Also in this issue:
- Tools to Fight Strokes
- Better Measurements of Sediment
- The Next Generation of Laser Targets

The New Science of High Explosives
The researchers announced their findings at the Seismological Society of America annual meeting, held in April in Honolulu. Their simulation for a sophisticated computer code developed at Livermore and a seismic velocity model developed at Berkeley.

Defence research yields commercial benefits

Defense research at Lawrence Livermore may help U.S. companies get a head start in the fiercely competitive international computer chip market, according to Dan Belzer, author of a new study about the Laboratory’s effect on the economy.

Belzer, a principal consultant with Bay Area Economics in Berkeley, quoted industry giants Intel Corp. and Microsoft as saying that breakthroughs at Lawrence Livermore have been critical to putting more information onto tiny microchips. The companies said the Lab’s cutting-edge research tools and wide pool of scientists from diverse disciplines enabled micropitch breakthroughs such as EUL lithography, a technique for putting information on chips more precisely with strokes that are about a thousandth of the width of a human hair.

Belzer’s report said that the planned National Ignition Facility laser could push the state of the art in several technology areas over the next 10 to 15 years but cautioned that “economic benefits can only be realized if the national labs continue to have strong interactive relationships with private industry.”

Lawrence Livermore’s high profile in arms control

In an address to Lawrence Livermore employees in April, Ambassador Thomas Graham, Jr., U.S. negotiator and special representative of the President at the U.S. Arms Control and Disarmament Agency, applauded the Laboratory’s contributions and its high-profile role in achieving a global treaty to end nuclear testing.

According to Graham, Lawrence Livermore was the only one of the nation’s three nuclear weapons laboratories represented directly on the U.S. negotiating team for the test ban.

The Laboratory’s representative, physicist William Dunlop, said that the Laboratory’s role in arms control is critical to our commitment to understanding the aging of high explosives in the stockpile and predicting their useful lifetime.

Current energetic materials research and development in support of stockpile stewardship focuses on several areas. In the important area of enhanced surveillance, we are developing new, minimally invasive methods of detecting the products of high explosives decomposition as well as pursuing theoretical and experimental work to predict and characterize potential decomposition pathways.

Our continuing emphasis on safety, performance, and reliability drives an intense effort to improve our ability to model the behavior of energetic materials under both normal and abnormal conditions. This research necessitates the acquisition of additional equation-of-state data and better modeling of the very complex coupling of thermodynamic, chemical-kinetic, and hydrodynamic behavior in a burning high explosive.

We also have a continuing responsibility to assist DOE’s Pantex Plant in meeting the needs of the stockpile; we must also meet the requirements of our own hydrotesting programs. For example, we are currently doing research focused on improving the chemical synthesis processes for high explosives (e.g., a new route to the synthesis of the insensitive high explosive TATB), and we maintain a viable synthesis, processing, and assembly area at Site 300.

Department of Defense and Other Activities

Livermore’s role in energetic materials has broadened beyond its primary nuclear weapon-related mission. Today, there are extensive activities in advanced conventional weapons, rocket and gun propellants, antiterrorist work, demilitarization, and industrial applications of energetic materials. We are actively assisting the Department of Defense in a wide range of activities in this area, particularly those focused on insensitive high explosives, environmentally sound demilitarization of surplus high explosives and propellants, and modeling the performance and safety of high explosives and propellants.

Two current examples of Department of Defense projects are the development of molten salt as an environmentally benign means of destroying energetic materials and the exploration of new synthesis routes to reduce the cost of high explosives.

In support of Livermore’s nonproliferation program, we are developing the means to reliably detect and identify high-explosive compounds and formulations, with the added interest of potentially determining their origin.

Providing the Scientific Foundation

The excellent science carried out at Livermore enables the outstanding advances in energetic materials research and development described above and in the following article. This work ranges from understanding detonation science at the molecular level to predicting structures for exciting new high explosives. This continuing excellence in the science and technology of energetic materials has made possible the wide range of Livermore contributions since its inception and promises significant breakthroughs in the years ahead.

Hal Graboske is Associate Director of Chemistry and Materials 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.

EW 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.

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/DDO “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 leading 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.
Energetic Materials

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 (triaminotriazine, 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, sensitivity to mechanical insult, 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 synthetic chemists. Theoretical chemists tend to suggest more “flammable” 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 luckes 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

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

Table 1. Codes used in developing energetic materials.

<table>
<thead>
<tr>
<th>Code</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALEID</td>
<td>Hydrodynamic code used in safety analyses such as “cookoff” simulations spanning a remarkably wide time span. (Developed at LLNL.)</td>
</tr>
<tr>
<td>CHEETAH</td>
<td>Transforms predicted formation energy and density of molecules into performance measures such as detonation velocity, pressure, energy, impulse, and impetus. (Developed at LLNL.)</td>
</tr>
<tr>
<td>GAUSSIAN</td>
<td>Determines the three-dimensional shape of the molecule and the energy binding its atoms.</td>
</tr>
<tr>
<td>HOLPAK</td>
<td>Packs molecules together into a low-energy configuration.</td>
</tr>
<tr>
<td>TOPACHEM, PALM</td>
<td>Predict changes in thermal and chemical properties caused by different accident, battlefield, and aging scenarios. (Developed at LLNL.)</td>
</tr>
</tbody>
</table>

Table 2. Molecular structure of important energetic materials.

<table>
<thead>
<tr>
<th>Material</th>
<th>Molecular Structures</th>
</tr>
</thead>
<tbody>
<tr>
<td>TNT (trinitrotoluene)</td>
<td><img src="structure_of_tnt.png" alt="Structure of TNT" /></td>
</tr>
<tr>
<td>HMX (cyclo-tetramethylene-tetranitramine)</td>
<td><img src="structure_of_hmx.png" alt="Structure of HMX" /></td>
</tr>
<tr>
<td>TATB (triamino-trinitrobenzene)</td>
<td><img src="structure_of_tatb.png" alt="Structure of TATB" /></td>
</tr>
<tr>
<td>LX-19</td>
<td><img src="structure_of_lx19.png" alt="Structure of LX-19" /></td>
</tr>
<tr>
<td>CL-20 in LX-19</td>
<td><img src="structure_of_cl20_in_lx19.png" alt="Structure of CL-20 in LX-19" /></td>
</tr>
<tr>
<td>TATB</td>
<td><img src="structure_of_tatb.png" alt="Structure of TATB" /></td>
</tr>
<tr>
<td>TNT</td>
<td><img src="structure_of_tnt.png" alt="Structure of TNT" /></td>
</tr>
</tbody>
</table>

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 synthetic chemists. Theoretical chemists tend to suggest more “flammable” 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 luckes 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
Energetic Materials

Energetic Materials

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 procedure that 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

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

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 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 procedure that 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

* Experimental molecules are designated by an LLM number for Lawrence Livermore molecules. Experimental formulations are designated by an RX number for research explosives. Once the material is in production, it acquires an LX designation for Livermore explosive. DoD experimental munitions receive an XM number.
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 a computational model that could eliminate inherently unstable molecules from consideration before they are synthesized. Fellow theoretical chemist Al Nichols has been working 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 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.

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 does not feel that Livermore has 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 to 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. Tests of performance, thermal 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.

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, 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.

The ALE3D computer code is capable of simulating a “test-bed” safety test by modeling the rate of deformations in a slowly heated high explosive over a wide time span. (c) A model of the test 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-diameter device at the rate of 3.3°C per hour. (b), (c), and (d) are snapshots of the simulation of the material’s deformations 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.

The ALE3D computer code is capable of simulating a “test-bed” 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 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-diameter device at the rate of 3.3°C per hour. (b), (c), and (d) are snapshots of the simulation of the material’s deformations 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 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 (510) 423-0379 (simpson5@llnl.gov).

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.

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 MAIENSCHIEB, 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.
Recognizing that Lawrence Livermore has capabilities in microfabrication and other technologies that could be used to reduce the size of medical devices, the Center for Healthcare Technologies established a program to create a new standard of stroke care.

Critical to defining this standard was the “Workshop on New Technology for the Treatment of Stroke,” which the Center sponsored in March 1995. The workshop was attended by internationally recognized stroke clinicians and researchers, cardiologists with experience in medical devices used to treat heart attack, and scientists and engineers from Lawrence Livermore and Los Alamos National Laboratories. Instead of the typical conference agenda of success stories, clinicians described significant areas of unmet need for diagnosing and treating stroke victims, particularly the want of medical devices that might satisfy those needs.

Out of the workshop grew a vision of the future of stroke care and a framework for the priorities of a multidisciplinary team of Laboratory researchers who, with the help of Laboratory Directed Research and Development funding, are developing much-needed tools to diagnose and treat stroke. The Lawrence Livermore stroke initiative team’s vision of the future of stroke care is summarized in Figure 1. It focuses on the greatest unmet clinical needs—restoring blood flow, preventing hemorrhage, improving treatment decisions with sensors, and identifying the at-risk population with new screening technologies. (For a primer on the kinds, causes, and treatment of stroke, see the box on p. 19.)

The Livermore team consists of specialists in biomedical engineering, biology and bioscience, laser medicine and surgery, micro-engineering, microsensors, and computer simulation. It also has key collaborators from academic medical centers and private companies. These partnerships are the basis for rapidly moving the medical device concepts from the research laboratory through development, clinical trials, regulatory approval, and manufacture so that the resulting new tools can have a timely impact on the lives of the thousands of people who have strokes each year.

Since the workshop, the stroke initiative team’s research has developed several proof-of-principle prototypes. The work falls into four categories: microsensors for brain and clot characterization, optical therapies for breaking up clots in the blood vessels of the brain, laser–tissue interaction modeling, and microtools for treating aneurysms (a leading cause of hemorrhagic stroke).

Sensors to Diagnose Clots

The Laboratory’s stroke initiative has made substantial progress in developing microsensors that improve understanding of the biochemistry of stroke as well as offer the potential to identify the types of clots that cause stroke, to monitor patients during therapies that dissolve clots or protect brain cells with drugs, and to determine the health of brain or blood vessel tissue at a stroke site prior to treatment.

Development and use of these sensors, like much of the team’s work, are predicated on the availability of microcatheters. These tiny, hollow tubes, which are available from a number of manufacturers, can contain optical fibers to which microsensors and other diagnostic, treatment, and monitoring tools being developed at the Laboratory are attached (Figure 2).

Inserted in the femoral artery, the microcatheters are guided by microwires through the circulatory system to the clot...
Livermore scientists have, for example, demonstrated in vitro fiber-optic and electrochemical sensors for measuring pH at stroke sites. These sensors can establish brain tissue viability by direct measurement of pH in brain tissue or through indirect measurement in blood near the stroke site. Livermore scientists have developed miniature intracranial (direct brain tissue) electrochemical and fiber-optic pH sensors, which neurosurgeon collaborators at the State University of New York at Buffalo have used for in vivo animal testing.

The measurement of blood pH is one of a number of chemical “markers” that have been identified to assess the health of blood-vessel tissue at the site of a stroke, thereby providing guidance in stroke therapy. When tissue dies, lactic acid builds up and blood pH decreases. So if blood pH is below normal (7.4) at or near the stroke site, then brain cell death has occurred, and the use of neuroprotectant drugs to minimize brain damage is unwarranted. If, on the other hand, pH is close to normal, cell death has not occurred, and neuroprotectant drugs become a therapeutic option.

In the Laboratory’s fiber-optic pH sensor, a pH-sensitive dye, seminaphthorhodamine-1-carboxylate (SNARF-1C), is mixed with transparent silica sol-gel and dip-coated onto an optical fiber tip. In laboratory tests, the tip is placed in blood, and the dye is excited by a tungsten–halogen light source or a low-energy density laser. The emission spectra of the dye is pH sensitive. These tests showed that the sensor had good sensitivity in the pH range of 6.8 to 8.0, indicating possible use for in vivo sensing of blood pH in the neighborhood of a stroke site.

Livermore scientists are also developing a D-dimer biosensor to monitor stroke patients during therapies to dissolve blood clots in the vessels of the brain. D dimer is a substance with antigenic properties (i.e., capable of stimulating an immune response) and is produced as a result of a complex biochemical process when clot-dissolving drugs are injected via a microcatheter into blood clots.

Livermore’s D-dimer biosensor can act as a diagnostic tool by indicating whether the blockage is caused by plaque or by a clot. Clot-dissolving drugs will not dissolve plaque; therefore, if an elevated concentration of D dimer is not detected at the site of blockage, then the blockage may be caused by something other than a clot, and alternative therapy is needed. In addition, because treatment using clot-dissolving drugs is highly variable, the D-dimer biosensor could help eliminate the guesswork related to the dosage and infusion rates. It could help physicians develop a diagnosis and treatment plan faster and reduce the risk of hemorrhage resulting from treatment to dissolve clots.

Medical Photonics

Members of the stroke-initiative team are developing a catheter-based system that uses laser energy to break up clots. The system will deliver low-energy laser pulses through a fiber-optic microcatheter (Figure 3). The laser energy will be directed at a cerebral clot, and by conversion of optical light to acoustic stress waves, it will break up the clot and restore blood flow in cerebral arteries. The concept is simple. The challenge is to determine the proper pulse strength needed to break up the clot without damaging the blood vessel.

Research has focused on the optical and mechanical material strength and failure properties of the clots and tissue found in the cerebral blood vessels. Using a tunable optical parametric oscillator (OPO) laser system at Livermore’s Medical Photonics Laboratory (Figure 4), the medical-lasers team has conducted in vitro experiments to send laser pulses to dissolve blood clots in vessels of the brain. D dimer is a substance with antigenic properties (i.e., capable of stimulating an immune response) and is produced as a result of a complex biochemical process when clot-dissolving drugs are injected via a microcatheter into blood clots.
into a blood phantom (water colored with red food coloring). They have identified two distinct regimes of dynamic response, one due to strong laser light absorption, the other to moderate absorption.

In both cases, the confined stresses imparted to the liquid are substantial and determine most of the important dynamics. In the strong absorption case, energy is deposited in a thin zone near the fiber tip (Figure 5a). A thermally generated vapor bubble develops around the tip, and the initial stress wave, which can generate high peak pressure within 400 nanoseconds (billionths of a second), quickly propagates away from the tip. In the moderate case, energy is deposited in an extended zone beyond the fiber tip (Figure 5b). The initial stress evolves from the heated region within 500 micrometers (millionths of a meter) of the end of the tip, and the largest stress gradients, which develop within 20 nanoseconds, are directed radially and are situated in the immediate vicinity of the tip.

Eventually (within 100 nanoseconds), a cloud of tiny bubbles develops in response to the stress caused by laser heating. In both cases, this expansion and collapse of bubbles exert pressure and shear forces on a clot, which lead ultimately to its breakup.

The Laboratory recently entered into a Cooperative Research and Development Agreement (CRADA) with EndoVasix Inc. of Belmont, California, which will eventually market the laser “clot-busting” technology.

Figure 5. Livermore researchers use a tunable opto-parametric oscillator (OPO) laser to create a series of laser back-lit images (see Figure 5b) of the pressure distribution of laser energy within a blood-like fluid.

Brain Attack Facts*

Stroke (or “brain attack”) results from vascular disease affecting the arteries supplying blood to the brain and occurs when one of these vessels bursts or is clogged. Part of the brain is deprived of the oxygen and nutrients it needs to function, the nerve cells die within minutes, and the part of the body controlled by these cells cannot function. Sometimes the devastating effects of stroke are permanent because the dead brain cells are not replaced.

Brainstem thrombosis occurs when a blood clot (a thrombus) forms in an artery in or leading to the brain, blocking the blood flow. It is the most common cause of ischemic stroke. Ischemic strokes are the most common, hemorrhagic strokes the most deadly.

Cerebral hemorrhage occurs when a blood clot (a thrombus) forms in an artery in or leading to the brain, blocking the blood flow. It is the most common cause of ischemic stroke. Cerebral hemorrhage or subarachnoid hemorrhage causes hemorrhagic strokes. Ischemic strokes are the most common, hemorrhagic strokes the most deadly.

Cerebral thrombosis occurs when a blood clot (a thrombus) forms in an artery in or leading to the brain, blocking the blood flow. It is the most common cause of ischemic stroke. Cerebral hemorrhage or subarachnoid hemorrhage causes hemorrhagic strokes. Ischemic strokes are the most common, hemorrhagic strokes the most deadly.

There are two main types of strokes, ischemic and hemorrhagic: Clots—cerebral thromboses or cerebral embolisms—cause ischemic strokes. Cerebral hemorrhage or subarachnoid hemorrhage causes hemorrhagic strokes. Ischemic strokes are the most common, hemorrhagic strokes the most deadly.

Cerebral thrombosis occurs when a blood clot (a thrombus) forms in an artery in or leading to the brain, blocking the blood flow. It is the most common cause of ischemic stroke. Cerebral hemorrhage or subarachnoid hemorrhage causes hemorrhagic strokes. Ischemic strokes are the most common, hemorrhagic strokes the most deadly.

Cerebral thrombosis occurs when a blood clot (a thrombus) forms in an artery in or leading to the brain, blocking the blood flow. It is the most common cause of ischemic stroke. Cerebral hemorrhage or subarachnoid hemorrhage causes hemorrhagic strokes. Ischemic strokes are the most common, hemorrhagic strokes the most deadly.

Stroke is the leading cause of permanent disability in the U.S. and the third leading cause of death. Each year, 550,000 Americans have strokes. One-third of them die. Many of the survivors, who currently total over 3 million, have decreased vocational function (75%); of these 16% remain institutionalized, and 35% need assisted care. The personal cost is incalculable; the annual cost for treatment, post-stroke care, rehabilitation, and lost income to victims (but not their family caregivers) is $30 billion.

Types of Stroke

There are two main types of strokes, ischemic and hemorrhagic: Clots—cerebral thromboses or cerebral embolisms—cause ischemic strokes. Cerebral hemorrhage or subarachnoid hemorrhage causes hemorrhagic strokes. Ischemic strokes are the most common, hemorrhagic strokes the most deadly.

Cerebral thrombosis occurs when a blood clot (a thrombus) forms in an artery in or leading to the brain, blocking the blood flow. It is the most common cause of ischemic stroke. Cerebral hemorrhage or subarachnoid hemorrhage causes hemorrhagic strokes. Ischemic strokes are the most common, hemorrhagic strokes the most deadly.

Cerebral thrombosis occurs when a blood clot (a thrombus) forms in an artery in or leading to the brain, blocking the blood flow. It is the most common cause of ischemic stroke. Cerebral hemorrhage or subarachnoid hemorrhage causes hemorrhagic strokes. Ischemic strokes are the most common, hemorrhagic strokes the most deadly.

Imaging of stroke is the first step in diagnosis and treatment. One of these is the Doppler ultrasound test, which can detect blockages in the carotid artery. Another is carotid phono-angiography, wherein a stethoscope or sensitive microphone is put on the neck over the carotid artery to detect abnormal sounds (bruits) that may indicate a partially blocked artery. Yet another is digital subtraction angiography, in which dye is injected into a vein in the arm and an x-ray machine quickly takes a series of pictures of the head and neck. From these x-rays, doctors can determine the location of any blockages, how severe they are, and what can be done about them.

Surgery to remove plaque from artery walls, drugs that prevent clots from forming or getting bigger, acute hospital care, and rehabilitation are all accepted ways to treat stroke. Sometimes treating a stroke means treating the heart, because various forms of heart disease can contribute to the risk of stroke, particularly those caused by clots that form in a damaged heart and travel to the brain. But compared to the diagnosis and treatment tools that have been developed for heart attack, those for brain attack seem extremely limited and have not advanced greatly in recent years.

* Heart and Stroke Facts (The American Heart Association, Dallas, Texas, 1994), pp. 21–27. This booklet is available from the American Heart Association’s National Center, 7372 Greenville Avenue, Dallas, Texas 75231-4596 (telephone: 1-800-242-8721).

Science & Technology Review June 1997

Science & Technology Review June 1997
New Vision of Stroke Cure
The work of the stroke initiative at Lawrence Livermore hopes to remedy the paucity of tools for diagnosing and treating strokes. Its vision of stroke care includes medical devices for screening people without symptoms for stroke risk. It places special emphasis on the development of tools to provide earlier rather than later diagnosis of stroke type and assessment of brain cell damage so that appropriate treatment can be initiated rapidly. It has guided Livermore researchers in the development of technology to break up stroke-causing clots with laser energy as well as sensors and microtools to assist in the diagnosis and treatment of various kinds of brain attack. And it looks forward to providing the means for more instances of full recovery, fewer stroke-related disabilities, and less need for chronic care. —Dean Wheatcraft

Key Words: brain attack, laser “clot-busting,” laser–tissue interaction modeling, LATIS code, medical photonics, microsensors, neuroprotectant drugs, shape-memory microgripper, stroke.

Science & Technology Review June 1997

Figure 6. Microtools such as this silicon microgripper with “shape memory” will be used to treat the cerebral aneurysms that lead to hemorrhagic stroke. The microgripper is less than 1 cubic millimeter, that is, about the size of the head of a straight pin. (Approximate size.)
Laser Targets

The Next Phase

It will take a community of workers to bring the goals of the National Ignition Facility (NIF) to fruition. While national attention has been focused on the funding and construction of the 192-beam laser facility, scientists at Lawrence Livermore are working on myriad problems whose solutions are necessary to NIF’s success. A group of materials scientists, for example, is developing techniques to produce round, hollow shells about 2 millimeters in diameter—smaller than BB-gun pellets. This work seems incongruous in a project dominated by a football-stadium-size facility. But when filled with deuterium or deuterium-tritium fuel, these shells become the targets for NIF’s inertial confinement fusion (ICF) experiments. The goal of these experiments is to create fusion ignition—intense temperatures and pressures like those at the centers of stars for a small fraction of a second.

Steve Letts and Evelyn Fearon of the Laser Programs Directorate’s Target Area Technology Program are among the materials scientists continuing Lawrence Livermore’s more than 20 years of research and development on laser targets. Their focus now is on targets for NIF experiments. With 40 times more energy and 10 times more power than Nova (currently the world’s largest operating laser), NIF will require targets about 2 millimeters in diameter, 4 times larger than those used previously, which are about half a millimeter in diameter.

The increased shell size must be achieved in tandem with making the shell very smooth and symmetrical. During an ICF experiment, extremely high laser energies are absorbed by the mandrel and the other pyrolysis, leaving a spherical, hollow plasma polymer target shell.

Livermore scientists have developed a technique for producing hollow laser-target shells by starting with a poly(alpha-methylstyrene) (PAMS) mandrel and then overcoating it with thermally more stable plasma polymer. The coated mandrel is heated to 300°C over 30 hours or more. The PAMS decomposes and passes through coating, leaving a spherical, hollow plasma polymer target shell.

Successful Pyrolysis

During pyrolysis, the shells can collapse, burst, deform, or shrink. While collapse is mainly caused by nonuniform cooling, the other problems result from thermal effects. To avoid them, the researchers devised a temperature program that controls the rate of PAMS decomposition. It consists of raising the pyrolysis temperature by 10°C every minute until 200°C is reached, holding it there for 30 minutes to allow low-pressure PAMS and lowering the overcoating temperature, but the adjustments did not wholly overcome the distortion problem.

The Target Area group turned to hollow mandrels made by dot-to-dot technology and the other fabricators ground commercial PAMS beads into smaller sizes, put them through a sieve, and suspended them in water so that they would float and be evenly coated with plasma polymer. Two-millimeter, poly(alpha-methylstyrene) (PAMS) bead mandrels are molded into a smooth, spherical, thin-walled hollow shell about 2 millimeters in diameter, 4 times larger than those used previously, which are about half a millimeter in diameter. The shell is transparent, which allows fusion experimenters to diagnose the contained fuel layer. It can be used to coat the mandrel because it can withstand PAMS pyrolysis temperatures and is permeable to the gaseous, depolymerizing PAMS.

Plasma polymer is well suited to be fuel–shell material. It is transparent, which allows fusion experimenters to diagnose the contained fuel layer. It can be used to coat the mandrel because it can withstand PAMS pyrolysis temperatures and is permeable to the gaseous, depolymerizing PAMS. However, they tended to distort from the heat generated during overcoating and become nonsymmetrical or coat unevenly. To overcome the heat effects, Fearon experimented with higher molecular weight PAMS and lowered the overcoating temperature, but the adjustments did not wholly overcome the distortion problem.

The Progression of ICF Targets

Letts and Fearon’s technique for making shells uses an entirely new approach. Previously, plastic shells were produced when droplets of polystyrene solution were dropped down a heated drop tower, where evaporation first caused a skin to form on the droplets and then further vaporization of the solvent inside the skin caused the droplets to expand into hollow shells. Because the drop-tower technique produced shells of a limited size range, researchers tried micro-encapsulation. Micro-encapsulation techniques to increase shell sizes. They encapsulated droplets of water in a polymer solution suspended in an aqueous phase; the solvent containing the polymer would slowly disintegrate into the aqueous phase, leaving behind a polymer shell. However, the resulting shells were uneven in thickness and had bubbles in their walls. Steve Letts explains that these techniques frequently “wouldn’t produce round shells most of the time, so those that were round would have to be carefully picked out—not an easy task with such tiny things.”

He came up with a new idea. While measuring mass loss in polymers when they were heated, he identified one polymer material that evolved into a gas when heated to about 300°C, disappearing completely without any trace or residue. He figured out a way to take advantage of the material’s unique combination of characteristics.

That material was poly(alpha-methylstyrene), or PAMS. In Letts’s new fabrication method, an amount of PAMS is shaped into a smooth sphere, or mandrel, which is overcoated with a thermally stable plasma polymer to a desired thickness. The overcoated mandrel is heated to about 300°C, at which temperature the PAMS decomposes into a gas, diffuses through the plasma polymer overcoat (which is thermally stable up to 400°C), and leaves behind a hollow plasma polymer shell (see the figure on p. 23).

Letts postulated that this method would be feasible for producing fuel capsules of the size needed for NIF if a suitable PAMS mandrel could be formed. In addition, because the shell is built outward from the PAMS mandrel, it might be feasible to incorporate various layers during the overcoating process, which would be useful for diagnosing shell performance. The method would be successful if good quality mandrels could be made, an even overcoat could be deposited on the mandrel, and pyrolysis (heat treatment) could be accomplished without distorting or collapsing the resulting shell.

Spherical, Smooth Mandrels

Evelyn Fearon coordinated PAMS mandrel production. She and the other fabricators ground commercial PAMS beads into smaller sizes, put them through a sieve, and suspended them in water so that they would float and be evenly coated with plasma polymer. Two-millimeter, poly(alpha-methylstyrene) (PAMS) bead mandrels are molded into a smooth, spherical, thin-walled hollow shell about 2 millimeters in diameter, 4 times larger than those used previously, which are about half a millimeter in diameter.

Two-millimeter, poly(alpha-methylstyrene) (PAMS) bead mandrels are molded into a smooth, spherical, thin-walled hollow shell about 2 millimeters in diameter, 4 times larger than those used previously, which are about half a millimeter in diameter.

Letts’s new fabrication method, an amount of PAMS is shaped into a smooth sphere, or mandrel, which is overcoated with a thermally stable plasma polymer to a desired thickness.

Two-millimeter, poly(alpha-methylstyrene) (PAMS) bead mandrels are molded into a smooth, spherical, thin-walled hollow shell about 2 millimeters in diameter, 4 times larger than those used previously, which are about half a millimeter in diameter.
temperature volatiles to escape, and then ramping it up by 0.2°C every minute up to 300°C, where it is held for 30 hours or more, depending on the size of the shell. The plasma polymer shrinks gradually and uniformly during pyrolysis, and thus the sphericity is maintained. Experimenters observe and measure the shrinkage only to predict the size of a completed shell.

An optical microscope is used to measure the wall thickness and diameter of pyrolyzed shells, a scanning electron microscope is used to determine how smooth and free of particle defects shell surfaces are, and an atomic-force microscope is used to make detailed measurements of the sphericity and roughness of the shell.

Challenges Ahead

The techniques described here have now been adopted by General Atomics as the preferred method for making 0.5-millimeter-diameter capsule targets for Nova ICF experiments at Livermore and 0.9-millimeter-diameter capsules for ICF experiments at the Omega Laser facility at the University of Rochester. The success in moving this research proof of principle to actual target production is certainly encouraging. However, significant challenges still face Livermore’s laser-target scientists.

Currently the development efforts at Lawrence Livermore are focused on adapting the technology developed by Letts and Fearon to the production of 2-millimeter-diameter capsules for NIF. This effort has two parts. The first, being led by Ken Hamilton, is to develop micro-encapsulation techniques to form PAMS microshells with the required outer surface sphericity and surface finish. To meet NIF specifications, these shells must be no more than 1 micrometer, and a millimeter of a meter, out of round; that is, the radius to the outer surface can vary by no more than 1 micrometer (out of 1,000) as one moves across the surface. Solving this extremely difficult problem will require significant improvements in current micro-encapsulation technology. Once it is solved, the second part will be to maintain the sphericity of the shell through the coating and thermal treatment to remove the PAMS.

Members of the Laboratory’s Target Area Technology Program will continue to refine laser target technology. Beyond making targets for current ICF experiments, they must focus on developing targets for the real NIF event—ignition. The PAMS technique is being investigated for that mission.

---

**Key Words:** laser target, National Ignition Facility (NIF), inertial confinement fusion (ICF), fuel capsule, plasma polymer, polymershell, micro-encapsulation, poly(alpha-methylstyrene) (PAMS), hydrodynamic instability.

---

For further information contact Steve Letts (510) 422-0937 (letts1@llnl.gov) or Evelyn Fearon (510) 423-1817 (fearon2@llnl.gov).

---

### Patents

<table>
<thead>
<tr>
<th>Patent issued to</th>
<th>Patent title, number, and date of issue</th>
<th>Summary of disclosure</th>
</tr>
</thead>
<tbody>
<tr>
<td>John S. Tippet</td>
<td>Method for Optical and Mechanically Coupling Optical Fibers U.S. Patent 5,560,760 October 1, 1996</td>
<td>An inexpensive technique to splice optical fibers that does not cause deformation of the host fibers, does not require repeated thermal cycling of the optical fibers, does not cause thermal and photonic degradation of the fibers even at high power applications, does not cause the fibers to prematurely deteriorate with age, and is suitable for use with optical fibers having a core diameter of as much as 1,000 micrometers or greater. A solder-glass fit having a melting point lower than the melting point of the optical fibers is used to splice the two optical fibers together.</td>
</tr>
<tr>
<td>Rex Booth</td>
<td>Charge Line Quad Pulser U.S. Patent 5,563,457 October 8, 1996</td>
<td>A quartet of parallel planar triode triodes that is removably mounted in a quadrilateral-shaped PCB structure. Releasable brackets and flexible means attached to each triode socket make triode cathode and grid contact with respective conductive coatings on the PCB and with a detachable cylindrical conductive element enclosing and contacting the triode anodes. The configuration permits quick and easy replacement of faulty triodes. By such orientation, the quad pulser can convert a relatively low and broad pulse into a very high and narrow pulse. A maximum impedance mismatch within a planar triode circuit of less than 10% is maintained.</td>
</tr>
<tr>
<td>Thomas E. McIver</td>
<td>Precision Digital Pulse Phase Generator U.S. Patent 5,565,605 October 8, 1996</td>
<td>A timing generator comprising a crystal oscillator connected to provide an output reference pulse. A resistor–capacitor combination is connected to provide a variable-delay output pulse from an input connected to the crystal oscillator. A phase monitor is connected to provide duty-cycle representation of the reference and variable-delay output pulse phase. An operational amplifier drives a control voltage to the resistor–capacitor combination according to currents integrated from the phase monitor and injected into summing junctions. A digital-to-analog converter injects a control current into the summing junctions according to an input digital control code.</td>
</tr>
<tr>
<td>Kurt H. Weber</td>
<td>Process for Forming Retrograde Profiles in Silicon U.S. Patent 5,565,377 October 15, 1996</td>
<td>A process for the formation of retrograde profiles in silicon, either previously doped crystalline or polycrystalline silicon, or for introducing dopant into amorphous silicon so as to produce the retrograde profiles. This process involves the formation of higher dopant concentrations in the bulk than at the surface of silicon. By this process, n- and p-well regions in CMOS (complementary metal oxide silicon) transistors can be formed by a simple, flexible, and inexpensive manner. This technique has particular application in the manufacture of silicon integrated circuits where retrograde profiles are desired for the n- and p-well regions of CMOS transistor technology and for buried collectors in bipolar transistors.</td>
</tr>
<tr>
<td>Daniel W. Shiner, Arnold C. Lange</td>
<td>E-Beam High Voltage Switching Power Supply U.S. Patent 5,566,060 October 15, 1996</td>
<td>A circuit device for generating a ground-level voltage feedback signal for controlling the output voltage of one of a plurality of dc–dc converter modules having their outputs connected in series to form a supply output lead. Each module includes a switching device for producing a pulsating voltage of controlled duty cycle, an inductor mechanism for converting the pulsating voltage into a smooth direct current, and an inverter mechanism for producing from the direct current an alternating current through the primary of a transformer. The transformer has at least one secondary winding inductively coupled to the primary winding for producing an output voltage of the module.</td>
</tr>
<tr>
<td>Patent issued to</td>
<td>Patent title, number, and date of issue</td>
<td>Summary of disclosure</td>
</tr>
<tr>
<td>------------------------------------------</td>
<td>---------------------------------------------------------------------------------------------------------</td>
<td>----------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>George P. Roberson</td>
<td>Image Matrix Processor for Fast Multidimensional Computations U.S. Patent 5,566,341 October 21, 1996</td>
<td>An apparatus for multidimensional computation that comprises a computer engine, including a plurality of processing modules. The processing modules are configured in parallel and compute respective contributions to a computed multidimensional image of respective two-dimensional data sets. A storage system is provided that stores the multidimensional data sets, and a switching circuit routes the data among the processing modules in the computer engine and the storage system. The processing modules include a programmable local host, by which they may be configured to execute a plurality of different types of multidimensional algorithms.</td>
</tr>
<tr>
<td>Michael F. Skeate</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gary W. Johnson</td>
<td>Apparatus for Controlling the Scan Width of a Scanning Laser Beam U.S. Patent 5,568,255 October 22, 1996</td>
<td>A system wherein the scan width of a swept-ring dye laser or a semiconductor diode laser can be measured and controlled in real-time with a resolution better than 0.1%. Scan linearity, or conformity to a nonlinear scan waveform, can be measured and controlled. The system consists of a Fabry-Perot interferometer, three CAMEX interface modules, and a microcomputer running a simple analysis and proportional-integral control algorithm. With additional modules, multiple lasers can be simultaneously controlled. Also included is an embodiment implemented on an ordinary personal computer with a multifunction plug-in board.</td>
</tr>
<tr>
<td>Kurt H. Weiner</td>
<td>Method for Shallow junction Formation U.S. Patent 5,569,624 October 29, 1996</td>
<td>A doping sequence that reduces the cost and complexity of forming source-drain regions in complementary metal oxide silicon (CMOS) integrated circuit technologies. The process combines the use of patterned excimer laser annealing, dopant-saturated spin-on glass, silicide contact structures, and interference effects created by thin deuterium-layers to produce source and drain junctions that are ultrashallow in depth but exhibit low sheet and contact resistance. The process uses no photolithography and can be achieved without the use of expensive vacuum equipment. The process margins are wide, and yield loss due to contact of the ultrashallow dopants is eliminated.</td>
</tr>
<tr>
<td>Alexander R. Mitchel</td>
<td>Vicarious Nucleophilic Substitution to Prepare 1,3-Diamino-2,4,6-Trinitrobenzene or 1,3,5-Triamino-2,4,6-Trinitrobenzene U.S. Patent 5,569,783 October 29, 1996</td>
<td>A process that is milder and more environmentally benign to easily convert nitroaromatic compounds to DATB, TATB, or mixtures thereof by using processes that avoid strong acids (H₂SO₄, HNO₃) at elevated temperatures (100 to 150°C) and the need for noxious materials such as ammonia, thionyl chloride, and hydrogen sulfide. DATB and TATB can be useful specialty explosives. TATB can also be used for the preparation of tetrabenzoxazine, a starting material for the synthesis of novel materials such as optical imaging devices, liquid crystals, and ferrimagnetic compounds.</td>
</tr>
<tr>
<td>Philip F. Pagoria</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Robert D. Schmidt</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Howard Nathel</td>
<td>Method for Detection of Dental Caries and Periodontal Diseases Using Optical Imaging U.S. Patent 5,570,182 October 29, 1996</td>
<td>A method of optical imaging that may be used both for the detection of dental caries and for the diagnosis and monitoring of gingivitis. Optical radiation is used in the wavelength region between 500 and 1,400 nanometers, where various dental tissues is much more strongly absorbing than healthy tissue, so that transmitted or reflected optical radiation can be used to create a shadowgraph of structures within the dental tissue. The same wavelength region used for the detection and location of tissue boundaries may be used to diagnose and monitor the progress and treatment of gingivitis.</td>
</tr>
</tbody>
</table>

**Awards**

Laboratory scientists Paul Coronado, Dan Calef, Bob Sanner, and Lucy Hall were recently selected by the Society of Automotive Engineers to be honored by the Partnership For New Generation Vehicles (PNGV) for their contribution to the development of affordable, energy-efficient, nonpolluting vehicles to get up to 80 miles per gallon. On March 31 in Washington, D.C., they received medals from Vice President Al Gore. PNGV is a collaboration of eight federal agencies, the U.S. Council for Automotive Research, Chrysler, Ford, General Motors, and 18 laboratories, among them Livermore, Los Alamos, and Sandia national laboratories. Its goal is to select the most promising new technologies by 1997 and produce a concept car by the year 2000. The Livermore team was honored for the development of aerogels to be catalysts for the next-generation vehicles. Sanner, a materials chemist, made materials that Coronado, a chemist, developed into aerogels, which were tested for use as a catalyst. Calef, a theoretical chemist, did modeling to determine which metals would or would not work in an aerogel environment, and Hair, a chemical engineer, served as principal investigator on the project.

<table>
<thead>
<tr>
<th>Patent issued to</th>
<th>Patent title, number, and date of issue</th>
<th>Summary of disclosure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Joseph T. Salmon</td>
<td>Split-Field Pupil Plane Determination Apparatus U.S. Patent 5,570,189 October 29, 1996</td>
<td>An apparatus for locating a pupil plane following relay telescope optics along an optical path using a pair of optical wedges disposed side by side on the optical path for splitting an incident beam of collimated light on the optical path to provide two parallel side-by-side beams of collimated light on the optical path, the parallel side-by-side beams of collimated light being provided such that they diverge while being parallel to the path of the incident beam of collimated light.</td>
</tr>
<tr>
<td>George C. Pollock</td>
<td>Precision Control of High Temperature Furnaces Using an Auxiliary Power Supply and Charged Particle Current Flow U.S. Patent 5,597,301 January 20, 1997</td>
<td>A high-temperature furnace with two power supplies. A main power supply connected to a heating element in the furnace heads the furnace in the traditional manner. An auxiliary power supply introduces a current flow through charged particles between the heating element and an object holder. The main power supply provides the bulk heating power; the auxiliary provides temperature control.</td>
</tr>
</tbody>
</table>

**Awards**
Transforming Explosive Art into Science

Livermore researchers have studied and synthesized high explosives for decades because they are an integral element of every nuclear weapon. Today their work encompasses a wide range of basic research and programmatic activities. 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.

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 are also designing new paths to synthesizing existing energetic molecules that are cheaper and easier on the environment. In a parallel effort, experiments are being done to better understand the fundamental physics and chemistry of energetic materials, particularly with regard to their stability, sensitivity, and performance. Livermore chemists are also working to improve efficiencies in the production of these materials.

Contact:
Randall Simpson (510) 423-0379 (simpson5@llnl.gov).

On the Offensive against Brain Attack

The Center for Healthcare Technologies at Lawrence Livermore National Laboratory has undertaken a stroke initiative whose purpose is to provide the medical community with the tools that will allow doctors to diagnose and treat stroke as aggressively as they do heart attack. A multidisciplinary team of stroke-initiative researchers is collaborating with academic medical centers and private companies to move these tools from the research and development stage through clinical trials, regulatory approval, and manufacture so that they can benefit many thousands of people who have strokes each year. Tools the team has developed fall into four categories: microsensors for brain and clot characterization, a catheter-based system using laser energy to break up clots in the blood vessels of the brain, laser-tissue interaction models in support of laser “clot busting,” and microtools for treating the aneurysms that cause hemorrhagic stroke.

Contact:
J. Patrick Fitch (510) 422-3276 (healthcare@llnl.gov).