December 2009

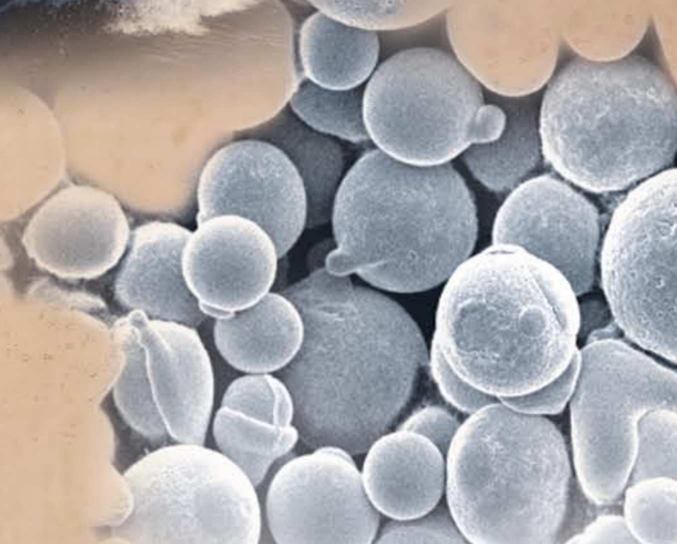
Science & Technology
REVIEW

National Nuclear
Security Administration's
Lawrence Livermore
National Laboratory

Protecting Materials in Harsh Environments

Also in this issue:

- **Asteroids on a Collision Course with Earth**
- **A Test Bed for Computing Technologies**
- **Isolating Biomolecules for Faster Diagnosis**



About the Cover

Livermore scientists in collaboration with researchers at other institutions have developed two iron-based amorphous metal alloys that are harder and tougher than stainless steel. The new alloys, SAM2X5 and SAM1651, also offer improved corrosion resistance and higher neutron absorption capabilities than crystalline, nickel-based alloys. Designed for use in coatings to protect ships and spent nuclear fuel containers from exposure to harsh environments, the alloys might also extend the life of wind turbine components, offshore drilling platforms, and oil- and gas-transmission pipelines. The cover shows the *USS Freedom* (center), a U.S. Navy warship built for littoral (close-to-shore) operations, and (bottom right) a micrograph of SAM2X5. In the background are x-ray diffraction data for various formulations of iron-based amorphous alloys. (*USS Freedom* photograph courtesy of the Department of Defense.)

Cover design: Daniel Moore

About the Review

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

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National
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Berni Alder Receives National Medal of Science

Retired Laboratory physicist and computational pioneer Berni Alder was one of nine researchers to receive the National Medal of Science from President Barack Obama on October 7, 2009. Alder is regarded as the founder of molecular dynamics, a type of computer simulation used to study the motions and interactions of atoms over time. In 1980, he was one of the first scientists to apply large-scale simulations to solve quantum mechanics problems. In addition, his work led to changes in kinetic molecular theory, showing that simulations can significantly affect a scientific field.

Alder completed his undergraduate work at the University of California (UC) at Berkeley. In the late 1940s, while studying for a Ph.D. at the California Institute of Technology, he met computer designer Stan Frankel. Together, they developed a computer technique, now called the Monte Carlo method, for calculating results from random sampling.

Alder continued developing his ideas at UC Berkeley and became a consultant to Lawrence Livermore when it opened in 1952, providing him with access to some of the only electronic computers in the nation. He joined the Laboratory full-time in 1955 and published his pioneering work on molecular dynamics in 1956.

The National Medal of Science is the highest honor bestowed by the U.S. government on scientists, engineers, and inventors. The other recipients for 2009 are Francis Collins, National Institutes of Health; Joanna Fowler, Brookhaven National Laboratory; Elaine Fuchs, Rockefeller University; James Gunn, Princeton University; Rudolf Kalman, Swiss Federal Institute of Technology; Michael Posner, University of Oregon; JoAnne Stubbe, Massachusetts Institute of Technology; and J. Craig Venter, J. Craig Venter Institute.

In presenting the awards, President Obama said, "These scientists, engineers, and inventors are national icons, embodying the very best of American ingenuity and inspiring a new generation of thinkers and innovators. Their extraordinary achievements strengthen our nation every day—not just intellectually and technologically, but economically, by helping create new industries and opportunities that others before them could never have imagined."

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Prototype Combines Bio and Nano Technologies

Laboratory researchers have developed a versatile hybrid platform that uses lipid-coated nanometer-size wires to build prototype bionanoelectronic devices. These devices, which combine biological components with electronic circuits, could boost the operating efficiency of various technologies, from biosensors and diagnostic tools to neural prosthetics and computers.

The circuits in modern communication systems rely on electric fields and currents to carry information. Biological systems, however, are much more complex, using an arsenal of membrane receptors, channels, and pumps to control signal transduction. For example, the processing involved in converting sound waves into nerve impulses is unmatched by even the most powerful computer application, yet the human ear has no trouble performing it. Electronic circuits that use biological components have the potential to significantly increase a system's efficiency.

For the bionanoelectronic platform, the Livermore researchers covered silicon nanowire transistors with a shell of lipid membranes. Because these membranes are virtually impenetrable to ions and molecules, the shell forms a barrier between the nanowire surface and the solution species. "This 'shielded wire' configuration ensures that the membrane pores are the only pathway for the ions to reach the nanowire," says Livermore scientist Aleksandr Noy, who led the project team.

Lipid membranes can also house an unlimited number of protein machines that perform critical cell functions. As a result, says Noy, "We can use the nanowire device to monitor specific transport and to control the membrane protein." In addition, changing the gate voltage on a device will open and close a membrane pore electronically. The team published its research results in the August 18, 2009, issue of *Proceedings of the National Academy of Sciences*.

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Simulations Examine Blast-Wave Effects

Hydrodynamic simulations on the effects of blast waves are providing new information about traumatic brain injuries. The research, which was conducted by scientists at Lawrence Livermore and the University of Rochester, could lead to improved designs for combat helmets and other protective equipment.

The simulations showed that even when blast pressures are nonlethal, the wave action can flex, or deform, the skull enough to generate potentially damaging pressure in brain tissue. In fact, the mechanical loads caused by a nonlethal blast wave can be comparable to those in an injury-inducing impact, such as in a motor vehicle or sports accident. The simulations also revealed that blasts and impacts affect the brain differently. An impact accelerates the head, whereas a blast wave sweeps over it, deforming the skull and squeezing the brain tissue. Although the skull flexure from a weak (100-kilopascal) blast wave is only about 50 micrometers (the width of a human hair), the deformation may be great enough to induce injury.

By comparing the mechanisms involved, researchers can better understand the potential damage to both soldiers and civilians and determine how helmets might be designed to minimize the two types of head injuries. Results from the team's research appeared in the September 4, 2009, issue of *Physical Review Letters*.

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Advanced Materials for Our Past, Present, and Future

LAWRENCE Livermore has a tradition of excellence in materials science. Throughout our history, we have applied creativity and innovation to designing materials in support of the Laboratory's missions, our sponsors, and the nation. Our work was essential in tests to determine the effects of aging on the lifespan of plutonium pits in the nuclear weapons stockpile and in a major initiative aimed at developing a new generation of multifunctional materials and sensors. In some cases, we have built on past research to create enhanced materials with new functionalities. For example, in the 1980s, Livermore researchers adapted aerogels for use in various national security applications. Today, they are redesigning these nanofoams for technologies that improve catalysis, energy efficiency, and environmental cleanup.

The Laboratory's successes in materials science are a direct result of our comprehensive approach to the development process, which begins with understanding a material at its most fundamental level. Through computational modeling and rigorous testing, Livermore scientists glean valuable data about a material's structure, composition, properties, and behavior and by implication how these characteristics affect performance. This methodology, which encompasses simulation, characterization, synthesis, and experimentation, not only broadens our knowledge of existing materials, but it also helps us design and produce new materials for a wide range of applications. As a result of these efforts and our scientists' expertise and foresight, we can make scientific breakthroughs that contribute to the nation's security and economic competitiveness.

The article beginning on p. 4 describes a perfect example of materials science at work and how we use the Laboratory's expertise in this discipline to meet important national needs. In collaboration with other government agencies, universities, and private industry, the Laboratory spearheaded the High-Performance Corrosion Resistant Materials (HPCRM) project. This project focused on developing a new class of materials known as iron-based amorphous metal alloys for the Defense Advanced Research Projects Agency and the Department of Energy.

Amorphous metal alloys have been applied as thermal spray coatings to surfaces on naval ships, submarines, and spent nuclear fuel containers to protect the underlying materials from corrosion and wear. They have also demonstrated exceptional neutron absorption capabilities—a necessary attribute for criticality control. With further research and development, the alloys may be useful for coating other materials such as machine components, steel bridges, and steel-reinforced concrete structures.

The ability to redesign, innovate, and reapply materials to solve new problems is at the heart of the HPCRM project. Leveraging modeling techniques and accelerated testing methods from past work on crystalline nickel-based alloys for reinforcing spent nuclear fuel containers, the HPCRM team determined the essential properties of different amorphous alloy compositions. Ultimately, their research led to the development of two alloy formulations that are harder, tougher, and more corrosion resistant than the best stainless steels and nickel-based alloys.

Lawrence Livermore will carry on this tradition of excellence in materials science for the foreseeable future. As outlined in our science, technology, and engineering roadmap—a five-year investment strategy for strengthening the Laboratory's capabilities—materials science will play a pivotal role in emerging 21st-century priorities as well as our enduring missions. This roadmap promotes the discovery of new materials with applications in high-energy-density science, including targets for experiments at the National Ignition Facility; fusion energy and advanced energy systems such as the Laser Inertial Fusion Energy engine; and sophisticated diagnostics and detector systems for laser experiments.

Our roadmap for the future builds on Livermore's culture of strategic thinking, innovation, and success. The HPCRM team provides just one example of our accomplishments. In the coming years, we will focus on developing a new generation of advanced materials in support of the Laboratory's missions. Successful endeavors will contribute to renewable and reliable sources of energy, a healthier environment, and improved human health and will strengthen national security.

■ Tomás Díaz de la Rubia is acting principal associate director for Science and Technology.

A Defensive "Coat"

Iron-based amorphous alloys can be applied as thermal spray coatings to protect materials exposed to harsh environments such as (counterclockwise from top left): oil- and gas-transmission pipelines, tunnel-boring machines (courtesy of the Department of Energy), and aircraft carrier decks (courtesy of the Department of Defense).

for Materials under Attack

Thermal spray coatings made with amorphous metal alloys enhance protection of ships and containers in corrosive environments.

FROM complex polymers and plastics to more common items such as window glass and candle wax, amorphous materials abound. These noncrystalline solids are not only prevalent in everyday life but also are an important research area at Lawrence Livermore. By varying the composition of different elements, Laboratory scientists have created novel materials such as amorphous carbon films to prevent wear and friction on computer hard disks (see *E&TR*, August/September 1994, pp. 4–5) and complex nanolaminates with unusual ductility (see *S&TR*, November/December 2008, pp. 10–16). In the last few years, Livermore researchers working on the High-Performance Corrosion-Resistant Materials (HPCRM) project have developed amorphous metal alloys, also known as metallic glasses, that can withstand corrosive environments.

Established in 2003, the HPCRM project was cosponsored by the Defense Advanced Research Projects Agency (DARPA) and the Department of Energy (DOE). The project's goal was to develop ultrahard, iron-based amorphous alloys for use as coatings to protect materials in harsh environments. For DARPA and the Department of Defense, such materials improve the corrosion resistance of ships and other military vehicles that spend most of their service life in saltwater and abrasive sand. For DOE, the coatings reduce the long-range expense of protecting spent nuclear fuel (SNF) containers while offering enhanced neutron absorption and criticality control.

Livermore chemical engineer and corrosion scientist Joe Farmer, who initiated and led the HPCRM project, is no stranger to high-performance, corrosion-resistant materials. In the early 1980s, he worked with a DOE team developing alloy C-22, a crystalline, nickel-based alloy designed to reinforce containers for long-term storage of nuclear waste. "Much of the Laboratory's early work with the nickel-based alloy was the first of its kind," says Farmer. "For example,

Iron-based amorphous alloys can be applied as thermal spray coatings to protect materials exposed to harsh environments, such as containers used for the long-term storage of spent nuclear fuel.

our thermochemical modeling showed that alloy C-22 had sufficient stability to survive the storage periods required for an underground repository, where containers would have to withstand temperatures near the boiling point in nearly saturated geothermal brines." The HPCRM team applied many of the same techniques learned during the repository studies to the DARPA challenge, thus providing the nation with additional benefit from the original investment.

DARPA approached the Laboratory in 2003 for help with a new iron-based material the agency had developed. Although this material was harder, stronger, and more wear resistant than virtually any known steel, it lacked corrosion resistance. "DARPA asked us to manipulate the material's composition to improve this essential property," says Farmer. Shortly thereafter, DOE's Office of Civilian and Radioactive Waste Management joined the effort as a cosponsor because the materials could be used for DOE mission work.

Together with colleagues from Livermore, other government laboratories, universities, and private industry, the HPCRM team developed and tested more than 40 compositions of iron-based amorphous alloys before determining the two most promising ones—SAM2X5 and SAM1651. "These materials are four to five times harder and more wear resistant than the best stainless steels and nickel-based alloys," says Farmer. "Tests showed the corrosion resistance of these two alloys was far superior to that of stainless steel and comparable to or better than that of the nickel-based alloy C-22, the gold standard for the SNF container."

SAM2X5 and SAM1651 are also less expensive, costing about $15 per kilogram ($7 per pound) compared with up to $80 per kilogram ($37 per pound) for alloy C-22. In addition, the high-boron alloys could absorb three to four times more thermal neutrons than the borated stainless steels commonly used for criticality control.

A Winning Combination

In a crystalline alloy, atoms form a three-dimensional lattice, but those in an amorphous solid are disordered and have no crystalline structure. Some materials are naturally amorphous, but others must be processed to maintain their glassy state. The cooling rate of this processing must be fast enough to prevent the atoms from forming a crystalline structure.

For amorphous metals and alloys, the minimum, or critical, cooling rate to prevent crystallization is extremely fast, as high as millions of degrees per second. Materials with lower critical cooling rates are thus much easier to process. As with corrosion resistance, the critical cooling rate can be controlled by carefully manipulating an alloy's composition. "For example, adding yttrium to some formulations will increase melt viscosity and slow the crystallization kinetics, which reduces the critical cooling rate dramatically," says Farmer.

The iron-based alloys developed by the HPCRM team combine several elements, each of which performs an important function. Iron gives the materials strength at an affordable price. Chromium, molybdenum, and tungsten are the necessary ingredients for enhanced corrosion resistance. Boron promotes glass formation and is an outstanding thermal neutron absorber, an important attribute for criticality control in various DOE applications. In fact, an unusually high level of boron is homogenously dispersed throughout SAM2X5 to make it an effective neutron absorber.

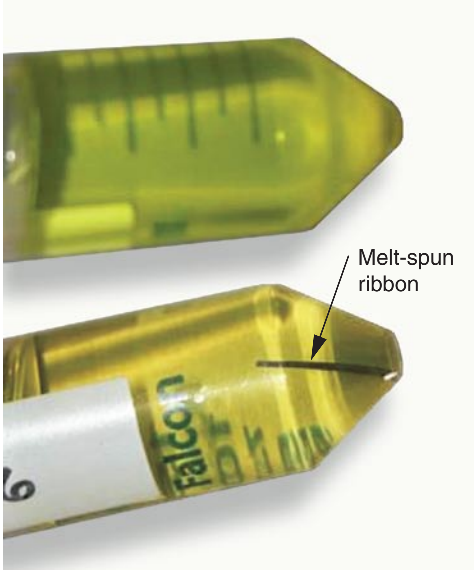
Eliminating the Competition

The 40-plus candidate materials underwent accelerated testing for periods of months to years to measure such characteristics as passive film stability, corrosion resistance, hardness, wear resistance, strength, fracture toughness, and absorption of thermal neutrons. Results for candidate materials were then compared with those of more conventional stainless steels, nickel-based alloys, and borated steels. “We conducted our tests using the quality assurance standards established for SNF repositories, which increased the confidence of external stakeholders in our work,” says Farmer. “Test results showed not only that we were meeting the performance requirements established by our sponsors, but also in many cases, we were doing much better.”

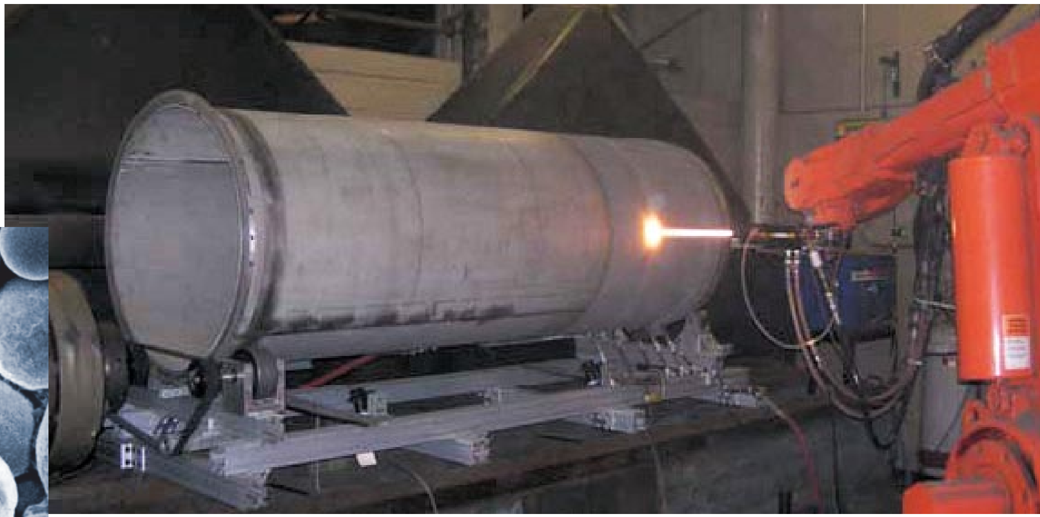
The testing series conducted by the Laboratory was similar to a competition with elimination rounds, where only the best performers progress to the next stage. In the first round, each material was made into a melt-spun ribbon. In this process, the liquid form of the amorphous material is dripped onto a supercooled copper wheel, which quenches the metal and transforms it into a solid ribbon a few millimeters wide and only 150 micrometers thick. “This method is the easiest way to make a metallic glass because it requires the least amount of material and prep work to produce a workable sample,” says Farmer.

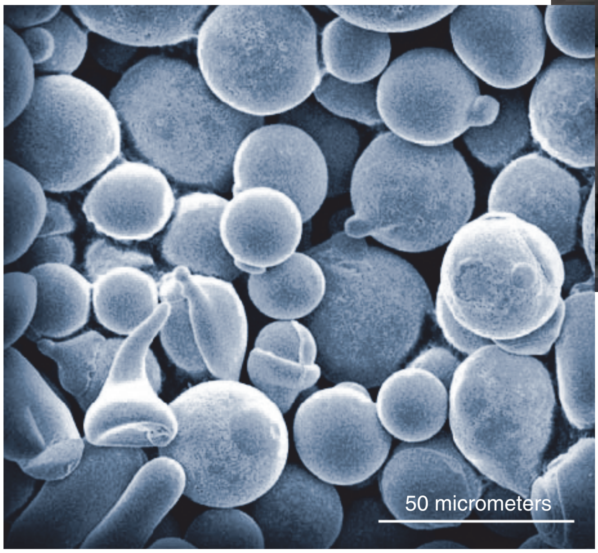
Formulations that passed the first stage were used to create drop-cast ingots. These tube-shaped casts, which were larger and thicker than the ribbons, were fabricated at Oak Ridge National Laboratory. Tests with the ingots allowed the researchers to determine if thicker sections of the material could be cooled fast enough to maintain a glassy state. Winners of the ingot “competition” then moved on to the next round, where gas atomization transformed each formulation into a fine powder.

At this stage, the Livermore team used characterization tools such as scanning

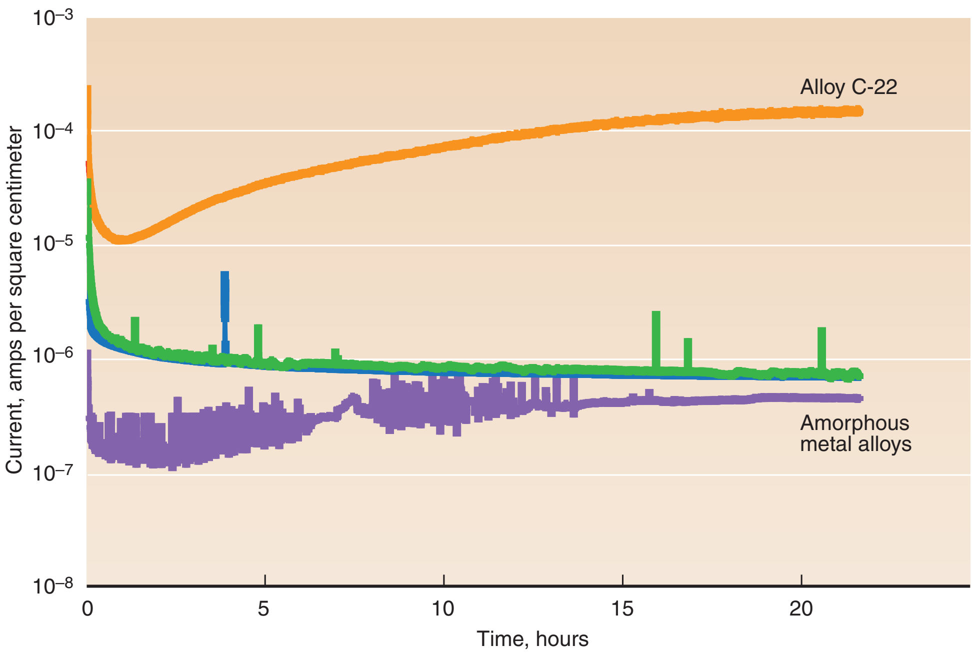


In tests using melt-spun ribbons, alloy C-22 (top) easily dissolved when submerged in a boiling acid solution. A formulation of the new iron-based amorphous alloy (bottom) remained intact, even after long-term exposure.





In one test, the Livermore team used a high-velocity oxy-fuel process to melt amorphous powders (left) for use in a thermal spray coating. The coating was applied with a hypersonic torch at extremely high pressures to a half-scale prototype spent nuclear fuel container (above).



Polarization tests subjected the iron-based alloy SAM2X5 and the nickel-based alloy C-22 to a constant applied potential for prolonged periods. The increase in current for alloy C-22 (orange curve) indicated a breakdown in its passive film. SAM2X5 remained stable as a melt-spun ribbon (purple) and in course (blue) and fine (green) powder form.

electron microscopy, x-ray diffraction, and transmission electron microscopy to measure each powder's particle crystallinity, size distribution, and morphology. Powders that met the desired specifications were applied as thermal coatings to stainless-steel substrates using the high-velocity oxy-fuel process. Finished coatings ranged in thickness from 375 micrometers to 2 centimeters.

The melt-spun ribbons, drop-cast ingots, and coated substrates were subjected to a battery of tests to determine each material's physical, mechanical, and thermal properties. X-ray diffraction experiments provided data on any residual structures, such as crystalline precipitates, which might reduce a material's corrosion resistance and effectiveness in the targeted applications.

The team also used energy-dispersive x-ray spectroscopy to determine a material's exact elemental composition. Through differential thermal analysis and differential scanning calorimetry, the researchers measured material changes in response to temperature and identified glass transition and crystallization temperatures, melting points, and other important characteristics.

When the iron-based alloys are exposed to aqueous environments, such as hot geothermal brines, seawater, or salt fogs, passive oxide films form a protective layer on a material's surface, which prevents corrosion. In wet, salty environments, such as the ocean, this protective layer can break down in the presence of aggressive elements such as chloride. The rate of breakdown depends on film quality, exposure time, and temperature. Higher temperatures accelerate the rate of attack.

To determine corrosion rates, passive film stability, and the effects of thermal aging on corrosion resistance, the Livermore team immersed the sample ribbons, ingots, and coated substrates in concentrated brines near the boiling point and in natural seawater at elevated temperatures for periods ranging from days to months. "We applied standard electrochemical techniques to evaluate the corrosion mechanisms and rates as functions of alloy composition and environmental conditions," says Farmer. "Electrochemistry is an extremely sensitive tool that allows us to study material degradation processes in situ, without having to periodically remove the sample from the harsh test environments. More recently, we have extended such measurements to high-temperature molten salts and have made in situ observations of alloy degradation at temperatures up to 1,000°C."

Nanocrystallites can form in amorphous alloys at elevated temperatures, causing the alloys to lose their corrosion resistance. To determine when the materials start to crystallize, the team heat-treated, or annealed, melt-spun ribbons at various temperatures. Subsequent electrochemical testing established the upper limit of the operating temperature. The researchers also used indentation methods to measure material hardness as a function of temperature and impact testing to establish the damage tolerance of the coatings. They also determined how well the coatings resist abrasion and wear.

After initial tests identified SAM2X5 and SAM1651 as the most promising materials, coating processes based on the two formulations were increased to commercial-scale production. Coated prototypes underwent salt-fog testing at a facility used by the Marine Corps in Fredericksburg, Virginia. Salt-fog testing is a standard method used by the automotive industry to measure corrosion resistance. In these tests, researchers evaluated SAM2X5 and SAM1651 coatings on various steel substrates, including half-scale prototype SNF containers and criticality control assemblies. In addition, they performed seawall tests using sail cover plates from submarines, and they applied coatings to panels inside air ducts aboard amphibious ships for testing during deployment.

“We demonstrated that the new alloys could be produced in significant quantities under industrial conditions, and we tested their performance in realistic scenarios,” says Farmer. “Under a wide range of harsh conditions, we found no significant corrosion—the materials appear to have passed the Admiral’s test with flying colors.”

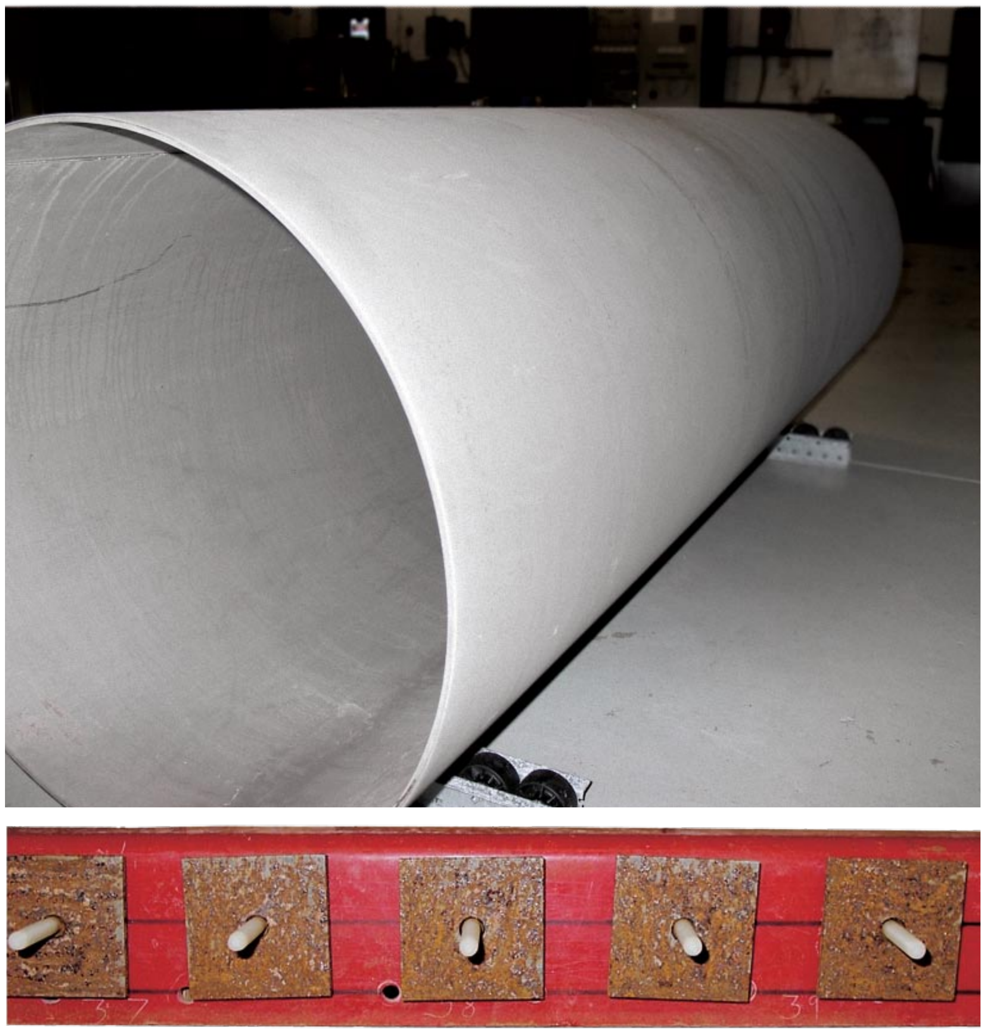
In the final round of experiments, the research team exposed several families of the SAM2X5 and SAM1651 alloy compositions to intense neutron irradiation in the 1.5-megawatt TRIGA reactor at McClellan Nuclear Radiation Center operated by the University of California at Davis. These tests demonstrated the phase stability of the materials at neutron irradiations corresponding to between 4,000 and 10,000 years inside an SNF container—the most realistic conditions that could be found for the applications of interest to DOE.

Through this extensive testing program, the Livermore researchers verified the corrosion resistance and mechanical properties of each formulation. They then worked with several industrial partners to prepare the powders to specifications for real-world applications. Carpenter Powder Products of Pittsburgh, Pennsylvania, optimized the SAM1651 gas atomization process, and Caterpillar in Peoria, Illinois, developed the SAM1651-based high-performance coatings. The NanoSteel Company in Idaho Falls, Idaho, produced the SAM2X5 powder, and Plasma Tech, Inc., in Torrance, California, developed those coatings.

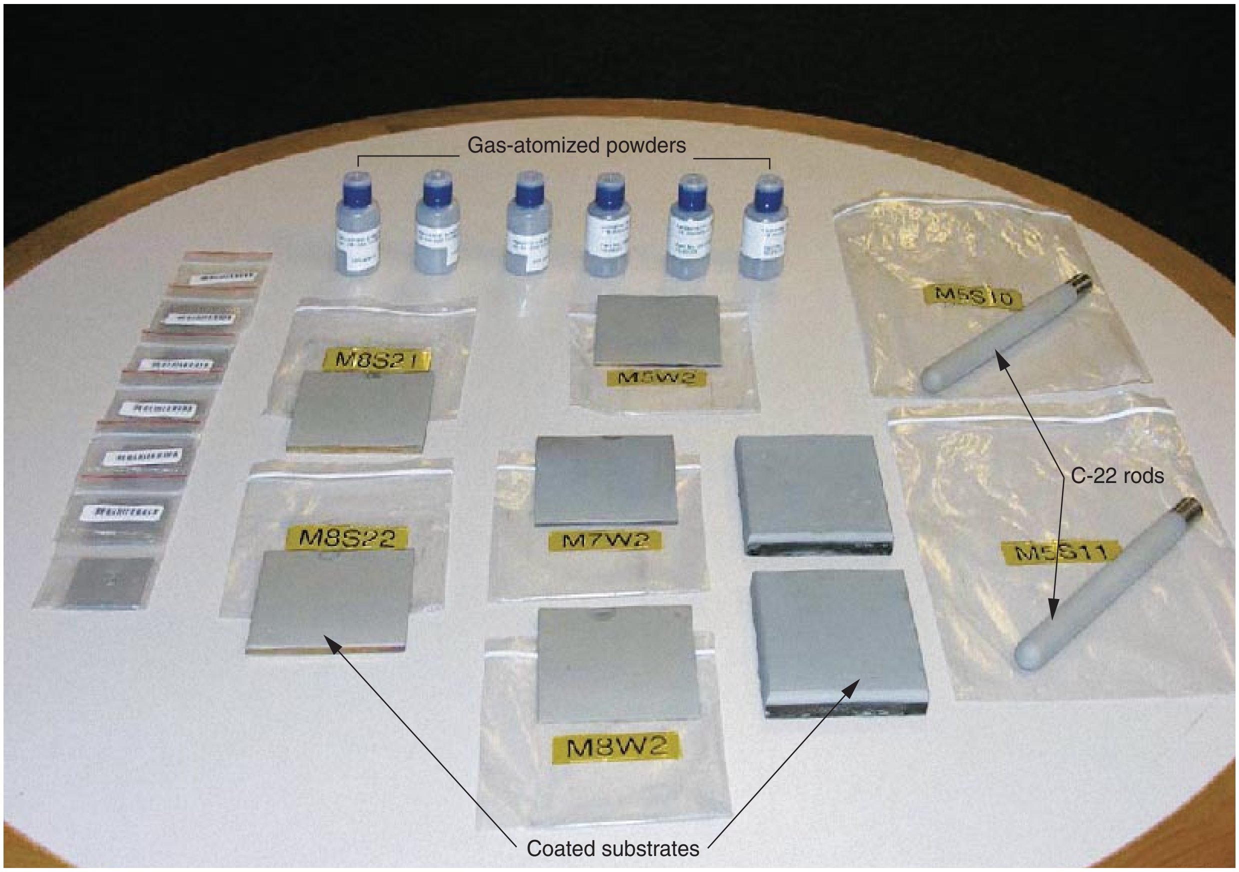
Meeting the Sponsors’ Needs

In the future, the high neutron absorption capability of alloys could be exploited for advanced reactor systems with complex geometries, such as the Laboratory’s Laser Inertial Fusion Energy engine. (See *S&TR*, April/May 2009, pp. 6–15.) Systems that can achieve a high burnup of fission fuels present particularly challenging problems because materials must withstand intense neutron bombardment over long periods. Much of the neutron damage affects the crystal lattice. One intriguing question is whether materials without lattices would be less prone to such damage. Perhaps future investigations will lead to even more resilient alloys for nuclear energy conversion applications.

The extreme hardness and abrasion resistance of iron-based amorphous alloys also makes them valuable for DOE’s tunnel-boring operations. In collaboration with Oak Ridge, the Colorado School of Mines, and Herrenknecht USA, the HPCRM team conducted several tunnel-boring experiments after applying the amorphous materials to disc cutters. “In laboratory tests at Colorado, the coating showed no signs of spalling even after more than 100 cuts on granite,” says Livermore scientist Frank Wong, who led



In salt-fog tests, a steel container coated with SAM2X5 (top) had remarkably better corrosion resistance than plates of uncoated carbon steel (bottom).



Test samples of the iron-based amorphous metals included powders, coated rods, and substrates.

the disc-cutter collaboration. "These tests marked the first time in 25 years of tunnel-boring research that a coating of any kind could survive rock impact."

Field experiments with a Herrenknecht tunnel-boring machine were equally impressive. The coatings survived under dynamic cutter loads that are typical of hard rock excavation. Compared with the measured wear on standard cutters, the amorphous alloy reduced wear on the discs by 15 to 20 percent for normal load-bearing operations and 10 to 28 percent for the severe loads of transition boring.

"Coatings were clearly visible on the crown of all the test cutters even after 14 meters of tunnel advance," says Wong, "and the coatings remained effective for up to 23 meters." In comparison, no other coating had previously survived more than 1 to 3 meters of tunnel advancement. By using the iron-based amorphous materials on essential components, DOE could potentially reduce the overall maintenance expense and extend the life of tunnel-boring equipment.

Because many applications of interest to DARPA involve ships, the Livermore team collaborated with colleagues at the Naval Research Laboratory. Prototype parts collected from various naval shipyards were refurbished and coated with the amorphous alloys for testing under realistic conditions. For example, submarine sail cover plates coated with the amorphous metal alloys were exposed for several months to the standard seawall testing at a naval facility in Key West, Florida, to determine how well the alloys performed in warm, wet, salty conditions with abundant sea life.

The Navy is particularly interested in improving antiskid surfaces on decks of littoral, or close-to-shore, combat ships. Exhaust from jet engines during takeoff can torch epoxy antiskid coatings on the upper decks. Lower decks are periodically flooded by seawater and exposed to heavy traffic from troops, tracked vehicles, and chains. "Our team learned to texture the coatings, just like the conventional epoxy coatings, to provide better traction in these mission-critical areas," says Farmer. Trials are still in progress, but testing thus far has been very successful.

The Department of Transportation is evaluating the metal alloys in coatings applied to rebar and other structural components to reinforce steel bridges. Annual maintenance and repair costs for bridges throughout the U.S. are estimated at billions of dollars. If new coatings could strengthen existing components and slow the progress of corrosion, bridge repairs could be safely scheduled less frequently, thus reducing the overall maintenance cost.

Branching Out

The HPCRM team is finding many potential applications for alloy-based coatings. For example, they could prevent wear on the bearings and shafts of wind turbines and improve the corrosion resistance of offshore drilling platforms and oil- and gas-transmission pipelines.

"Our work with these enhanced coatings is a good example of how the Laboratory can transition a mature program into other applicable areas," says Farmer. In addition, the HPCRM project shows how collaborations with industrial partners, other government agencies, and universities can speed development of advanced technologies. The new iron-based amorphous alloys are already proving to be a more effective means of protecting our national and military infrastructure and may soon offer more benefits for our technological future.

—Caryn Meissner

Key Words: amorphous metal alloy, corrosion resistance, criticality control, metallic glass, neutron absorption, thermal spray coating.

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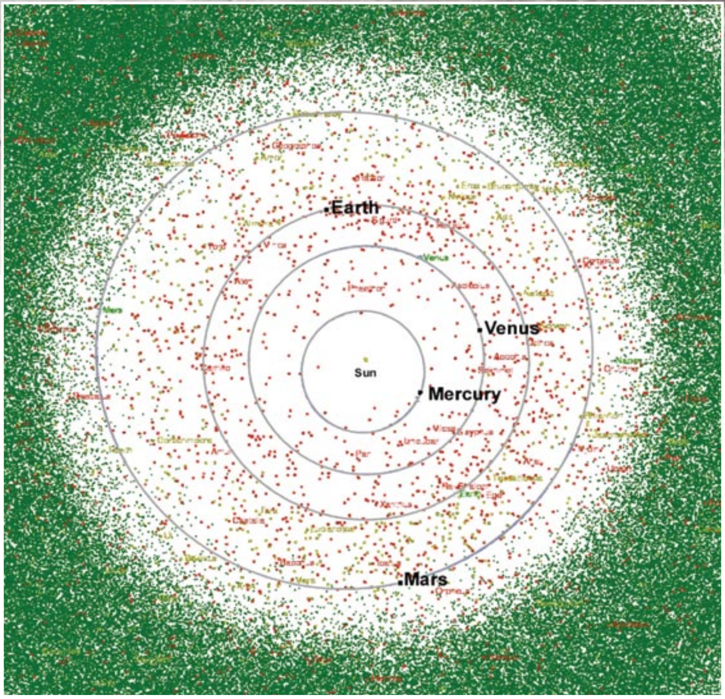
Potential applications for Livermore's alloy-based coatings include improving the corrosion resistance of materials used for oil- and gas-transmission pipelines.

Too Close for Comfort

Thousands of years ago, a 50-meter object traveling at several kilometers per second created the Barringer Crater near Winslow, Arizona. The crater is 1,200 meters in diameter and 170 meters deep.



Data from space surveys conducted in 2006 show the recorded near-Earth objects of various sizes that either cross (red) or are outside (green) Earth's orbit. (Courtesy of National Aeronautics and Space Administration/Jet Propulsion Laboratory.)

ASTEROIDS impacting Earth and causing mass devastation are a familiar topic in science fiction books and movies, but many people think such an event has little basis in reality. Scientists who study our solar system know better. For space-savvy professionals, this seemingly fantastical idea is not just fodder for entertainment purposes; it is a real concern. To prevent such a catastrophic event, scientists across the nation, including Livermore astrophysicist David Dearborn, are analyzing techniques to disrupt or divert asteroids on a collision course with Earth.

First discovered in the 1800s, asteroids—also known as minor planets—have become a hot topic in the last three decades, when space surveys began recording high concentrations of these celestial bodies in our solar system. As telescopes and other astronomical survey tools have become more precise, they have revealed that the number of asteroids within Earth's orbit is significantly greater than previously predicted. In addition, evidence of past impacts indicates that the collisions may have caused widespread devastation.

In 1998, the National Aeronautics and Space Administration (NASA) started the Spaceguard Near-Earth Object Survey to acquire data on objects that orbit close to the Sun. Survey data, such as those shown in the figure above right, allow researchers to estimate the potential danger of the many objects within Earth's orbit. The NASA program has primarily focused on identifying asteroids and comets that are larger than 1 kilometer in diameter.

"An object of this size would have approximately 1 billion tons of mass," says Dearborn, who works in the Laboratory's Science and Technology Principal Directorate. "If it traveled at 30 kilometers per second, it would have explosive power equivalent to 100 billion tons of TNT." In the event a 1-kilometer-size asteroid impacted Earth, the energy released would have global-scale effects.

Dearborn serves on a research panel, spearheaded by the National Academy of Sciences, tasked with evaluating methods to divert potentially hazardous objects—those that could hit Earth in the next 100 years. The panel is considering several diversion

This view of the 52-kilometer-long asteroid 243 Ida is a mosaic of five image frames acquired by the Galileo spacecraft on August 28, 1993. (Courtesy of National Aeronautics and Space Administration/Jet Propulsion Laboratory.)

technologies, but for Dearborn, nuclear explosives provide the best solution for dealing with catastrophic asteroids.

Dearborn has extensive experience in designing and testing nuclear and conventional explosives and leads the effort to model the impact of a nuclear explosion on an object's trajectory in space. Ultimately, Congress, the National Science Foundation, and NASA will use the information to determine the most effective strategy for deflecting asteroids.

Deflection or Fragmentation

Scientists use an asteroid's size, speed, kinetic energy, and orbit to determine whether it is potentially hazardous. An impact occurs when the orbits of an asteroid and Earth intersect and the two bodies reach the same point simultaneously. As the asteroid enters Earth's atmosphere and plummets toward the ground, it picks up speed, increasing its kinetic energy. The potential hazard depends on the asteroid's composition and size. "Small asteroids typically break apart in the atmosphere, burn up, and pose no real threat," says Dearborn.

However, in 1908, an asteroid 30 to 50 meters in diameter broke apart in the atmosphere, and the resulting airburst sent a shock wave to the ground, destroying 2,000 square kilometers of forest near the Tunguska River in Russia. "Because of the increased population density in many parts of the world," says Dearborn, "a similar impact today could affect several hundred thousand people." He adds that even more damage would occur if the object were to reach the ground intact.

Such an event can be avoided by nudging the asteroid off course or by fragmenting it. The action needed depends on the object's size and the time available before impact. According to Dearborn, nuclear explosives are the optimal method for diverting large asteroids or those that are too close to Earth—less than a decade away in time—to be deflected through other means. One benefit is that nuclear explosives are an established technology. "They are well tested and characterized," says Dearborn, "and the outputs and effects of explosions are well understood." In addition, nuclear explosives have a high energy-to-weight ratio, so they offer the lowest mass method for transporting energy to the asteroid.

To evaluate the effectiveness of different approaches, Dearborn and his colleagues used the Laboratory's multidimensional hydrodynamic codes to simulate three scenarios in which a nuclear explosive diverts an inhomogeneous, 1-kilometer-diameter structure. For each scenario, the team altered nuclear outputs, explosives energies, distances from the object, and the height or depth at which the explosion occurs.

In the first scenario, called the standoff approach, the nuclear explosive is detonated at a distance from the asteroid. The x rays, gamma rays, or neutrons produced by the explosion heat a hemispheric area of the asteroid. The energy applied to the body's surface vaporizes or obliterates the heated area, reducing the object's mass and giving it a "push." This push changes the asteroid's speed by a fraction of a centimeter to a few centimeters per second—just enough to prevent a collision.

The second scenario, also designed to reduce an asteroid's mass and push it slightly, involves detonating a low-yield explosive on its surface. The third scenario—a last resort—is for asteroids that are too close to Earth. In this approach, a nuclear explosive is detonated a few meters below the object's surface, fragmenting it.

Each simulation produced data on the deformation and speed change induced by the explosion and the resulting dispersion of material within space. By viewing these simulations, Dearborn and his colleagues can determine whether a nuclear explosive would have the desired result and whether the fragmented material would pose additional threats.

The simulated results indicate that in all three scenarios, the fragments created would be small and fast enough to avoid collisions with Earth. Future studies will vary the simulated object's shape, density, and porosity to determine how an asteroid's composition affects the outcome.

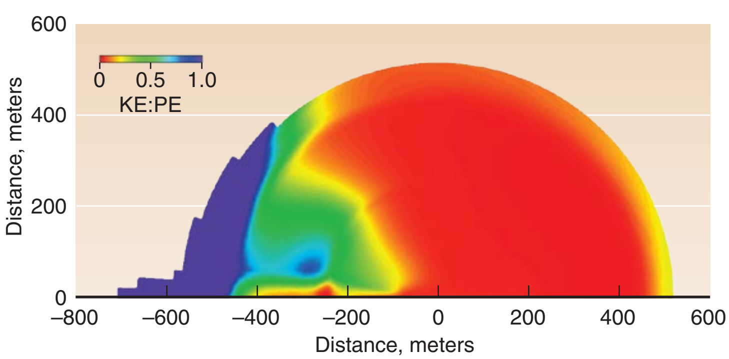
Exploring Options

Some potential deflection technologies are proving to be too expensive or too heavy to be feasible. Others would require too many technological advances to be implemented in the near future. One proposal is to attach rockets to an asteroid and push it out of its current orbit. This method would provide an adequate speed change and keep the bulk of the asteroid intact. However, asteroids have extremely low surface gravity, so attaching a rocket to one would be a logistical nightmare. "On a 1-kilometer asteroid, a 200-pound person would weigh less than one-fifth of an ounce," says Dearborn, "and a normal walking speed would be nearly two times escape velocity," that is, the speed needed to break free of the asteroid's gravitational field. Thus, the slightest pressure applied to the asteroid would push the rocket farther away, out of reach of the asteroid.

The rocket method could also be quite expensive. "Even if we ignore the challenges associated with anchoring a rocket engine to a rotating asteroid and with pushing an asymmetric object, a rocket would need thousands to millions of tons of fuel for successful diversion," says Dearborn. The closer the object is to Earth, the more fuel is required to produce the speed change needed. Deflecting an asteroid that is 20 to 30 years away would require about 10,000 tons of fuel. Significantly more fuel would be needed for objects less than a decade away.

NASA is evaluating impactor technology as a possible solution to diverting asteroids. These devices are designed to collide with the asteroid and change its momentum. "Tests during NASA's Deep Impact mission showed that impactors can divert smaller bodies, such as asteroids up to approximately 300 meters in size," says Dearborn.

Another diversion method is the gravity tractor. In this deflection scheme, the gravitational attraction between the asteroid and a spacecraft allows the spacecraft to move the asteroid off course over time, a process that could take years or even decades.



Simulation results show the effects of detonating a 1-kiloton nuclear explosive 150 meters above the surface of a 1-kilometer-diameter object. Colors indicate the ratio of kinetic energy (KE) to potential energy (PE) produced by the impact. The explosion obliterates the ejected debris (purple). In the bound areas (light blue to red), the object receives a "push," which changes its speed by a few centimeters per second.

According to Dearborn, this method may be advantageous for only about 5 percent of asteroids and would require major advances in technology before a spacecraft could carry out the mission successfully. Lasers have also been proposed, but even the most powerful lasers in existence would have to function over thousands of years to have any effect.

Methods that rely on elaborate launching stations or that add components to spacecraft could require putting an extra 20 tons of material into deep space. Conversely, nuclear explosives, with their high energy-to-weight ratio, would need comparatively less material to do the same job.

Dispelling Criticism

Not everyone shares Dearborn's enthusiasm and confidence in using nuclear explosives to deflect asteroids. Yet, in the face of skepticism, Dearborn remains resolute. "Part of my job is to respond to criticism and to dispel myths related to the use of nuclear explosives," he says. A common objection is that nuclear explosives will break the asteroid into large chunks and scatter debris all over Earth. Some critics are also concerned that radiation generated by the explosive will spread throughout the solar system and have undesirable effects. "This assumption is not true," says Dearborn. "Debris from the explosion would be spread over a solar system already full of cosmic rays. The solar wind would sweep the debris out of the solar system. If for some reason it did not, by the time the radiation was swept up by Earth, it would be a small amount compared to normal background levels."

Although there is some uncertainty in determining exactly when and where an asteroid could impact the planet, Dearborn notes that no asteroid currently being monitored poses an immediate threat. "But that doesn't mean we shouldn't have a deflection plan in place," he says. And nuclear explosives may prove to be the best technology for the job.

—Caryn Meissner

Key Words: asteroid, deflection, fragmentation, gravity tractor, impactor technology, Spaceguard Near-Earth Object Survey, nuclear explosive, space.

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Hyperion: A Titan of High-Performance Computing Systems

Hyperion is a large-scale test bed for high-performance computing technologies.

EVER bring home a new computer or software program only to find that it doesn't work as expected? Prerelease testing by the manufacturer can rarely evaluate all of the functions imagined by potential users. In performing full-scale operations, users often uncover hidden errors, or "bugs," that must be corrected in later upgrades.

Scientists working with high-performance computing (HPC) systems can empathize with that frustration. A fundamental challenge they face is establishing a testing phase rigorous enough to find the flaws in hardware or software designed for petaflops computing, where 1 petaflops is 1 quadrillion (10^{15}) floating-point operations per second.

To solve this problem, scientists in Livermore's Computation Directorate have teamed with 10 computing industry leaders to create Hyperion, the world's largest HPC test bed for developing, testing, and scaling Linux cluster technologies. A Linux cluster is a group of thousands of linked computers that together operate as a single, more powerful computing system. Each computer, or node, in the network uses the open-source Linux software as its operating system.

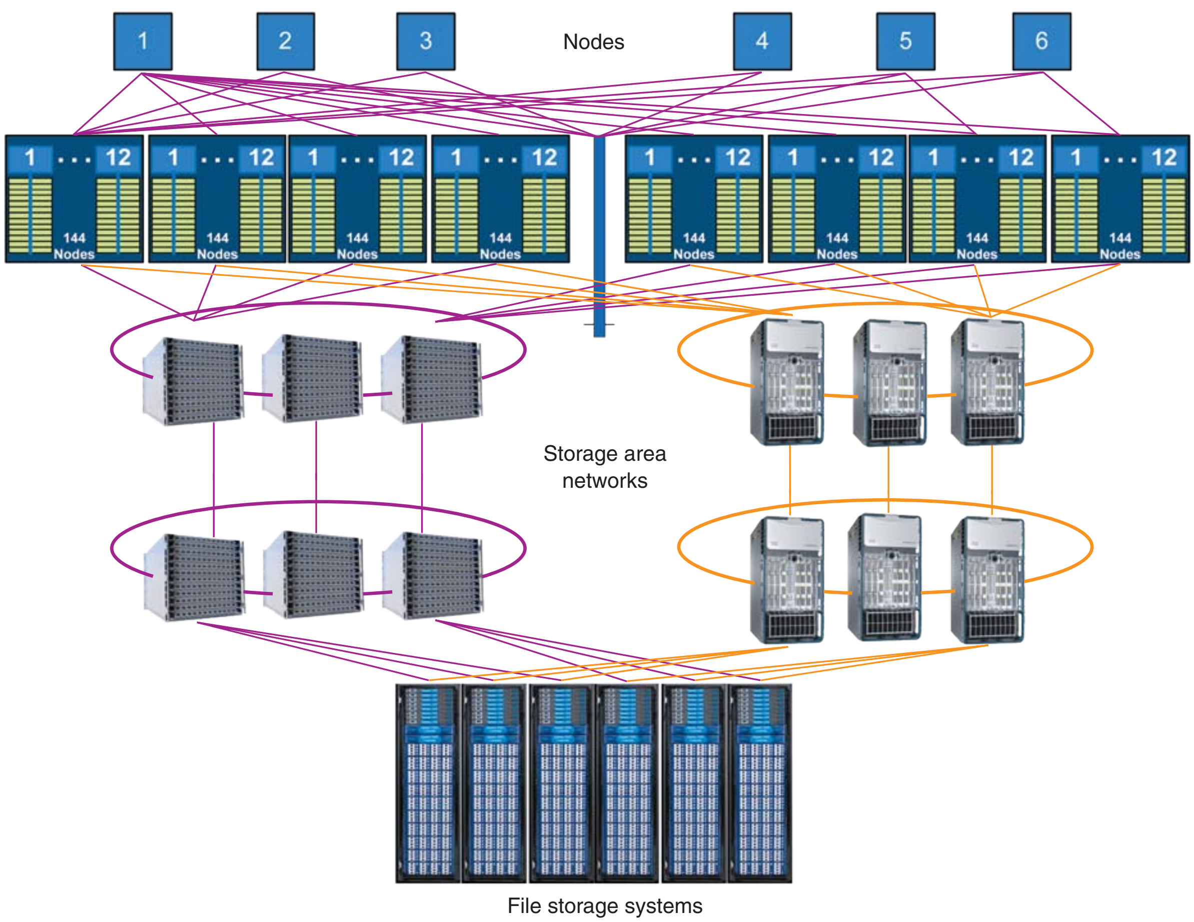
Mark Seager, who leads the Hyperion project at Livermore, is confident the large-scale test bed can find the bugs that often remain undiscovered on smaller testing systems. "Our slogan is, 'If you can make it, we will break it,'" says Seager. Hyperion provides an opportunity for the industrial partners to test their products in a realistic HPC environment, allowing them not only to improve new technologies but also to decrease the time it takes to bring those products to market. The collaboration also promotes long-term relationships between Laboratory researchers and the industrial partners, fostering continuity in HPC technology development.

Michael Dell, the chief executive officer of Dell, Inc., first announced the Hyperion project during his keynote speech at SC08, the annual International Conference for High Performance Computing, Networking, Storage, and Analysis. The National Nuclear Security Administration (NNSA) funds about half of the project as part of the Advanced Simulation and Computing (ASC) Program, which is a key component of NNSA's Stockpile Stewardship Program. The remainder is funded collectively by the 10 industrial partners: Dell, Inc.; Intel Corporation; Super Micro Computer, Inc.; QLogic Corporation; Cisco Systems, Inc.; Mellanox Technologies, Ltd.; DataDirect Networks, Inc.; LSI Corporation; Red Hat, Inc.; and Sun Microsystems, Inc.

The "Hype" in Hyperion

Installed at Livermore, Hyperion is available to the ASC tri-laboratory community—Lawrence Livermore, Los Alamos, and Sandia national laboratories—for developing the HPC technologies needed to maintain the nation's nuclear weapons stockpile without underground nuclear testing. Before deploying large-scale Linux clusters for ASC production applications, Hyperion team members run tests on sets of components as they scale up a new system. Tests are designed to evaluate operating systems, high-performance networking software, and the parallel file systems that distribute data across the servers. In addition, each industrial collaborator is allotted computing time in proportion to its funding contribution to run full-scale system tests of new products before they are released to market.

By rigorously testing a product at scale prior to release, companies can make improvements at the development stage, which is more cost-effective than fixing bugs after a product is deployed. This approach allows the computing industry to make



The Hyperion cluster architecture includes eight scalable units (1,152 nodes), two storage-area networks, and high-performance storage systems. Violet lines indicate InfiniBand network links, and orange lines indicate 10-gigabit Ethernet links.

petaflops technologies more affordable and thus accessible to commerce, industry, and private research and development.

Hyperion is also helping collaborators develop the storage systems and storage-area networks required for ASC's next-generation supercomputer. Called Sequoia, this 20-petaflops system will be delivered to Livermore in 2011. ASC Sequoia will run large suites of complex simulations, allowing scientists to build more accurate models of physical processes, such as those occurring as a nuclear weapon detonates, and to explore frontier science and breakthrough technologies.

Working with a full-scale test bed will establish a blueprint for future petascale computing platforms by helping researchers develop and test processors, memory, networks, storage systems, and visualization technologies. "Hyperion represents a new way to do business," says Seager. "Collectively, we are building a system none of us could have built individually."

One Project, Two Phases

The Hyperion cluster was installed at the Laboratory in two phases. "All of the collaborators were interested in working on the system in 2008," says Matt Leininger, deputy director for Advanced Technology Projects in the Computation Directorate. "However, we wanted some of the hardware to include the new Intel Nehalem processors, which wouldn't be available until early 2009. Splitting the project into two phases was a compromise between starting quickly and waiting for the faster processors."

The first phase, which consisted of 576 nodes, was installed in September 2008. With that cluster, researchers tested the Lustre parallel file system and TOSS, the Red Hat–based operating system that supports several Linux clusters developed by ASC. They also evaluated software used by other HPC researchers, such as the OpenMP message-passing interface and the OpenFabrics high-performance networking software.

In the second phase, which was completed in May 2009, Hyperion doubled in size to 1,152 nodes. The additional nodes incorporated the Nehalem processors and increased the on-node memory by 50 percent, from 8 to 12 gigabytes. As a result, Hyperion has more than 11 terabytes (trillion bytes) of memory—enough to store about 450 high-definition movies—and a peak processing capability of about 90 teraflops.

The Power of 10

Each of the 10 industry leaders plays a vital role in the Hyperion partnership. Dell, Intel, QLogic, Mellanox, and Super Micro Computer built the processors and nodes and helped integrate the input/output system. QLogic, Cisco Systems, and Mellanox built the InfiniBand and Ethernet network components. DataDirect Networks, Sun Microsystems, and LSI created the storage hardware, while Red Hat is responsible for Linux testing and various system administration duties.

The industrial partners collectively contributed about $5.5 million to the Hyperion project, and NNSA contributed approximately $5 million on behalf of Livermore. Fair market value for the system is estimated between $15 and $20 million—a good investment indeed. "We're sharing the cost between NNSA and collaborators to build a place where people can test their equipment, and they don't have to front the full bill for the system," says Lynn Kissel, who recently retired as deputy ASC program leader. "ASC, in some sense, is the glue that makes this partnership happen because we're providing an environment where competitors can share a resource."

In 2009, *Federal Computer Week* selected Seager as one of the Federal 100 top executives from government, industry, and academia who had the greatest impact on government information systems in the past year. Seager credits the collective effort of the Hyperion collaboration, which he says allows the partners to build a scalability test bed that none could afford to build alone.

A Bright Future for Hyperion

"The Hyperion project will advance the state of the art in a cost-effective manner," says Seager. "It offers benefits both to the end users, such as the national security laboratories, and to the computing industry, which can expand the market with proven, easy-to-deploy, large- and small-scale Linux clusters."

Hyperion will help fulfill NNSA goals to provide computing capabilities for national security and to meet the nation's challenges in energy, climate, and other enduring needs. It will also promote scientific discovery in basic science and enhance U.S. competitiveness in HPC. "The Hyperion collaboration will help ensure continuity in developing petascale Linux clusters and the storage technologies for future HPC systems," says Leininger. "As a result, this project will lead to a wide range of economically viable products."

—Kristen Light

Key Words: high-performance computing (HPC), Hyperion, Linux cluster, petascale system.

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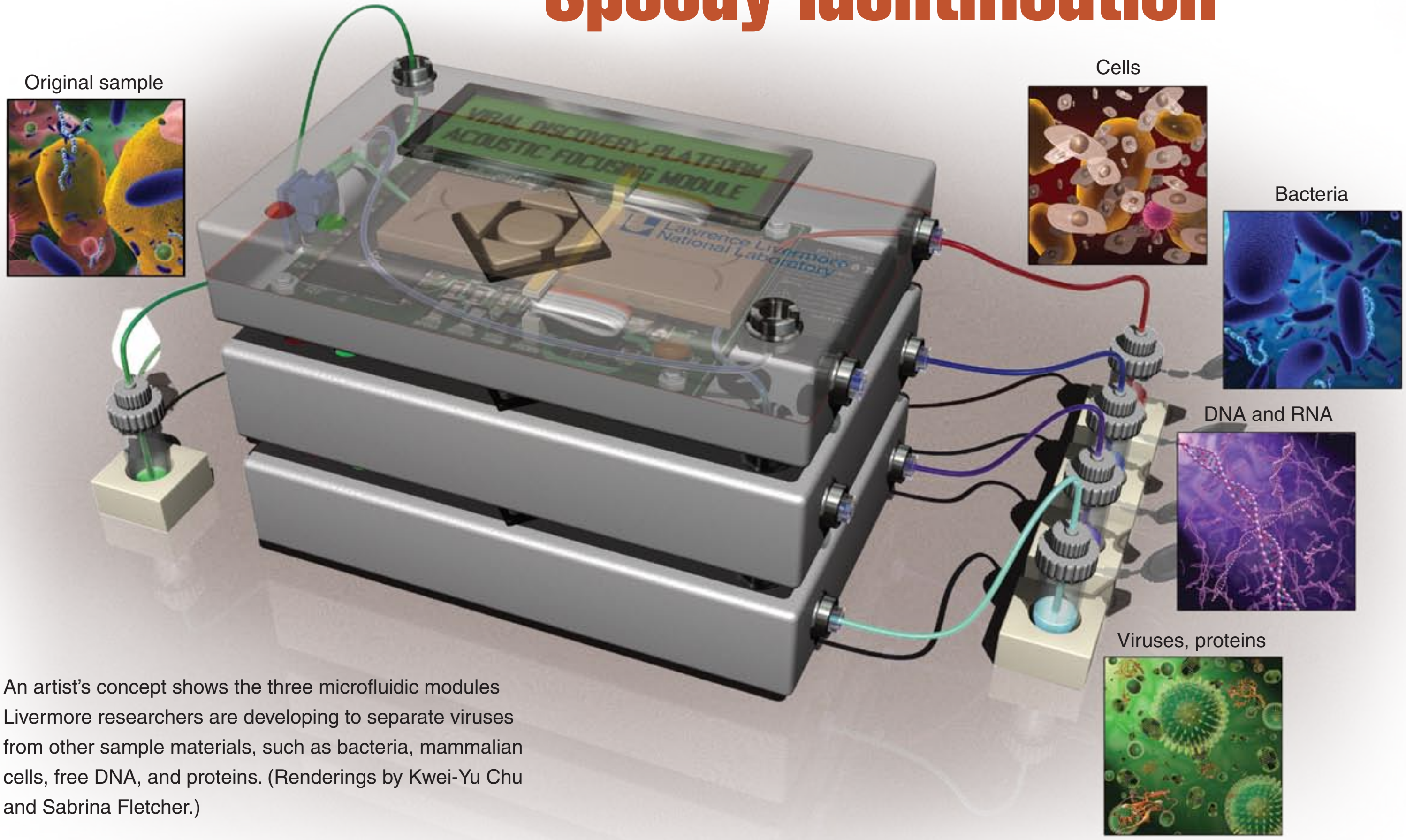
Isolating Pathogens for Speedy Identification



An artist's concept shows the three microfluidic modules Livermore researchers are developing to separate viruses from other sample materials, such as bacteria, mammalian cells, free DNA, and proteins. (Renderings by Kwei-Yu Chu and Sabrina Fletcher.)

QUICKLY identifying pathogens, especially viruses, can be crucial at the start of a disease outbreak such as H1N1 influenza, severe acute respiratory syndrome (SARS), or any of the many viruses that can initiate an epidemic. Rapid characterization could also speed the response following the deliberate release of a viral biological warfare agent.

However, distinguishing the components in a sample of blood, urine, or nasal mucus is a tedious and time-consuming process. The different materials—viruses, bacteria, mammalian cells, free DNA, and proteins—must be separated before they can be characterized, and the separation process requires the services of highly trained researchers or health-care workers.

A team of Livermore engineers and bioscientists is responding to the nation's critical need for a technology that quickly isolates viruses and other biological particles. The team's goal is to deliver a fully automated modular platform capable of accepting a diverse range of clinical and environmental samples, separating and "binning" the bioparticles, and removing background signals and contaminants that could distort the results.

The research project, led by mechanical engineer Klint Rose, is part of a Laboratory Directed Research and Development initiative led by Livermore scientist Chris Bailey to detect emerging viruses. "We want to identify existing pathogens and discover emerging ones quickly enough for public health officials to implement countermeasures such as quarantines and antibiotic prophylactic administration," says Rose, who works in the Laboratory's Science and Technology Principal Directorate.

The development effort focuses on introducing up to 1 milliliter of a raw sample into a device about the size of a hardcover book. Modules then separate the sample into components and concentrate the materials targeted for identification—all within 60 minutes. The Livermore separation method uses extremely small amounts of reagents such as saline and deionized water. Traditional methods require more expensive reagents and antibodies, and these technologies reduce the amount of virus available for analysis.

"Other techniques for separating bioparticles use beads that bind to specific types of cells, bacteria, and viruses," says Rose. "The beads must be extracted, and then the bacteria removed. We wanted a more generic approach that would separate all of the bioparticles in a sample, including the particles we have yet to identify. The most generic attribute we found was size." A typical sample contains a wide range of bioparticle sizes, from mammalian cells (which measure 2 micrometers in diameter and larger) to bacteria (0.5 to 2 micrometers in diameter), viruses (20 to 200 nanometers in diameter), and proteins (2 to 20 nanometers in diameter).

The Livermore instrument will use compact modules designed to accept various types of clinical samples, such as blood, urine, nasal washes, and dry and wet material trapped by environmental collectors. The team is focusing on nasal samples because a pandemic would likely start with a respiratory virus, and some virus particles would likely lodge in a patient's nostrils. Mucus is collected by flushing the nasal cavity with a wash, usually sterile saline. Samples contain cells, bacteria, viruses, loose genetic material, and proteins, representing a vast range of particle sizes.

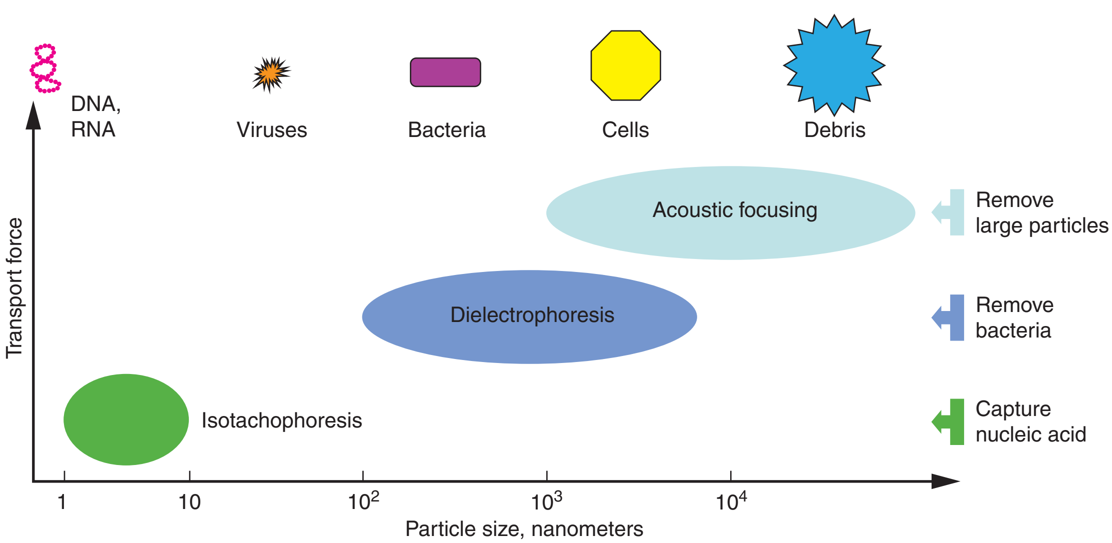
The sample preparation effort complements the work of two Livermore groups that are developing similar advanced modules for identifying purified virus fractions, or aliquots, using microarrays and a process called polymerase chain reaction (PCR). "Our modules will 'hand off' the cleaned-up sample to the analysis modules," says Rose. "We're in frequent contact with the other researchers to ensure that the different devices work well together." He notes that because PCR is based on amplifying DNA or RNA, the separation modules must remove all nonviral nucleic acids, including free-floating DNA and RNA, as well as cells and bacteria whose large genomes would complicate analyses.

Microfluidics Tap Subtle Forces

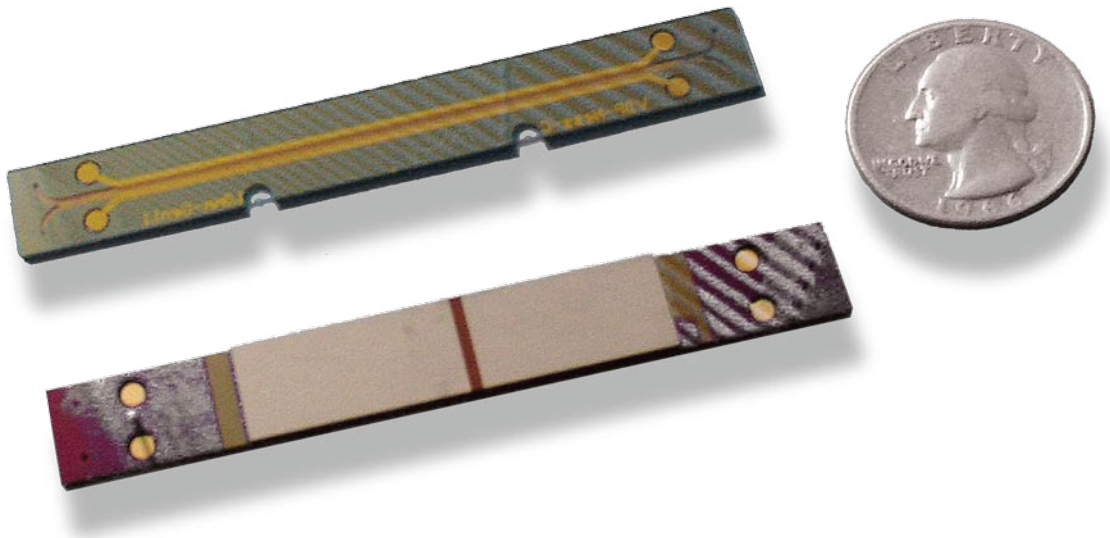
The development team is conducting its research at the Livermore Center for Micro- and Nanotechnology, which brings together researchers from diverse disciplines such as engineering, chemistry, biology, physics, materials science, and computer science. In addition, the team is collaborating with researchers from the University of California at San Francisco and Santa Barbara, San Diego State University, and Stanford University.

The modular separation technologies are based on microfluidics, a field aimed at manipulating particles suspended in extremely small volumes of liquid within microscopic channels. At the microscale, physical forces such as subtle electrical attractions and repulsions influence particle transport and component separation in ways that are not effective in larger-scale systems. For example, the weak electric forces of dielectrophoresis decay rapidly as a particle drifts more than a few micrometers away. Livermore researchers have been among the leaders in using microfluidic technologies to build experimental devices aimed at reducing costs, sample volumes, and time to complete a diagnostic test.

In the Laboratory's instrument, separation modules serve as "virtual filters" in which three microfluidic techniques—acoustic focusing, dielectrophoresis, and isotachophoresis—replace physical filters. The first two modules separate and concentrate a certain class of constituents according to size. Acoustic focusing extracts cells larger than 2 micrometers. Dielectrophoresis then removes bacteria and other particles small enough to pass through the acoustic separator. In the third module, isotachophoresis pulls out loose DNA and RNA molecules based on their electric charge



The Livermore device uses three microfluidic technologies to separate biomolecules. Acoustic focusing removes large particles, mainly mammalian cells. Dielectrophoresis isolates bacteria. Isotachophoresis then captures nucleic acids and separates them from virus particles.



In the acoustic focusing module, the vibration of sound waves pushes cells to the middle of an H-shaped channel (top), where they can be collected. Smaller components, including viruses, are then transferred to the next module. On the reverse side of the device (bottom), a piezoelectric transducer vibrates the channel walls as fluid flows through.

within the fluid. Once the viruses pass through the third filter, they are collected for analysis.

The microfluidic chips in the three modules are small, measuring about 5 centimeters by 2 centimeters by 1 millimeter thick, with channels 500 micrometers wide and 200 micrometers tall. Manufactured at Livermore from silicon and glass, they are relatively inexpensive and reusable. Together, they form a rugged, automated system.

Each module is built around a single microfluidic chip with an H-shaped channel geometry. With this geometry, samples can be injected at one end, fractionated, and then extracted at the other end. An automated system controls the chips' fluids and electronics. To optimize the module designs, the team ran simulations to determine how the different moving bioparticles respond to the subtle acoustic or electric forces.

Modules are connected so that as each one captures its designated class of bioparticle, it transfers the remaining sample to the next module. The first module uses acoustic waves to remove cells from the complex sample. A piezoelectric chip bonded to the back of the device generates acoustic forces that cause the channel walls to vibrate as fluid moves through. The acoustic waves push cells to the middle of the channel where they can be collected. Smaller constituents are then transferred to the second module, which uses dielectrophoresis.

The second module applies an electric field gradient to polarize particles and isolate them. In effect, the electric field pushes bacteria from the input stream to the recovery outlet, while permitting smaller bioparticles (DNA, RNA, viruses, and proteins) to pass through to the isotachophoresis stage.

In this third module, an electric field applied across specially designed electrolytes creates forces that focus, or pull, bioparticles into different zones depending on their electrophoretic mobility. In this way, DNA and RNA, which have a nearly uniform mobility for lengths greater than about 200 base pairs, can be separated from the viruses and proteins in the remaining sample.

The three-part separation process produces individual aliquots of cells, bacteria, DNA and RNA, and viruses. Although the team is focusing on viruses, other materials could just as easily be tapped for analysis.

Modular Process Improves Performance

In early tests, the Livermore modules recovered more than 80 percent of input viruses while removing more than 90 percent of the cells from the sample. These results compare favorably to more cumbersome bench-top techniques involving membrane filters or centrifugation, which recover about 50 percent of viruses and remove 99 percent of the cells. In addition, the modules can process samples ranging from 10 microliters to 1 milliliter at a rate of 10 to 100 microliters per minute, resulting in a total processing time of 10 minutes to about an hour. In contrast, current techniques can take several hours.

Over the next year, the team plans to integrate the three modules into a single device. Rose estimates that the Laboratory can transfer this technology to industry in about three years, where it could perform diagnostic tests more cheaply and quickly than is currently possible. The modular device could also be deployed on the front lines of biodefense, where aerosol environmental collectors search for evidence of biological warfare agents.

—Arnie Heller

Key Words: acoustic focusing, bacteria, Center for Micro- and Nanotechnology, dielectrophoresis, DNA, isotachophoresis, microfluidics, polymerase chain reaction (PCR), RNA, virus.

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The Laboratory in the News

Continued from p. 2

Superfund Cleanup Effort Steams to Record Time

Using a process initially developed with funding from Livermore's Laboratory Directed Research and Development Program, Southern California Edison has successfully cleaned up its Visalia Pole Yard. In September 2009, the Environmental Protection Agency removed the site from its National Priorities (Superfund) List. The Livermore-developed process combines dynamic underground stripping, which vaporizes contaminants, and hydrous pyrolysis/oxidation, which converts them to benign products such as carbon dioxide, chloride ions, and water. By introducing both heat and oxygen, the process effectively destroys all petroleum and solvent contaminants and cleans the groundwater to drinking water standards.

Southern California Edison had used the Visalia Pole Yard for 80 years to treat utility poles, dipping them in creosote or pentachlorophenol. By the 1970s, these toxic chemicals had seeped about 30 meters deep into the subsurface soil and groundwater. Research indicated that a permanent pump-and-treat operation would be required to prevent contaminated water from migrating off the 4-acre site.

After 20 years of pump-and-treat operations, Southern California Edison began using the faster process in 1997, working with SteamTech Environmental Services of Bakersfield, California, and consulting with Livermore scientists. Between June and August 1997, the team removed or destroyed about 135 metric tons of contaminants, a rate of about 22 metric tons per week—or 5,000 times the pump-and-treat removal rate. The new process shortened the cleanup time to 10 years, reduced costs from an estimated $100 million to $14 million, and showed that one of the most difficult types of Superfund sites can be cleaned and closed.

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Groundbreaking Science in Early Runs on Dawn

Initial research on Dawn, the newest high-performance computing system installed at Livermore, is generating exciting results. Dawn is an IBM Blue Gene/P system that can process 500 trillion floating-point operations per second. In the first few months of operation, it has demonstrated enhanced code performance and produced some of the largest, highest resolution simulations ever run in various scientific disciplines.

Researchers at Lawrence Livermore, Los Alamos, and Sandia national laboratories are using the system in their work for the National Nuclear Security Administration's Advanced Simulation and Computing Program. For example, a simulation showing how laser light scatters off plasma waves is helping researchers optimize target performance on the National Ignition Facility. Another study revealed the evolution of electron temperature as a high-energy beam heats a charged-particle plasma, providing insights into the plasma–beam interactions that might occur during a fusion fast-ignition experiment.

"The rapidly increasing performance of new supercomputers, such as Dawn, allows us to perform calculations unimaginable only a few years ago," says Denise Hinkel, who leads Livermore's Plasma Theory Group. "Today's supercomputers are the enabling technology for predictive laser–plasma interaction modeling, and recent large-scale simulations on Dawn are helping with focal-spot-size decisions for the National Ignition Facility beams and with ignition design optimization."

Contact: Mark Seager (925) 423-3141 (seager1@llnl.gov).

In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Lipid Bilayers on Nano-Templates

Aleksandr Noy, Alexander B. Artyukhin, Olgica Bakajin, Pieter Stoeve
U.S. Patent 7,569,850 B2
August 4, 2009
This method for fabricating a lipid bilayer on a nanotemplate includes steps for providing a nanotube or nanowire and forming a lipid bilayer around the polymer cushion. The lipid bilayer can include a protein pore, which can be designed to be sensitive to specific agents.

High Throughput Protein Production Screening

Peter T. Beernink, Matthew A. Coleman, Brent W. Segelke
U.S. Patent 7,585,815 B2
September 8, 2009
This cell-free approach uses polymerase chain reaction (PCR) and in vitro transcription (IVT) to produce proteins from prokaryotic or eukaryotic sequences, including human complementary DNA. It then applies fluorescence or immunoblot techniques to detect the proteins. Methods are designed to identify optimized PCR and IVT conditions, codon usages, and mutations. The methods are readily automated and can be used for high-throughput analysis of protein expression levels, interactions, and functional states.

Method for Ultrafast Optical Deflection Enabling Optical Recording via Serrated or Graded Light Illumination

John E. Heebner
U.S. Patent 7,587,103 B2
September 8, 2009
This method applies an optical control signal to a mask to deflect an optical input signal propagating through a waveguide. The deflected signal is then detected in parallel on an array of detectors. A beam-deflecting structure with at least one waveguiding layer and at least one masking layer can be used to modify the signal characteristics. Another approach is to propagate pulsed laser light toward an attenuating mask so that the mask pattern is applied to the waveguide, changing the material properties of at least part of the waveguide.

Biobriefcase Aerosol Collector

Perry M. Bell, Allen T. Christian, Christopher G. Bailey, Ladona Willis, Donald A. Masquelier, Shanavaz L. Nasarabadi
U.S. Patent 7,591,197 B2
September 22, 2009
This system collects air samples and analyzes the entrained particles to determine if potential bioagents are present. A collector directs air samples toward a liquid receiving surface designed to capture entrained particles. The surface tension of the receiving liquid and the velocity at which the sample impacts this surface are such that the liquid captures the particles. This impact causes minor turbulence on the surface, resulting in an insignificant level of liquid evaporation.

Shape Memory System with Integrated Actuation Using Embedded Particles

Patrick R. Buckley, Duncan J. Maitland
U.S. Patent 7,591,834 B2
September 22, 2009
This shape memory material uses embedded particles to integrate actuation. One design provides an apparatus with magnetic pieces included in the body of a shape memory material. Another method actuates a device to perform an activity on a subject. The device will position a shape memory material in a desired position with regard to the subject. It will also form the material into a specific primary shape and reform it into a secondary stable shape. The device then uses pieces embedded in the material to actuate the material, causing it to recover the specific primary shape and perform the desired activity.

Awards

Computer scientist **Panayot Vassilevski** received a **Fulbright Scholarship** to teach a graduate-level course in computational mathematics at the St. Kliment Ohridski University in Sofia, Bulgaria, where he received a Ph.D. in mathematics in 1984. The course is based on Vassilevski's book, *Multilevel Block Factorization Pre-conditioners*, which describes matrix-based analysis and algorithms for solving finite-element equations. Vassilevski works in Livermore's Center for Applied Scientific Computing, where he pursues his research interests in numerical linear algebra and finite-element methods at large—computational methods that are central to the Laboratory's mission-related research in areas such as stockpile stewardship and global climate modeling.

Edward Moses, principal associate director for the Laboratory's National Ignition Facility (NIF) and Photon Sciences, received the **2009 Edward Teller Medal** from the **American Nuclear Society** for his leadership in developing and completing the 192-beam laser. The Edward Teller Medal recognizes pioneering research and leadership in inertial fusion sciences and applications. It is named in honor of the late Edward Teller, director emeritus of Lawrence Livermore and a pioneer in inertial fusion sciences.

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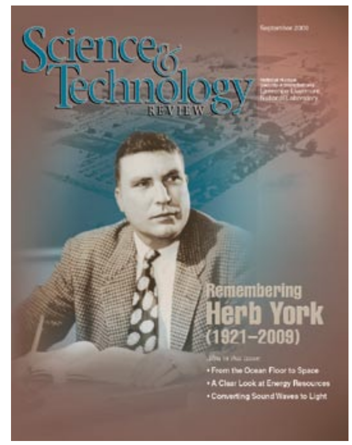

October/November 2009

December 2009

Abstract

A Defensive “Coat” for Materials under Attack

Partnering with other government laboratories, universities, and manufacturers in private industry, Livermore scientists have developed two iron-based amorphous metal alloys that can be applied as thermal spray coatings to protect materials in harsh environments. The new alloys, SAM2X5 and SAM1651, are harder and more wear resistant than stainless steels and nickel-based alloys. In addition, their corrosion resistance and neutron absorption capabilities are equal to or higher than those of alloy C-22, the crystalline, nickel-based material designed to reinforce containers for the long-term storage of nuclear waste. Yet, the amorphous alloys are substantially less expensive to manufacture than alloy C-22. Developed to protect spent nuclear fuel containers in underground respositories and ships exposed to saltwater and abrasive sand, the new alloys might also extend the life of wind turbine components, offshore drilling platforms, and oil- and gas-transmission pipelines.

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New Materials Enhance Detectors

The Laboratory, along with many partners, is developing more effective materials for use in radiation detection devices.

Also in January/February

• A Livermore-developed device can simultaneously distinguish up to five blood pathogens in minutes.

• Computer scientists are strengthening their ability to promptly identify malicious attacks on large computing networks.

• A Livermore–University of California team is modeling a new radiation detection scheme for identifying nuclear materials concealed inside cargo containers.

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