patterns; instead, we observe a smooth set of fringes or lines. Such is the case in our work.

If we look through a pair of gratings at an angle, the fringes are shifted from the original position they had in a perpendicular view. In moiré deflectometry, we can exploit the fringe shifts, and the connection between the angle of refraction and electron density, to obtain a measure of the electron density gradient along a plasma. To do so, we simply placed a pair of offset gratings just before the CCD detector in the experimental setup (Figure 5). We also added a combination of flat mirrors and a filter to the setup so that the detector would see a narrow range of radiation centered at 15.5 nm. We control the sensitivity of the deflectometer by varying the distance separating the gratings.

First, we created a deflectogram by using the x-ray beam, a CH target, and a pair of gratings without any plasma present. In this control experiment, the second beam of Nova was not used, so no target plasma was created to deflect the fringes. Figure 8a shows the control image, which consists of a uniform moiré pattern except where the beam was blocked by the side of the CH target.

Next, we obtained a deflectogram of a CH plasma. As in the control experiment, we used a 5-mm-square, 50-μm-thick CH foil, but this time, we irradiated the foil with the Nova laser. The pulse duration of the x-ray laser was about 200 ps, which is short enough to avoid significant blurring. In this experiment, the x-ray beam passed through the plasma about 1 ns after the start of irradiation. To maximize fringe shifts and demonstrate our ability to probe relatively large plasmas, we used a large, 3-mm-diameter Nova laser spot on the CH target.

Figure 8b is a deflectogram of a CH plasma. In areas that are far from the surface of the foil, which is once again viewed from the side, this image shows the expected unperturbed moiré pattern. Closer to the surface, fringe shifts (or displacements) by as much as about four fringe spacings are visible. Immediately adjacent to the surface, the fringes disappear because contrast is lost to very strong density gradients. (We can reduce this limitation by increasing the magnification and reducing the separation between rulings.) Subsequent analysis of the deflectogram—which assumes we know the boundary density far from the target surface—allows us to infer a density of slightly greater that 4×10^{21} cm^{-3}near the foil surface.

It is noteworthy that this type of deflectometry can be done with probes that are much weaker than our intense yttrium x-ray laser. In fact, the intensity

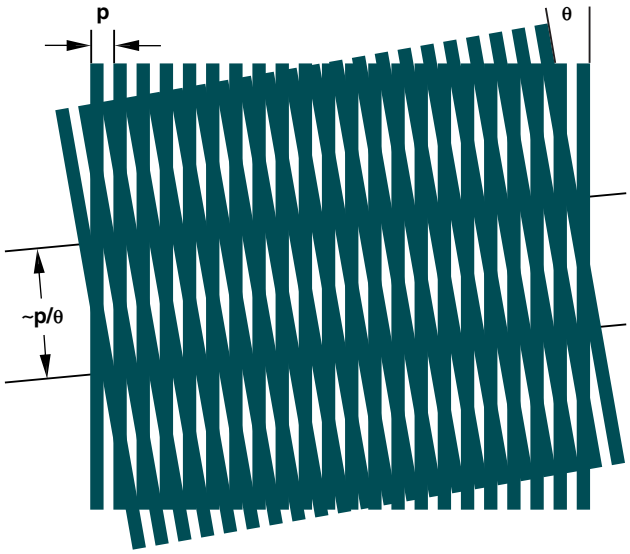


Figure 7. A moiré pattern, consisting of a set of dark bands or fringes, is produced when two one-dimensional gratings are overlaid and rotated slightly with respect to one another. By locating a pair of offset gratings like these just before the CCD detector in our experimental setup, we can measure the deflection of the fringes to obtain an electron density gradient along a

could be reduced by a factor of 25, and the image quality would still be acceptable. By making other modifications, such as reducing the thickness of filters used in our setup, we could optimize the system even further. This ability means that it should be possible to produce a deflectogram with low-energy x-ray laser systems, such as those that use selenium or germanium.

The primary disadvantage of deflectometry is that it gives us a measurement of the plasma density gradient, not the plasma density. The desired density measurement can be made by interferometry.

Interferometry

Our most recent technique is, in some respects, also our most useful tool in terms of its potential applications. Because an observed fringe shift is directly proportional to the electron density in a plasma being probed by interferometry, this tool can provide a direct measurement of density in two dimensions.

The technique of interferometry adds a reference beam to the system. The interference of the reference beam and the probe beam supplies information directly on the index of refraction of the target. Such an approach requires the use of beam splitters that are effective at x-ray laser wavelengths. Recently, LLNL researchers have developed and fabricated such beam splitters with reflectivity in the range of about 25% and transmission of about 20%. The beam splitters are similar to our multilayer mirrors and consist of eight layer pairs of molybdenum and silicon on a 100-nm-thick silicon nitride support. Our current beam splitters have a 1-cm-square aperture, and we are working on 2-cm-square apertures.

Figure 9 shows the experimental setup for soft-x-ray interferometry. In the terminology of optics, the arrangement includes a Mach-Zehnder interferometer. In essence, we add four multilayer mirrors to the setup we used for direct plasma imaging. Two of the mirrors are semitransparent (the beam splitters) and two are completely reflecting. Whereas the probe beam passes through the plasma, the reference beam does not. When the two beams recombine after the probe passes through the plasma, they interfere. The interference shows up as fringes on the detector. By measuring the number of fringe shifts and using the known values of the x-ray wavelength and the plasma path length, we can calculate the electron density from a simple equation.

In a control experiment, we obtained an interferogram without using the second beam of Nova to produce a target plasma. The results showed excellent fringe contrast and proved the viability of the technique.

Figure 10 is an interferogram we obtained after irradiating a 10-mm-thick coating of CH on a polished silicon substrate. The CH coating, viewed from the side in this image, was irradiated from the top of the picture with the Nova laser. For this experiment, the laser spot size was about 700 μm in diameter, and the intensity of the beam was 2.7×10^{13} W/cm^2. By counting the fringe shifts that are clearly visible above the CH surface in the center of the spot, we find that the maximum electron density is 3×10^{21} cm^{-3}. This value and the overall density profile of the plasma are in good agreement with computer simulations.

Current Work and Future Applications

Ultimately, the spatial resolution of a plasma image in two dimensions is

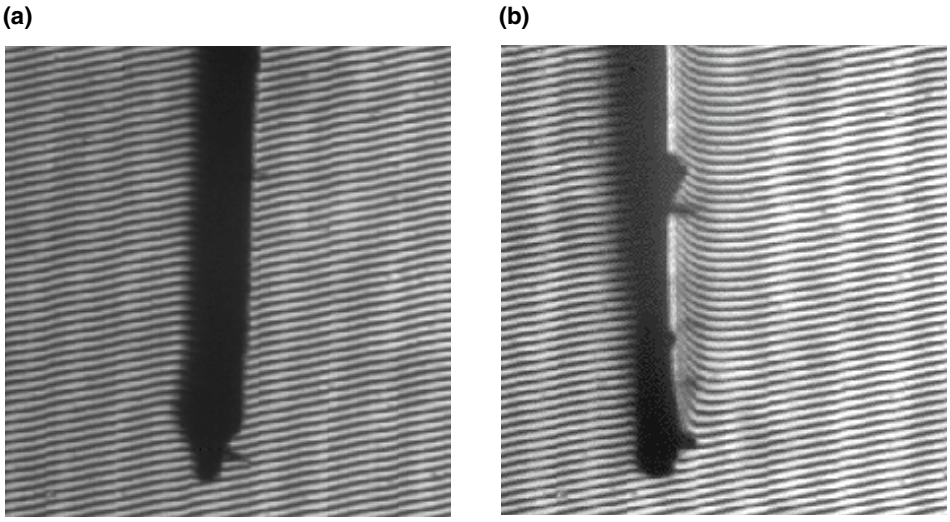


Figure 8. Two deflectograms of a polyethylene (CH) target viewed from the side. (a) A control image with no plasma present shows the expected unperturbed moiré pattern. (b) A deflectogram of a laser-irradiated CH foil target illuminated from the right side. This image shows distinct fringe shifts close to the target surface. We can use the deflections to infer the electron density gradient near the surface. The dark features associated with the target surface are probably caused by ripples in the CH material.

limited by the duration of the x-ray laser pulse. Therefore, to obtain better images and improved measurements of plasma density, we need to improve the x-ray laser itself.

In work that is in progress to reduce the pulse duration, we have begun to irradiate thin yttrium foils with multiple optical laser pulses. The first Nova pulse, which has less energy than those that follow, heats the thin foil target to produce a plasma. The subsequent pulses ionize the preformed plasma to produce conditions suitable for generating shorter-duration x-ray pulses.

When using multiple pulses in this way, we need to overcome the anticipated problem of limited gain (or brightness). One way to shorten the x-ray laser pulse and to maintain brightness at the same time is to use a so-called traveling wave. In this approach, the incident Nova wave front is tilted by inserting a grating so that the pulse, in effect, is swept along the 3-cm foil target. The technique matches the optical pump (the Nova pulse) to the propagation of the x-ray pulse along the plasma. Our early efforts have yielded an x-ray laser pulse duration of 45 ps.[4] To our knowledge, this is the shortest collisionally pumped x-ray laser to date. In the future, we expect to achieve pulse durations of less than 20 ps.

In the future, our x-ray laser can be applied as a probe to study the very dense plasmas that will be created at the proposed National Ignition Facility (NIF). The NIF would allow us to

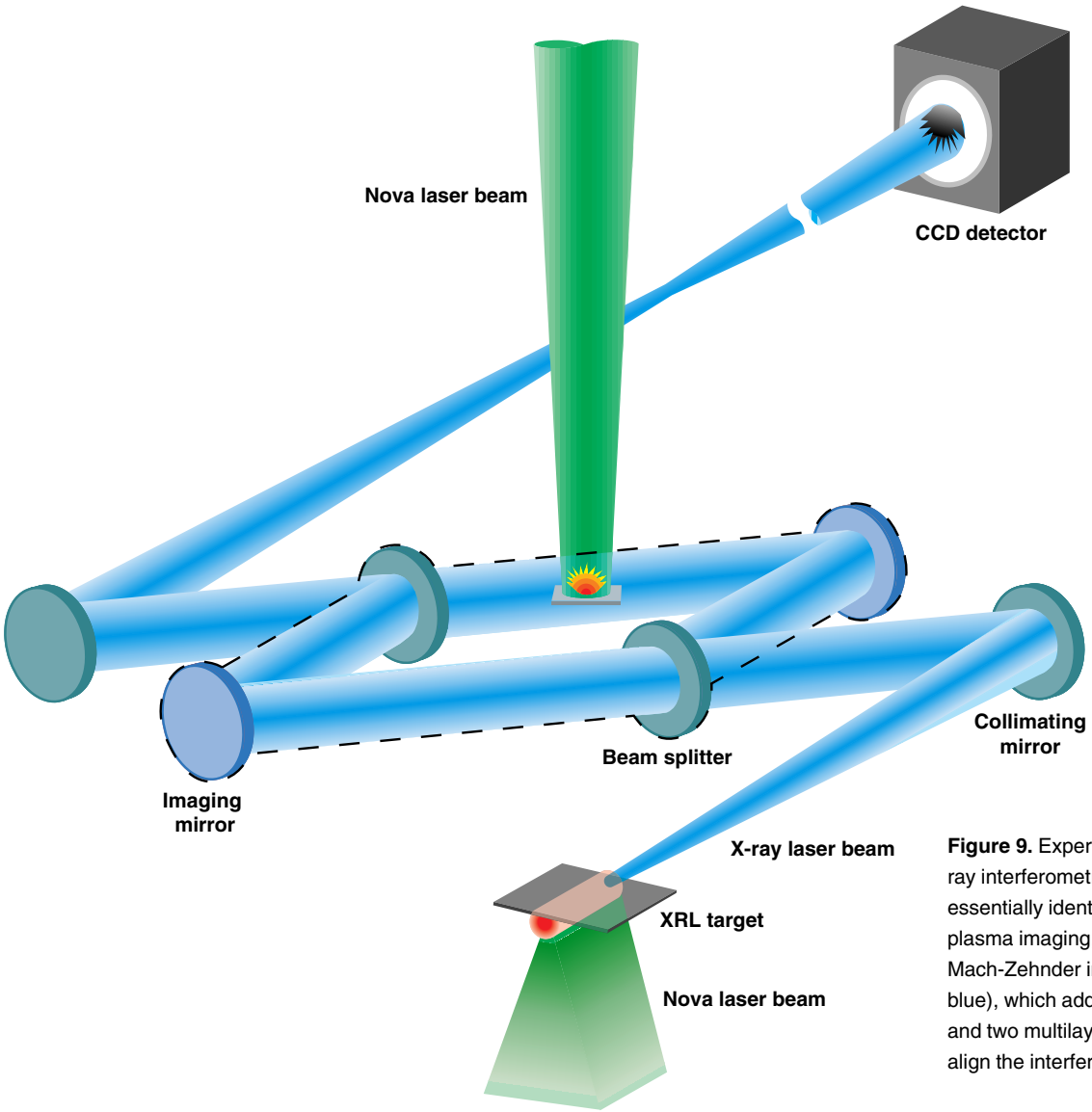


Figure 9. Experimental setup for soft-x-ray interferometry. This arrangement is essentially identical to that used for plasma imaging, but it also includes a Mach-Zehnder interferometer (shown in blue), which adds two multilayer mirrors and two multilayer beam splitters. We align the interferometer using white light.

extend collisionally pumped neonlike and nickel-like x-ray laser systems to shorter wavelengths and high output energies, which would make the x-ray laser an even more important diagnostic tool. For example, we estimate that we will be able to achieve wavelengths of about 2 nm and peak intensities of 1×10^{17} W/cm^2.

The short-pulse capabilities of NIF will also allow us to investigate a variety of new x-ray laser schemes, including recombination x-ray lasers. In recombination lasers, an atom is first stripped of several electrons, and then some of those electrons recombine with the ion into the upper lasing level. Recombination systems have long been viewed as an alternative to collisionally pumped systems, offering the potential for higher conversion efficiencies. To date, however, such systems have proven inefficient, in part because it is difficult to produce long, uniform plasmas suitable for x-ray propagation. A facility the size of NIF would allow recombination x-ray systems to be tested adequately.

Finally, x-ray lasers are well suited for a variety of other applications ranging from biological imaging to nonlinear optics. In the area of biological imaging, for example, x-ray microscopy offers a way to study wet, thick specimens with a demonstrated resolution that is about five times better than that of conventional optical microscopes. Electron microscopes are limited to thin samples (the limit is about 0.4 μm in thickness), and they cause radiation damage to and decomposition of the specimens being studied. In contrast, x-ray lasers have the potential to produce high-contrast, high-resolution images of whole cells or other structures that are 2 to 10 μm thick before significant damage occurs to the specimen.

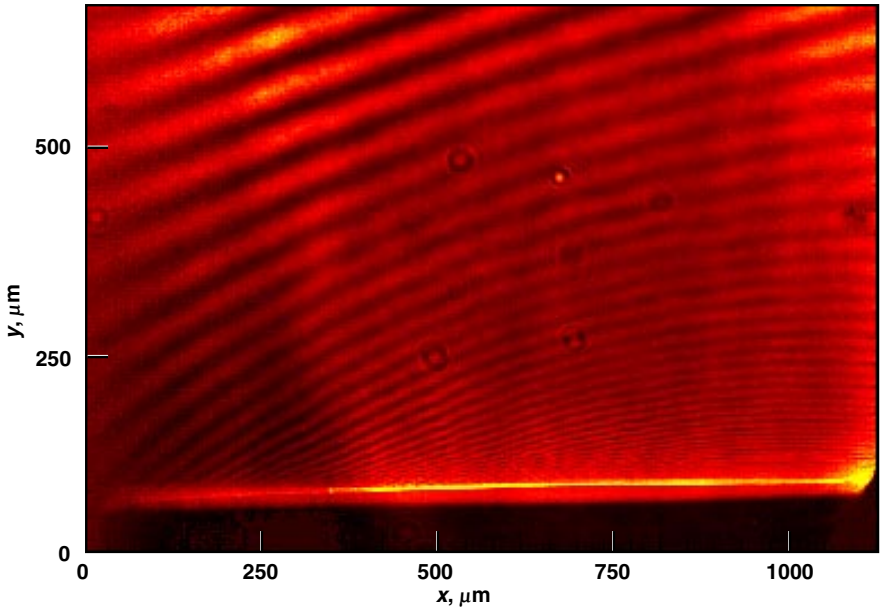


Figure 10. Interferogram of a laser-heated CH foil shown in a horizontal orientation and viewed from the side. The Nova drive laser, which produced the target plasma, is incident from the top of the picture. The fringe shifts are clearly visible just above the foil surface. One fringe shift corresponds to an electron density of 2×10^{20} cm^{-3}. By counting the shifts, we have determined that the maximum electron density near the foil surface is 3×10^{21} cm^{-3}.

Key Words: interferometry; moiré deflectometry; National Ignition Facility (NIF); plasma imaging; x-ray laser—plasma diagnostics.

Notes and References

1. For further reading on the proposed National Ignition Facility, see the December 1994 issue of *Energy and Technology Review*, UCRL-52000-94-12.
2. L. B. Da Silva, B. J. MacGowan, S. Mrowka, J. A. Koch, R. A. London, D. L. Matthews, and J. H. Underwood, "Power Measurements of a Saturated Yttrium X-Ray Laser," *Optics Letters* **18**, 1174 (1993).
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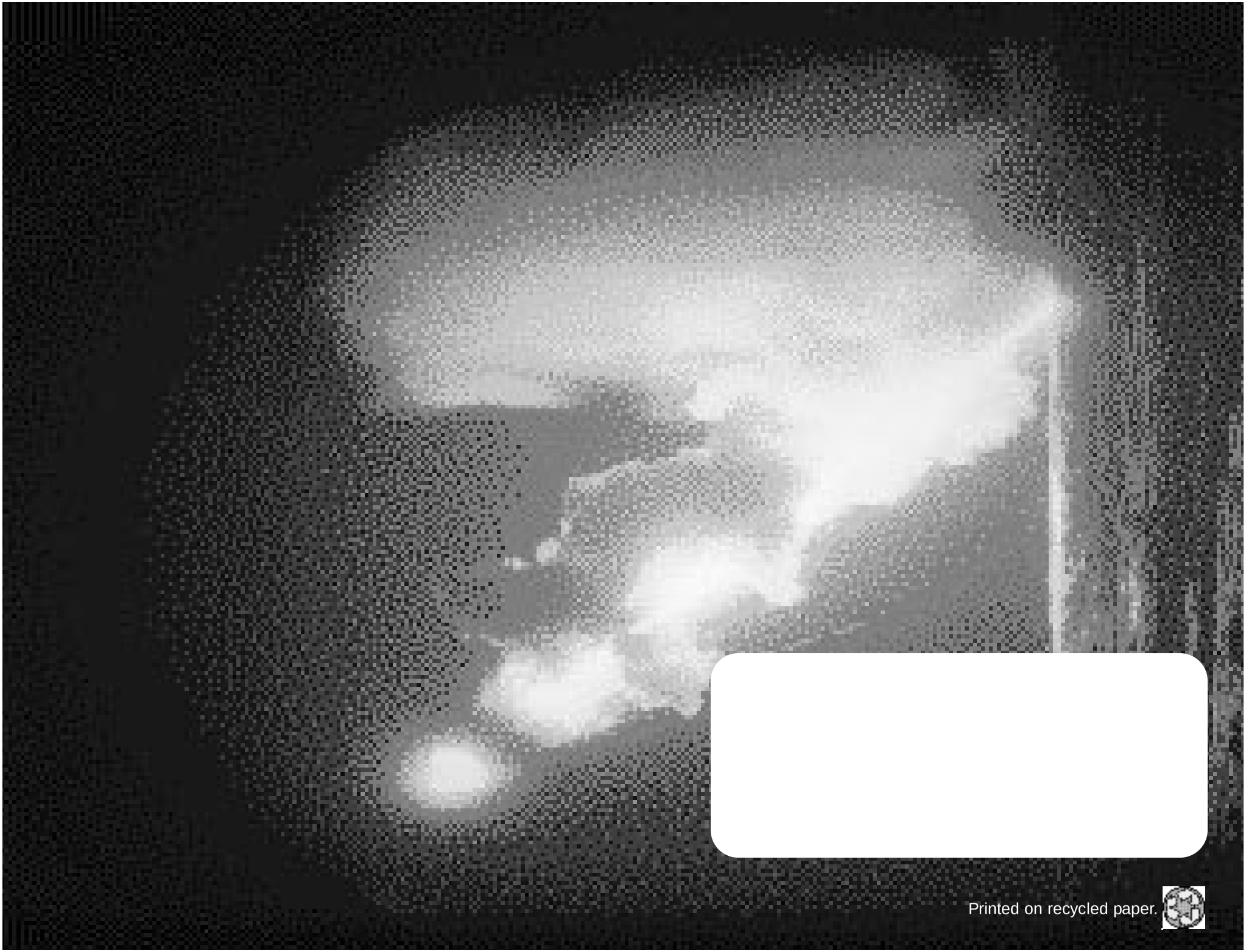

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