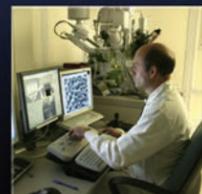


# CHEMISTRY AND MATERIALS SCIENCE DIRECTORATE

CHEMISTRY AND MATERIALS SCIENCE DIRECTORATE



# 2005

## ANNUAL REPORT

Lawrence Livermore National Laboratory

*About the Cover*

One of Livermore's emerging missions is to provide the nation with scientific capabilities for defense against biological threats and natural disease outbreaks. Our scientists apply expertise in materials and analytical methods to develop platforms for chemical and bioagent detection.

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A MESSAGE FROM

Associate Director

# Tomás Díaz de la Rubia



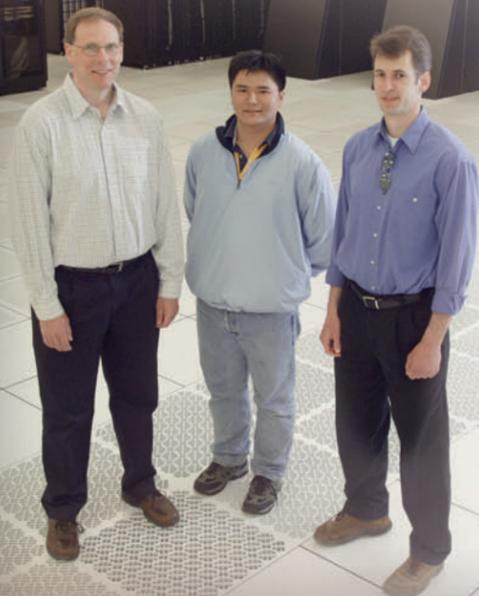
In 1952, we began laboratory operations in the barracks building of the Naval Air Station with approximately 50 employees. Today, the Chemistry and Materials Science (CMS) Directorate is a major organization at the Lawrence Livermore National Laboratory with more than 500 employees who continue to contribute to our evolving national-security mission.

For more than half a century, the mission of the Laboratory revolved primarily around nuclear deterrence and associated defense technologies. Today, Livermore supports a broad-based national-security mission, and our specialized capabilities increasingly support emerging missions in human health and energy security.

In the future, CMS will play a significantly expanded role in science and technology at the intersection of national security, energy and environment, and health. Our world-class workforce will provide the science and technology base for radically innovative materials to our programs and sponsors.

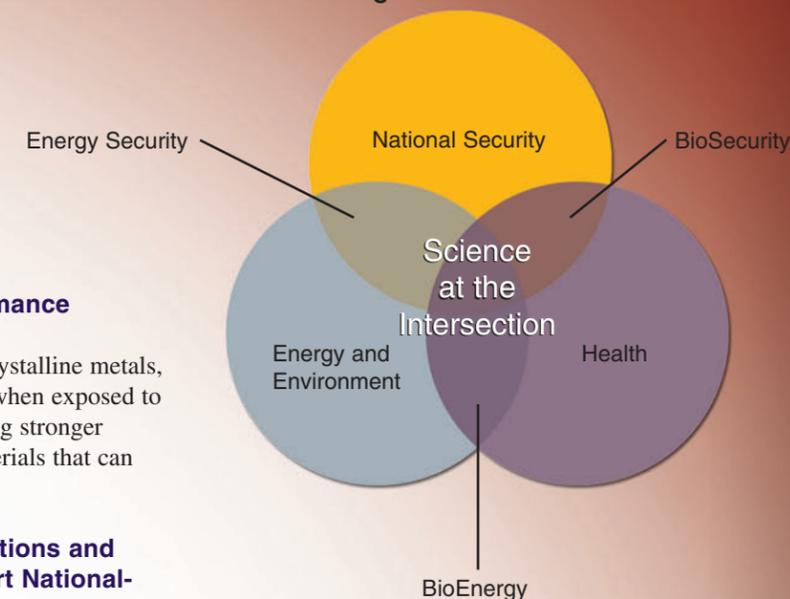
Our 2005 Annual Report describes how our successes and breakthroughs follow a path set forward by our strategic plan and four organizing research themes, each with key scientific accomplishments by our staff and collaborators.

Organized into two major sections—*research themes* and *dynamic teams*, this report focuses on achievements arising from earlier investments that address future challenges. The research presented in this annual report gives substantive examples of how we are proceeding in each of these four theme areas and how they are aligned with our national-security mission.



## CMS Directorate

Strategic vision for 2025



### Research Themes

#### Materials Properties and Performance under Extreme Conditions

We are developing ultrahard nanocrystalline metals, exploring the properties of nanotubes when exposed to very high temperatures, and engineering stronger materials to meet future needs for materials that can withstand extreme conditions.

#### Chemistry under Extreme Conditions and Chemical Engineering to Support National-Security Programs

Our recent discovery of a new source of coherent light adds a new tool to an array of methods we use to more fully understand the properties of materials. Insights into the early stages of polymer crystallization may lead to new materials for our national-security mission and private industry.

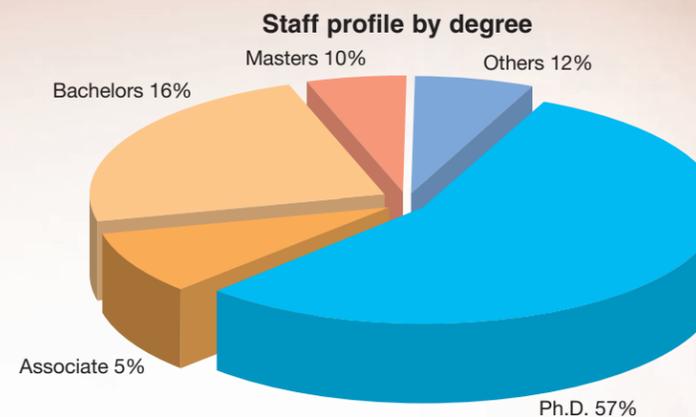
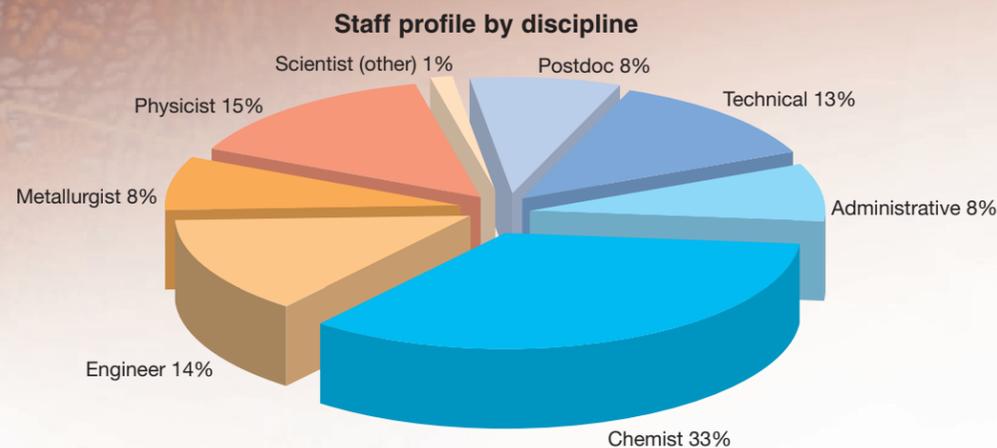
#### Science Supporting National Objectives at the Intersection of Chemistry, Materials Science, and Biology

We are improving drug binding for cancer treatment through the use of new tools that are helping us characterize protein-antibody interactions. By probing proteins and nucleic acids, we may gain an understanding of Alzheimer's, Mad Cow, and other neurodegenerative diseases.

#### Applied Nuclear Science for Human Health and National Security

Our work with cyanobacteria is leading to a fuller understanding of how these microorganisms affect the global carbon cycle. We are also developing new ways to reduce nuclear threats with better radiation detectors.





### Dynamic Teams

The dynamic teams section illustrates the directorate's organizational structure that supports a team environment across disciplinary and institutional boundaries. Our three divisions maintain a close relationship with Laboratory programs, working with directorate and program leaders to ensure an effective response to programmatic needs. CMS's divisions are responsible for line management and leadership, and together, provide us with the flexibility and agility to respond to change and meet program milestones.

- Materials Science and Technology Division
- Chemistry and Chemical Engineering Division
- Chemical Biology and Nuclear Science Division

By maintaining an organizational structure that offers an environment of collaborative problem-solving opportunities, we are able to nurture the discoveries and breakthroughs required for future successes.

The dynamic teams section also presents the work of CMS's postdoctoral fellows, who bring to the Laboratory many of the most recent advances taking place in academic departments and provide a research stimulus to established research teams. Postdoctoral fellows are selected for their scientific expertise, capability, and enthusiasm for working in a highly productive environment that places a premium on scientific innovation.

The staff members who make the science happen at Lawrence Livermore continue to receive recognition for their accomplishments from their peers through awards, honors, and fellowships from respected scientific societies.

### Financial and Operational Information

CMS is fully committed to the simultaneous excellence in both science and operations. Most of our \$91-million budget in 2005 was designated for mission-related research and development activities while maintaining a high standard of operational excellence in safety and security.

Our strategic investments are leading to groundbreaking technological advances, benefiting both our national-security mission and the scientific

community in general. In addition to internal Livermore programs directed by the National Nuclear Security Administration (NNSA), we have a growing portfolio of work funded by the Department of Energy, the DOE Office of Science, and industrial partners.

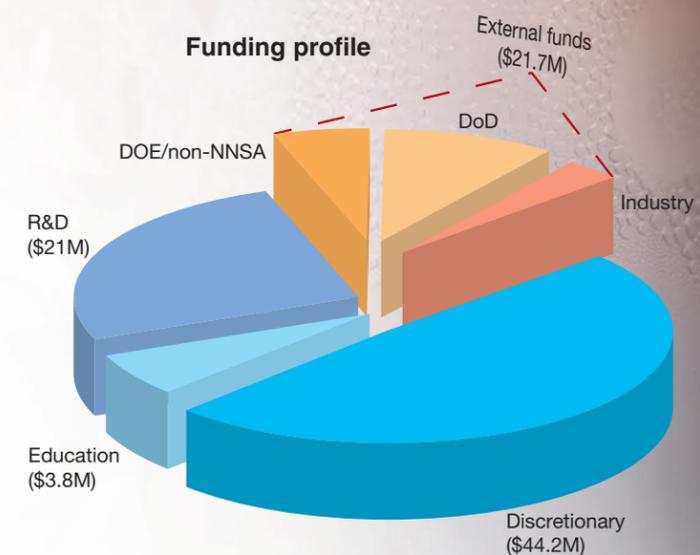
### Looking Forward

We have good reasons to be optimistic as 2006 unfolds and the Laboratory assumes increasing responsibilities in new programs ranging from homeland security and threat reduction, to transformation of the nuclear stockpile. CMS maintains an unambiguous role as both a partner and a technology leader for these responsibilities. More confident and committed than ever, we look forward to expanding frontiers of science and continuing our legacy of partnership with the Laboratory and the worldwide scientific community, as we apply science and technology to the important challenges of our time.

Sincerely,

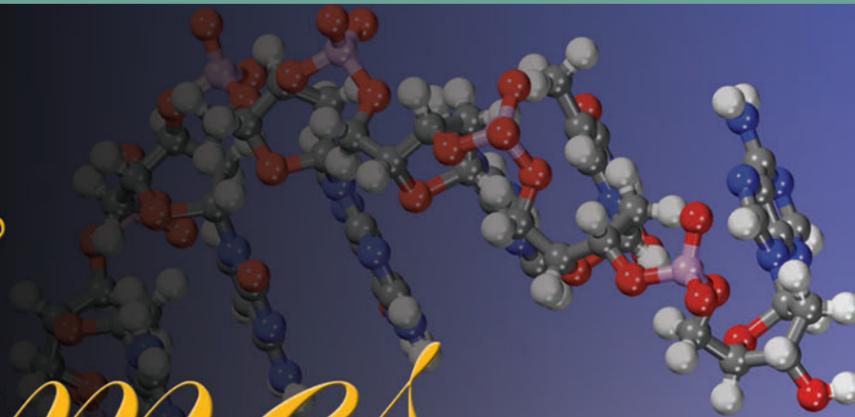
Tomás Díaz de la Rubia  
Associate Director, Chemistry and Materials Science

### Funding profile



# CHEMISTRY AND MATERIALS SCIENCE

# Research Themes



*The Research Themes section of our annual report gives substantive examples of our successes and breakthroughs, following a path set forward by our strategic plan and four organizing research themes. These four theme areas are closely aligned with our national-security mission. The key scientific accomplishments by our staff and collaborators focus on achievements arising from earlier investments while addressing future challenges.*

## ● **Materials Properties and Performance under Extreme Conditions**

Our emerging ability to control matter on the nanometer scale is leading to many entirely new types of novel materials that will find many national-security applications.

## ● **Chemistry under Extreme Conditions and Chemical Engineering to Support National-Security Programs**

Taking advantage of the immense computing resources at Lawrence Livermore, our scientists have unique tools to study extreme phenomena of matter at the atomic scale.

## ● **Science Supporting National Objectives at the Intersection of Chemistry, Materials Science, and Biology**

Many applications in nano- and biotechnology readily build on our unique mixture of disciplines. We are conducting research that will enable new technologies and tools to combat chemical and biological terrorism and enhance fundamental human-health research.

## ● **Applied Nuclear Science for Human Health and National Security**

Our nuclear science and isotopic techniques are proving critically important in defining and solving national and international problems related to the environment and global security.

# Ultrahard Nanocrystalline Metals

The strength or hardness of a metal depends on the properties of the constituent crystallites—known as grains—that compose it. By reducing the grain size of a metal to the nanometer scale, we can produce nanostructured materials that are much harder than their coarse grain counterparts. This characteristic provides opportunities for developing new materials for applications ranging from protection shields for spacecrafts and military vehicles to millimeter-sized targets for inertial confinement fusion experiments.

However, this strengthening characteristic is limited by mechanisms occurring at grain boundaries. One effect is that, as the dimension of the grains is reduced, they begin to slide over each other—a softening mechanism that imposes a limit to the maximum strength the material can have.

Combining terascale atomistic simulations and novel shock-loading experiments on nanocrystalline metals, our team has uncovered new deformation mechanisms and new approaches to optimize high-strength materials. Results on nanocrystalline nickel and copper showed that, by applying shock waves traveling faster than the speed of sound, the softening effects do not occur and can

be controlled by both high strain rate and high pressure.

## Relevance to CMS Research Themes

Many Laboratory missions, including stockpile stewardship, require an understanding of how metals respond to shock waves and subsequent high-strain-rate deformations. To assess the behavior under these conditions, it is important to study the origin of deformation and strength, and how defects within a crystal structure (known as dislocations) affect the properties of materials.

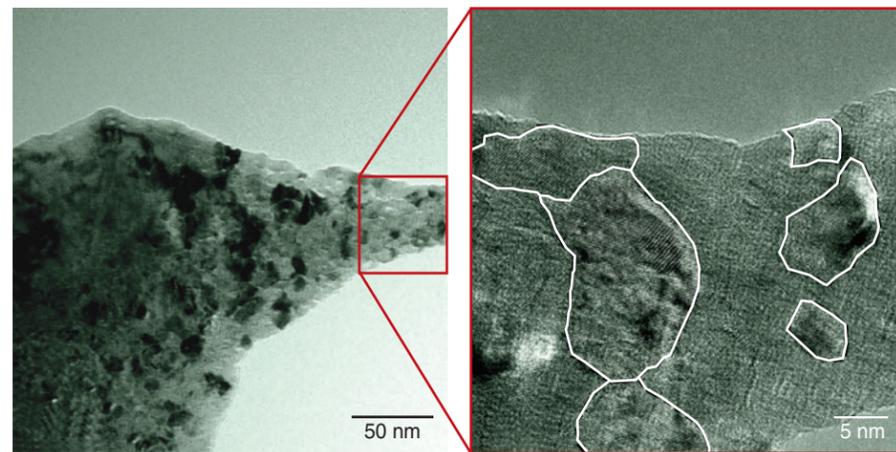
Measuring the dynamic deformation process during high-strain-rate loading at the nanoscale is difficult using experimental methods alone. However, by combining simulations with experiments, we can use our improved understanding of these processes to build numerical models that accurately predict the material's response under various temperatures and pressures over time. The information we glean will also bring us closer to the development of new materials with superior strength.

## Major Accomplishments in 2005

We carried out the largest atomistic simulations of shocked nanocrystalline

samples of nickel and copper to date, employing up to 4000 processors on Livermore's supercomputers. Shock waves move faster than the speed of sound and generate pressures nearly one million times larger than atmospheric pressure. The extremely short compression timescales (or very high strain rates) imply that dislocation formation and movement are the dominant plasticity mechanisms involved. Our simulations show that a large increase in pressure significantly reduces grain-boundary sliding, limiting the softening mechanism and doubling the flow stress.

In addition to the simulations, we also performed the first shock experiments on nanocrystalline metals at the same scale of our simulations. Because of experimental constraints, it is extremely difficult to directly measure the dynamic deformation process during high-strain-rate loading at the nanoscale. Using the Livermore JANUS laser, we shocked and recovered nickel samples, which were later studied with a transmission electron microscope (TEM) as shown in Figure 1. We observed clear experimental evidence of dislocation activity occurring inside grains, in agreement with our atomistic simulations. During loading at 50 GPa, our molecular

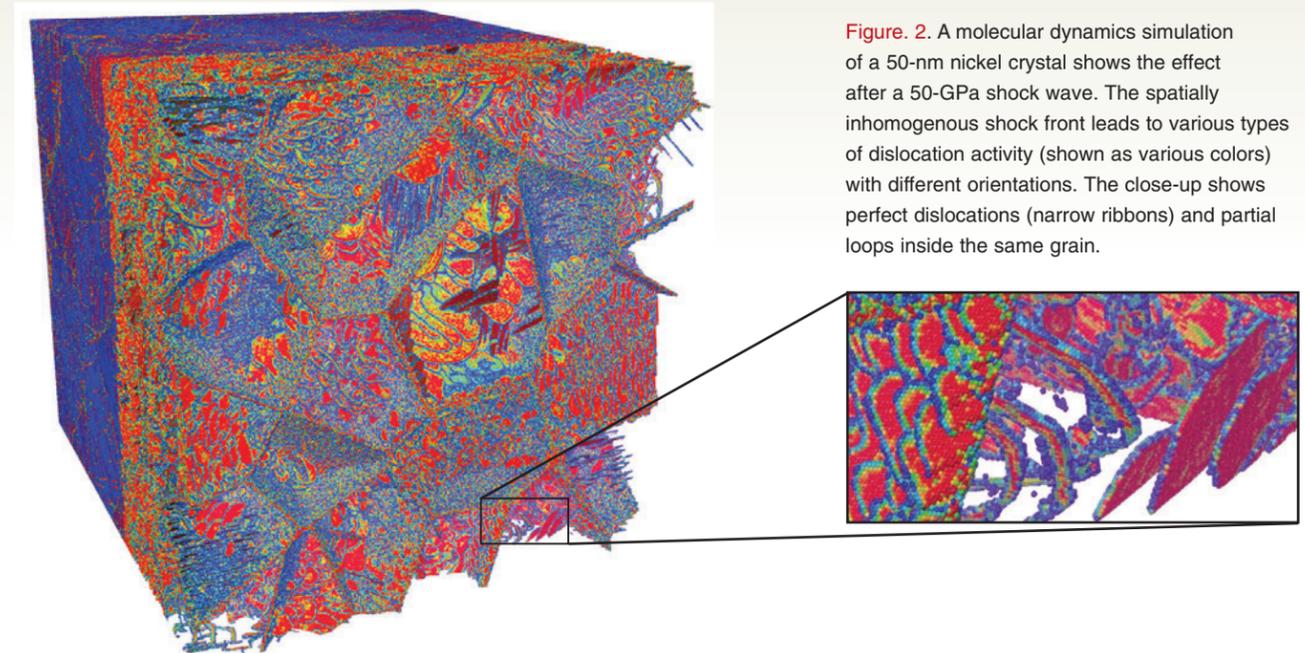


**Figure 1.** A transmission electron microscope image of a nickel sample with grains measuring 30–50 nm shows that the nanostructure remains intact after a shock pressure of 40 GPa. After the shock, some grains grow up to 300 nm, while others decrease in size (as in the grains marked by white lines in the right panel).

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**Figure 2.** A molecular dynamics simulation of a 50-nm nickel crystal shows the effect after a 50-GPa shock wave. The spatially inhomogeneous shock front leads to various types of dislocation activity (shown as various colors) with different orientations. The close-up shows perfect dislocations (narrow ribbons) and partial loops inside the same grain.

dynamics simulations predict a dislocation density of approximately  $10^{13}/\text{cm}^2$ .

Although the exact dislocation density in recovered samples is difficult to estimate, our high-resolution TEM images showed residual dislocations inside some nanograins. This is quite unusual in nanocrystalline materials and not typically achievable under normal deformation conditions. Our experiments also indicate an increase in hardness in the samples recovered after shock loading, as expected from the measured residual dislocation densities. By turning off the mechanism that softens the grains, we create a material that is harder during and following the shock-wave application.

## Scientific Impact

Connecting atomistic models with shock experiments performed on nanocrystalline metals advances our understanding of how extreme pressure affects the behavior of metallic materials

at the nanoscale. Specifically, our experiments on nickel confirm simulation results indicating that, at extremely short compression timescales, the dominant plasticity mechanisms are dislocation formation and movement (Figure 2). Our studies demonstrate that shock waves can be used to turn off the grain-boundary sliding that softens the metal, creating a much harder material. They also provide new insights that can be applied toward the construction of new computational models to better understand crystal plasticity.

## Related Publications

E. M. Bringa et al., "Wave Propagation in Polycrystals," *J. Met.* **57**, 67–70 (2005).

E. M. Bringa et al., "Ultra-Hard Nanocrystalline Metals by Shock Loading," *Science* **309**, 1838 (2005).

Y. W. Yang, E. M. Bringa, et al., "Deforming Nanocrystalline Nickel at Ultrahigh Strain Rates," *Appl. Phys. Lett.* **88**, 061917 (2006).

## NEW FRONTIERS

Studies on the behavior of metallic nanocrystals subjected to extreme conditions have helped us identify the mechanisms of shock-induced plasticity when grain-boundary effects cannot be neglected. Although our simulations and experiments were conducted on nanocrystalline copper and nickel, grain-boundary sliding under pressure should be a general feature of shock-loaded materials, including alloy and nonmetallic nanocrystals. Our findings could provide valuable information for the design of harder nanocrystalline materials for applications such as National Ignition Facility targets, spacecraft shielding, fusion energy production, and safer automobile frames.

# Manipulating Individual Nanotubes under Extreme Conditions



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Carbon nanotubes are cylindrical carbon molecules with unique properties that make them potentially useful for devices such as cell phones, computers, and personal handheld electronics. Nanotubes, measuring about one-thousandth of the diameter of a human hair, cannot be seen with the naked eye, yet they are one of the strongest known materials. In fact, their size is so small that their material properties have only been explored in bundles. This led to inaccuracy and misinterpretation of experimental data, preventing large-scale integration of carbon nanotubes into electronic devices.

Our research has focused on improving fundamental understanding of the structural, mechanical, and electrical transport behavior of these nanomaterials under various conditions. To accomplish this, we developed novel experimental tools to identify, manipulate, and measure the

properties of these nanomaterials while stretching them under extreme heat. Although we expected to confirm that carbon nanotubes are rigid materials, our data indicate that they show superplastic behavior at very high temperatures.

## Relevance to CMS Research Themes

Nanoscale materials possess many technologically useful properties. Carbon nanotubes, in particular, are broadly targeted for applications relevant to national security and defense, such as in biosensing and radiation-detection applications. Hence, the physical properties of these nanotubes under extreme conditions are of great relevance to fundamental science and also to essential missions of LLNL. Some of the projects that will benefit from our study include carbon nanotube lipid bilayer membranes for pathogen detection and carbon nanotube mixture explosives for photographic ignition of targets.

## Major Accomplishments in 2005

Despite more than a decade of studies, the manipulation of individual carbon nanotubes and the accurate determination of their electrical and mechanical properties remain grand challenges. To solve this problem, we have developed, in collaboration with Boston College, a manipulator that employs a piezoelectric device to precisely stretch the nanotube (Figure 1). We have also developed a resistance-heating method to heat individual nanotubes or nanowires to extremely high temperatures while stretching them. This allows us to investigate the mechanical and electrical transport behavior of these nanostructured materials under previously inaccessible conditions.

Using this new setup, we observed the stretched nanotubes at atomic resolution using a transmission electron microscope equipped with an in situ digital camera.

We investigated the mechanical properties and electrical conductance of a number of single-, double-, and multiwalled carbon nanotubes. Single-walled nanotubes are composed of a one-atom-thick layer of carbon formed into a cylinder. Double- and multiwalled nanotubes have two or more layers of carbon atoms.

Contrary to the belief that carbon nanotubes are rigid when stretched at room temperature, we discovered a superplastic behavior in all three types of nanotubes while they are deformed at temperatures over several thousand degrees Fahrenheit. We believe that nanotube plasticity is mediated by a new physical mechanism, called *kink nucleation*, and motion inside nanotube walls. Because of drastic dimensional changes during elongation of carbon nanotubes (Figure 2), we further observed a large adjustable

semiconducting band gap in carbon nanotubes. This allows us to tune the electronic properties of individual carbon nanotubes by straining, thereby providing a new route to investigate the fundamental electromechanical behavior of carbon nanotubes.

## Scientific Impact

Carbon nanotubes were previously thought to be a class of rigid materials that could not sustain stretch under normal conditions. Our discovery of superplastic behavior in carbon nanotubes at high temperatures opens the door for their potential application as strengthening agents in ceramics, high-temperature alloys, and nanocomposites that are subjected to extreme loading or heating conditions. The super-strain property we discovered can be employed to tune the electrical

properties of carbon nanotubes for insulating, semiconducting, metallic, or even superconducting applications. The physical properties observed at high temperatures also provide a foundation for a worldwide computational endeavor to understand the unique and versatile properties of carbon nanotubes.

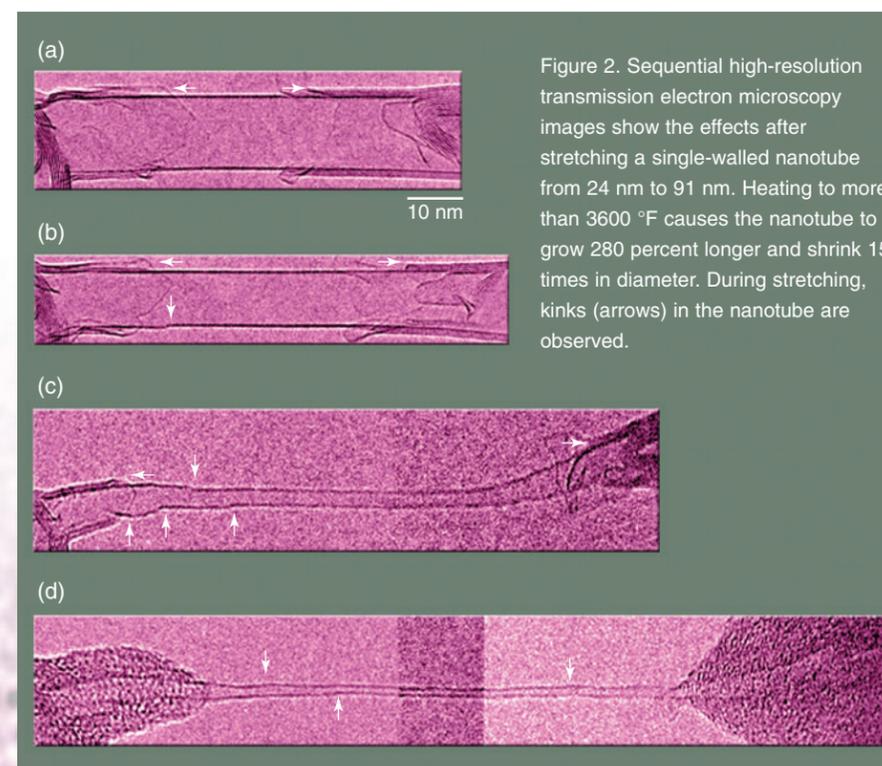
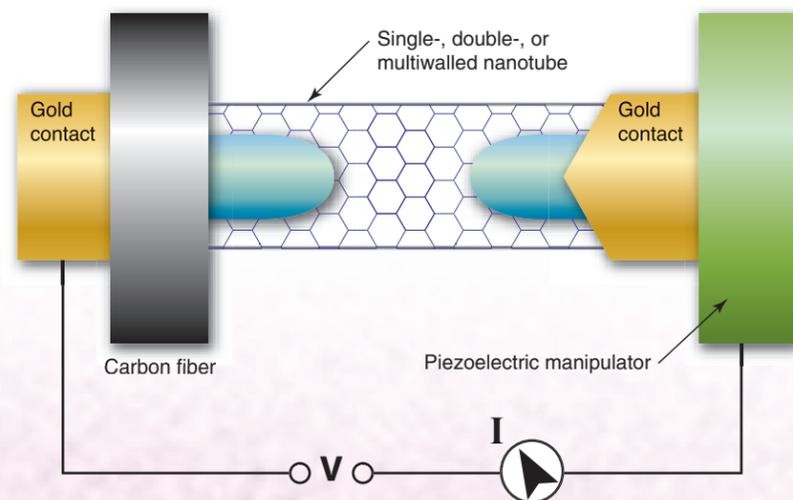
## Related Publications

J. Y. Huang, Y. M. Wang, et al., "Superplastic Carbon Nanotubes," *Nature* **439**, 281 (2006).

J. Y. Huang et al., "Atomic-scale Imaging of Wall-by-Wall Breakdown and Concurrent Transport Measurements in Multiwall Carbon Nanotubes," *Phys. Rev. Lett.* **94**, 236802 (2005).

CMS RESEARCH THEMES

**Figure 1.** A schematic shows how a piezoelectric device is used to manipulate a nanotube. The piezoelectric manipulator stretches the tube, revealing the tube's electromechanical behavior. This nanomanipulating device can also heat the nanotube to extremely high temperatures by applying a high bias (V) on both ends of nanotubes. The electrical conductance (I-V curve) of carbon nanotubes can be measured simultaneously.



**Figure 2.** Sequential high-resolution transmission electron microscopy images show the effects after stretching a single-walled nanotube from 24 nm to 91 nm. Heating to more than 3600 °F causes the nanotube to grow 280 percent longer and shrink 15 times in diameter. During stretching, kinks (arrows) in the nanotube are observed.

## NEW FRONTIERS

The nanomanipulation device we developed provides a platform to investigate the fundamental electromechanical behavior of many dimensionally small nanostructured materials under extreme conditions. Our discovery of the unexpected properties of carbon nanotubes is of particular importance because nanotubes and nanowires will likely be used to build innovative functional nanodevices with applications in radiation and biological agent detection, water desalination, and pressure diagnostics.

As we continue to investigate the fundamental physical properties of carbon nanotubes, we will start to incorporate them into various detection nanodevices that are relevant to our national-security missions. For example, single-walled carbon nanotubes can be used as piezoresistive strain gages for pressure sensing of materials at extreme conditions.

# Engineering Stronger Materials to Withstand Extreme Conditions

The Laboratory's energy- and defense-related missions require the strongest possible metals, capable of performing as required under extreme conditions. In order to engineer metals that will not fail under stress, our scientists are combining computational and experimental techniques to improve our fundamental understanding of materials and how they deform.

Most metallic materials are polycrystals—large assemblages of single-crystal grains that meet at grain boundaries. These boundaries are essential to material strength, in that they block large-scale plastic deformation by containing material damage within localized regions. We are engineering materials that have stronger boundaries spread throughout the material, breaking up networks of weaker boundaries. This notion of grain-boundary engineering has produced materials with five-fold improvements in resistance to intergranular failure, with minimal added cost.

We discovered that the strong boundaries tend to cluster together far more than first expected, affecting material performance. Using a

combination of mathematical theory, computation, and experiment, we are improving our material models by analyzing the mathematical correlations of grain-boundary networks and how they control the roughness scaling of fracture surfaces.

## Relevance to CMS Research Themes

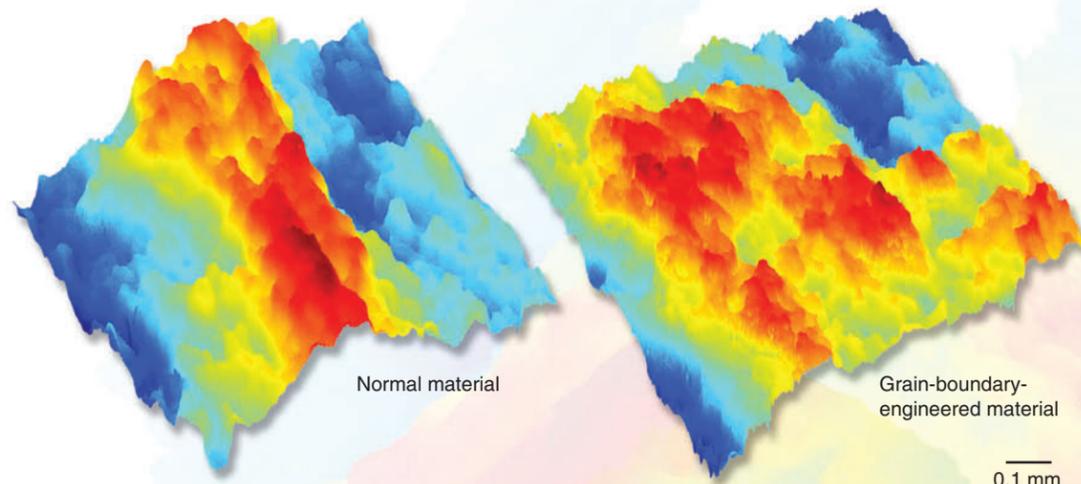
A common type of materials failure in hot, high-pressure, corrosive liquid environments—such as in certain nuclear reactor designs—is caused by intergranular stress-corrosion cracking. Because grain-boundary-engineered materials are much more resistant to intergranular cracking than normal materials, our studies of microstructural correlations are providing the scientific underpinnings that will lead to substantially improved materials for such extreme applications.

We are also interested in the effects of shock loading on materials that are used in defense systems. To gain a better understanding of these fundamentals, we are generating more realistic computational microstructures for use in plasticity models that will help us understand the strength of materials under shock-wave conditions.

## Major Accomplishments in 2005

The key to the effectiveness of grain-boundary engineering lies in the microstructure of what we are calling twin-related domains, or TRDs. Twinning, known for its symmetrical crystal structure, occurs when crystals are subject to stress or other extreme conditions. Materials engineered with the grain-boundary process tend to have large, well-developed TRDs, which significantly improve the materials' strength. A stress-corrosion crack encountering a TRD usually has to go around it; such a dense cluster of strong boundaries is too tough to crack. On the other hand, normal nonengineered materials have more weak boundaries and less well-developed TRDs, and a crack can easily find large, continuous paths of weak boundaries.

We discovered how strong boundaries tend to cluster into TRDs and how this clustering affects material performance in terms of failure resistance, uniformity, isotropy, and roughness of these fracture surfaces. Figure 1 shows how these surfaces roughened by corrosion look completely different in the two materials. While the normal material has prominent ridges and valleys aligned with the



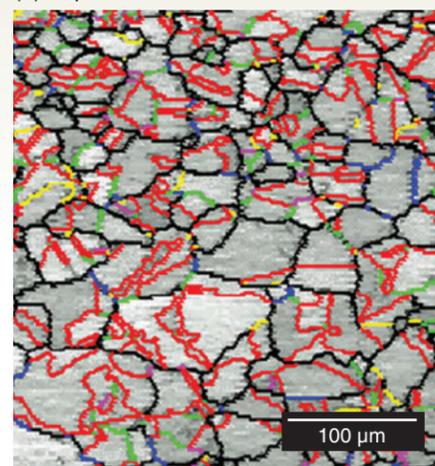
**Figure 1.** Perspective images of stress-corrosion crack surfaces from normal and grain-boundary-engineered materials. Not only do the engineered materials last up to five times longer, the difference in roughness shows that the material cracks in a completely different way that can be traced back to its grain-boundary structure.

For more information contact

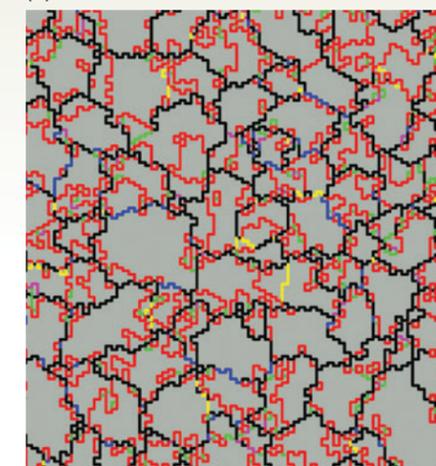


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(a) Experiment



(b) Model



- Twin boundary
- Weak boundary
- Nontwin strong boundary
- Nontwin strong boundary
- Nontwin strong boundary
- Nontwin strong boundary

**Figure 2.** This comparison of (a) an experimentally measured microstructure from grain-boundary-engineered copper and (b) an optimized computational model designed to mimic it shows good agreement and similarity. Our model tends to produce grain-boundary networks that are quite similar to those in the real material.

direction of the crack growth, the roughness in the engineered material is weaker, more uniform, and more random.

Our results have greatly clarified how these TRDs behave, how the boundaries connect together in networks, and how they control the fractal-like surfaces shown in the figure. The networks are highly correlated, so using a simple percolation theory of network connectivity was not sufficient to understand them.

Instead, we produced the first complete mathematical description of the relationships among the different types of strong boundaries, which enabled us to explore the constraints on grain-boundary networks in a simple, efficient, and mathematically rigorous manner. The constraints impose a degree of order and structure on the TRDs, and we have found that the resulting computer-generated microstructures tend to naturally fall into quite realistic patterns that can be optimized to closely mimic an experimentally obtained microstructure (Figure 2). The computational microstructure shows clearly defined TRDs with complex networks of boundaries inside. If we count the grain-boundary populations in detail, we find that the match is quantitative as well as qualitative. We can match the statistics measured

in real materials to within the limits of random sampling.

## Scientific Impact

Grain-boundary engineering techniques effectively improve fracture toughness, stress-corrosion resistance, and superconducting properties by factors of five. By understanding the laws governing grain-boundary network correlations and how they translate into material properties, we will create better grain-boundary-engineered materials designed for specific applications. There is a growing awareness that crystallographic correlations on supra-grain length scales are essential to the performance of many materials, and our techniques may be a key to understanding these length scales.

## Related Publications

B. W. Reed et al., "The Structure of the Cubic Coincident Site Lattice Rotation Group," *Acta Cryst.* **A60**, 263 (2004).

V. Y. Gertsman and B. W. Reed, "On the Three-Dimensional Twin-Limited Microstructure," *Z. Metallkd.* **96**, 1106 (2005).

B. W. Reed et al., "Mathematical Methods for Analyzing Highly-Twinned Grain Boundary Networks," *Scripta Materialia* **54**, 1029 (2006).

## NEW FRONTIERS

We are scaling up the microstructure generation algorithms to higher resolutions and will include specific physics for a much larger class of materials. Using the material-modeling expertise and world-leading computational capabilities at LLNL (including BlueGene/L and Thunder) and working in collaboration with Michigan State University, we plan to address the issue of dimensionality. Because percolation and network correlations behave extremely differently in two- and three-dimensional systems, we are currently studying this very challenging problem to understand exactly how the three-dimensional structure of a TRD translates into improved performance. This may help guide the development of new kinds of grain-boundary-engineered materials for a broad range of extreme-stress applications.

# Finding a New Source of Laser-like Radiation

Since its invention in 1958, the laser has found use in every segment of our society. In contrast to common light sources, which emit incoherent photons at many frequencies, laser beams are emitted from “coherent” or single-wavelength light sources. However, exceedingly few sources can generate the narrow-bandwidth, intense laser light.

We have found a new source of coherent optical radiation that is fundamentally distinct from lasers and other existing sources of coherent radiation. Using analytical theory and computational experiments, we have simulated a mechanical shock wave in simple table salt (NaCl) and observed a new light source. Where only incoherent photons and sparks would be expected to emerge from the NaCl crystal, we found much more. Remarkably, weak but measurable coherent light was

observed, typically in the frequency range 1–100 THz.

## Relevance to CMS Research Themes

CMS has several strategic themes that are directed toward understanding and clarifying the ultrafast dynamics of matter under shock compression. Using the coherent property of this light, we can develop new and novel experimental diagnostics to better understand the picosecond-timescale dynamics of shocked matter. For example, because the coherent emission frequencies are determined by the shock speed and the lattice constants of the crystal, they can potentially be used to determine atomic-scale properties of the shocked material.

## Major Accomplishments in 2005

In collaboration with the Massachusetts Institute of Technology, our preliminary

theoretical work suggested that coherent light might be emitted from shock waves under some circumstances. However, experimentally relevant predictions would require simulations of tens of millions of atoms.

In 2005, we performed molecular dynamics simulations of shock waves propagating through crystalline NaCl. The simulations of such large numbers of atoms were made possible by using the LLNL 23-TFLOP/s Thunder computer.

These simulations solved the classical equations of motion for each atom in the shocked NaCl crystal, addressing interaction, thermal effects, and deformation of the crystal lattice. Additionally, each atom in the crystal has a static charge. Our goal was to calculate the total electric current in the computational cell and relate it to the emitted electromagnetic radiation to make a prediction about the emission of coherent light.

Molecular dynamics simulations of NaCl in Figure 1 show coherent (narrow) peaks in the electric current for shocks propagating in two different crystallographic directions [111, 100]. The peak frequencies are in excellent agreement with our analytical results.

We discovered that, when a shock wave propagates through a crystal, the synchronized motion of large numbers of atoms can produce narrow-bandwidth radiation. The molecular dynamics simulations demonstrate coherence lengths on the order of millimeters (around 20 THz) and potentially greater, comparable to some lasers. Figure 2 shows the time- and space-dependent origin of the coherent currents in a simulation.

The emission frequencies are determined by both the shock speed and the lattice constants of the crystal and, therefore, can potentially be used to determine atomic-scale properties of the shocked material. We expect that this effect will be observable in a wide variety of material systems under

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realizable shock-wave conditions. The predicted spatial distribution of emitted radiation shows that the radiation can be concentrated in a particular direction (Figure 3).

## Scientific Impact

The generation of terahertz radiation caused by shocking crystals will have

significant basic science implications because other mechanisms are few and fundamentally different. In the near term, we expect to use this form of coherent light as a subpicosecond probe to understand properties of shock waves. The frequency, magnitude, and spatial distribution of the emitted radiation contain information about the shock speed, roughness or shape of the

shock front, and the degree of crystallinity of the lattice.

Potential longer-term applications include a practical source of long-time coherence radiation if the emission power level can be made sufficiently large. This new source of radiation may lead to new methods of medical imaging and new detectors for national-security applications.

## Related Publications

E. J. Reed et al., “Coherent Optical Photons from Shock Waves in Crystals,” *Phys. Rev. Lett.* **96**, 013904 (2006).

E. J. Reed et al., “Reversed Doppler Effect in Photonic Crystals,” *Phys. Rev. Lett.* **91**, 133901 (2003).

E. J. Reed et al., “The Color of Shock Waves in Photonic Crystals,” *Phys. Rev. Lett.* **90**, 203904 (2003).

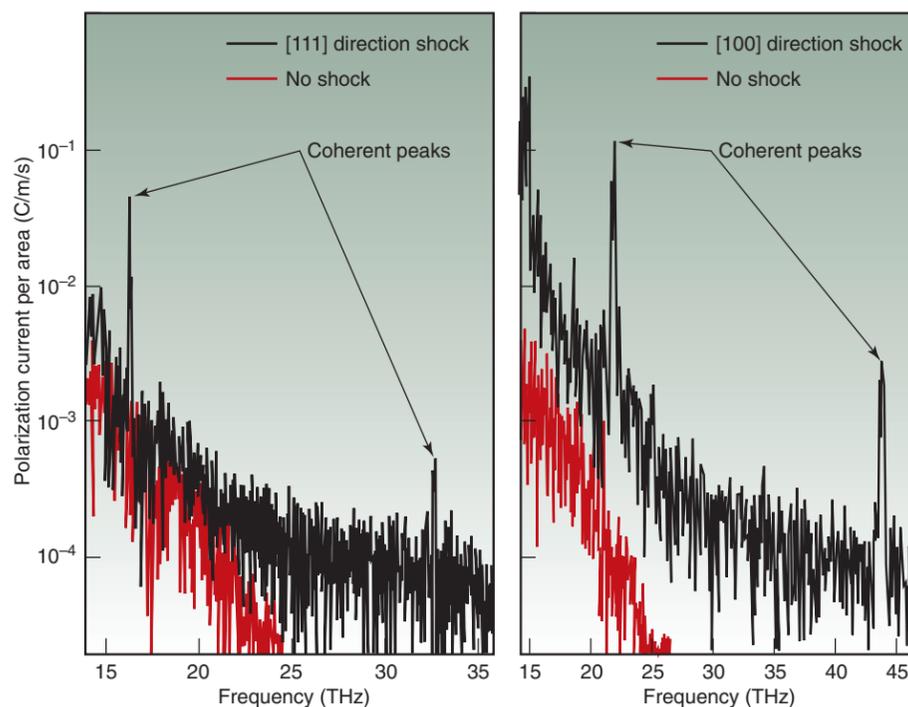


Figure 1. Simulations of a shock propagating through NaCl (black) show narrow-bandwidth coherent peaks that do not exist in the simulations without shocks (red). The emission frequencies show a coherence length of 5 mm from the 16-THz peak, comparable to that of some commonly used lasers.

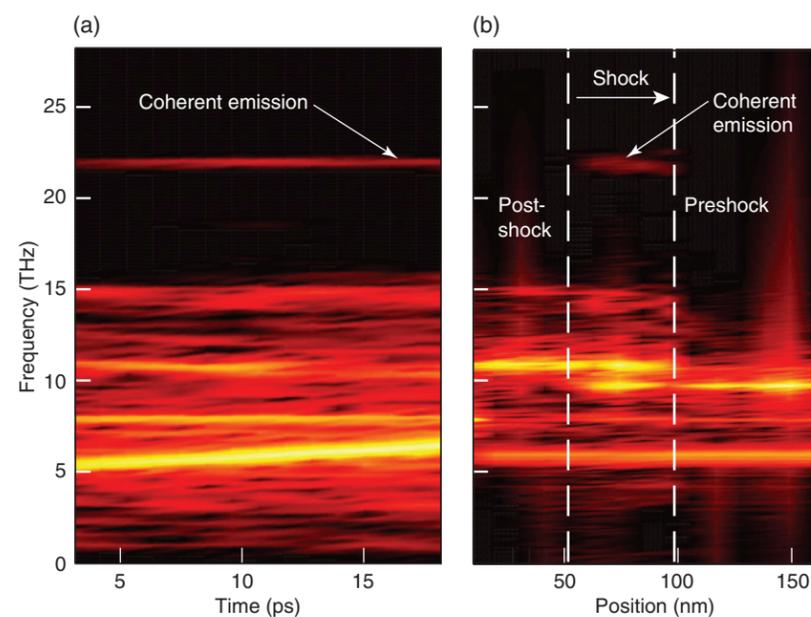


Figure 2. (a) The coherent polarization current occurs for the duration of the shock propagation with roughly constant amplitude. (b) The frequency as a function of position (in the shock propagation direction) shows that the coherent current originates at the shock front (between the white dotted lines) rather than behind it.

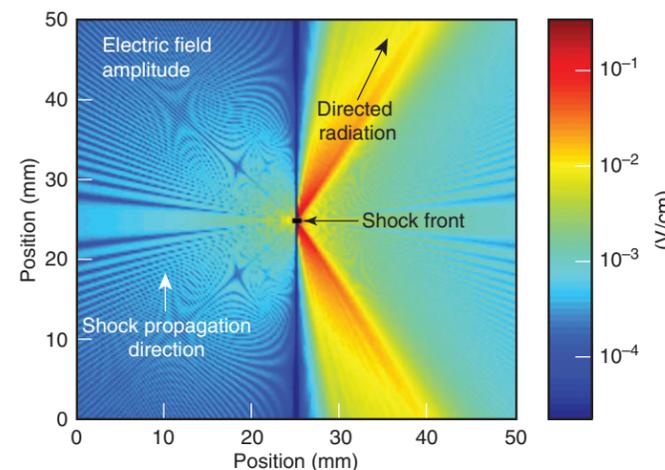


Figure 3. The calculated spatial distribution of the coherent electric field magnitude from a 1-mm<sup>2</sup> shock front shows that the emitted radiation can be concentrated in a particular direction under some circumstances.

## NEW FRONTIERS

We continue to explore the coherent emission effect through molecular dynamics simulations and are developing a theoretical picture of coherent effects in shocked crystals. In addition, we will verify our simulation results with physical experiments to observe the effect.

We anticipate that the biggest challenge will be to detect the weak signal using existing relatively inefficient detection techniques. However, our experimental approach incorporates a number of elements designed to boost the coherent signal strength. One element includes using a technique capable of generating repeated shock waves at rates of around 1 kHz.

In these experiments, we will employ ultrafast subpicosecond laser-driven shock waves in conjunction with an ultrafast terahertz detection scheme. At potentially subnanometer spatial resolution, our experiments will bring us close to the scale of our simulations.

# Insights into Early Stages of Polymer Crystallization

Because of their diverse physical and mechanical properties, polymers—such as polyethylene—have become essential materials in a variety of defense systems as well as medical, industrial, and environmental applications. Typically, polymers are composed of both crystalline and amorphous regions, and their properties are strongly influenced by the size and shape of the crystalline regions. Understanding how and why these regions form will help us control these properties, leading to new applications and improvements to existing materials.

However, the atomistic processes that lead to polymer crystallization are not well formulated, and experiments have not given us the level of detail we need. Using LLNL's terascale computational capabilities, we are able to further our understanding of these processes on an atomistic level.

## Relevance to CMS Research Themes

By increasing our understanding of polymer crystallization, we are gaining fundamental knowledge about the nature of crystal formation and, more specifically, the aging of technologically important materials in a variety of defense systems. The polymer materials in defense systems such as nuclear weapons must perform within predictable margins, and we are turning increasingly to simulations to ensure that these materials will perform as required.

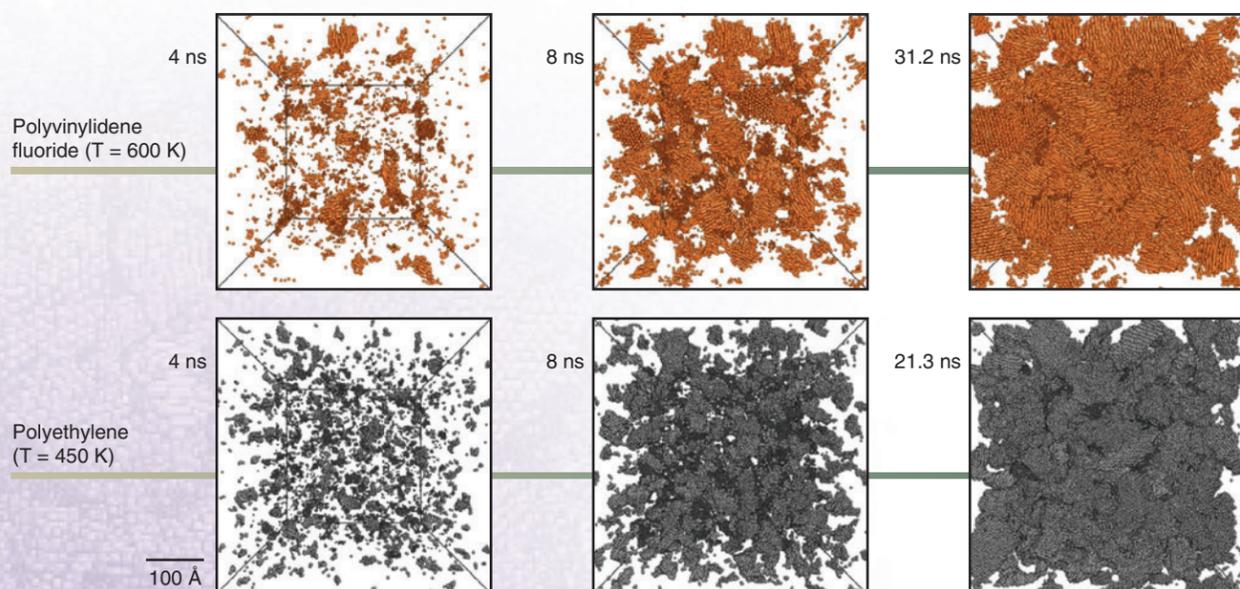
In our polymer crystallization investigations, we have focused on examining high-explosive aging phenomena relevant to the Stockpile Stewardship Program's Enhanced Surveillance Campaign. Our goal is to obtain, through accurate models, a lifetime assessment of physical and mechanical properties of polymers relevant to their use

in national defense systems. In a broader sense, the results of our work can also be applied in atomic-scale control of the physical and mechanical properties of polymers.

## Major Accomplishments in 2005

Under some circumstances, polymers nucleate almost instantly, in contrast to classical nucleation, where a crystal seed is formed over time. Using the LLNL 23-TFLOP/s Thunder supercomputer and other computational resources, we conducted the largest molecular dynamics simulations of polymer crystallization to date to test recent experimental findings and theoretical predictions that, when rapidly cooled, polymeric materials undergo instant crystallization (known as spinodally assisted nucleation).

Understanding the process of spinodally assisted nucleation at the atomistic level is

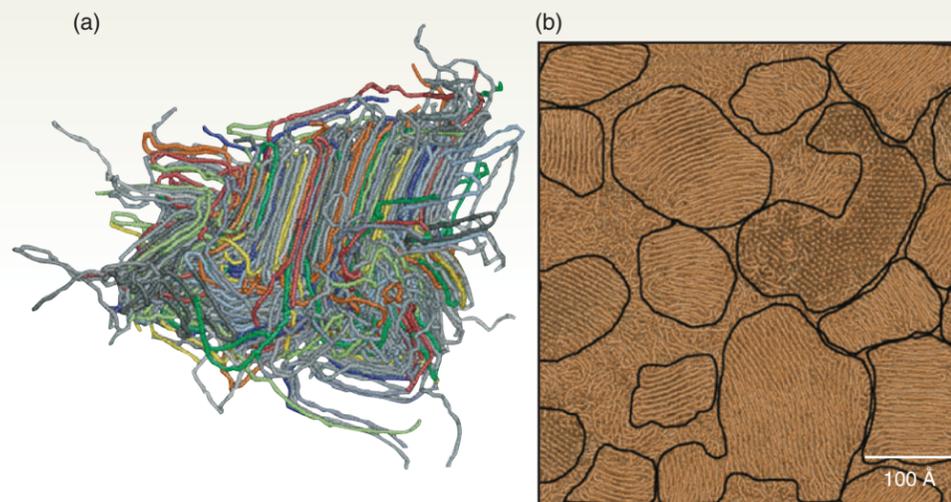


**Figure 1.** In the largest molecular dynamics simulations of polymer crystallization to date, our models show the evolution of the spinodal-assisted crystallization process for the polar (orange atoms) and nonpolar (grey atoms) polymers. The crystalline regions are explicitly shown, while the amorphous domains are shown as the white space in each panel.

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**Figure 2.** The first panel (a) shows a single ordered polymer domain with a morphology for the polar polymer model. Individual polymers are colored to illustrate polymer chains entering the amorphous region from an ordered region and adjoining two separate adjacent ordered domains (adjacent domains are not shown). The second panel (b) shows a representative ensemble of ordered domains.

the first step to elucidating the pretransition state of polymer crystallization.

We considered two classes of polymers: polar polymers (polyvinylidene fluoride, or PVDF) and nonpolar polymers (polyethylene, or PE). Both classes are made up of united atoms in chains, similar to a necklace of beads. We put these chains in a simulation cell and equilibrated them at several temperatures before we observed the almost instant chain ordering.

To address questions about the atomistic mechanism responsible for this instant ordering, our simulations used the length scale of 10 to 20 nm—the range at which spinodally assisted nucleation occurs. Using simulation cells twice the size of our length scale, our results provided atomistic information of polymer nucleation with unprecedented resolutions. (For example, the number of beads in one nonpolar melt was five million, and the size of the simulation cell was approximately 50 nm.)

Confirming earlier experimental findings, our simulations revealed microphase separation of bulk amorphous polymer ensembles into many ordered domains (Figure 1). These domains coalesce and grow, initially forming a small number of crystalline regions that grow to occupy most of the

simulation volume at the end of the runs. Figure 2a shows an enlarged ordered domain isolated from the sample, which reveals an interface between oriented and unoriented domains. Ordered crystalline domains are circled in Figure 2b to demonstrate the complex nature of the polymer morphology.

## Scientific Impact

As the first atomistic observation of the debated prenucleation, this work provides unambiguous insight into the physics of the early stages of polymer ordering leading to crystallization. Furthermore, with the unprecedented resolutions and details of our simulations, it was possible to compare and confirm our findings with laboratory experiments. Our results pertaining to crystallite size and structure as well as the critical length of polymer segments provide crucial information needed to form a fundamental understanding of the structure–property relationships of semicrystalline polymers.

## Related Publications

R. H. Gee et al., "Atomistic Simulations of Spinodal Phase Separation Preceding Polymer Crystallization," *Nat. Mater.* **5**, 39 (2006).

R. H. Gee et al., "Ultrafast Crystallization of Polar Polymer Melts," *J. Chem. Phys.* **118**, 3827 (2003).

## NEW FRONTIERS

We will use our findings about bulk polymer melts to give us greater control of the crystallite microstructure, orientation, density, and size—all of which contribute to performance. Not only can we find specific defense applications in the case of binding materials for high explosives, we also expect broader applications such as polymer transistors, which offer great flexibility at low cost. We are looking at ways to control the microstructure during manufacturing, when semiconductor films are deposited by various techniques (spin coating, jet printing, dip coating) on a dielectric surface.

Furthermore, our findings about spinodally assisted nucleation are applicable to other materials (such as metals), and we are using this process to develop new materials for National Ignition Facility targets and other applications. Powerful simulations on our terascale supercomputers will help us understand and control the microstructures of polymers and metals, leading to new and improved materials in a broad range of technologically and scientifically important devices.

# Improving Drug-Binding for Cancer Treatment

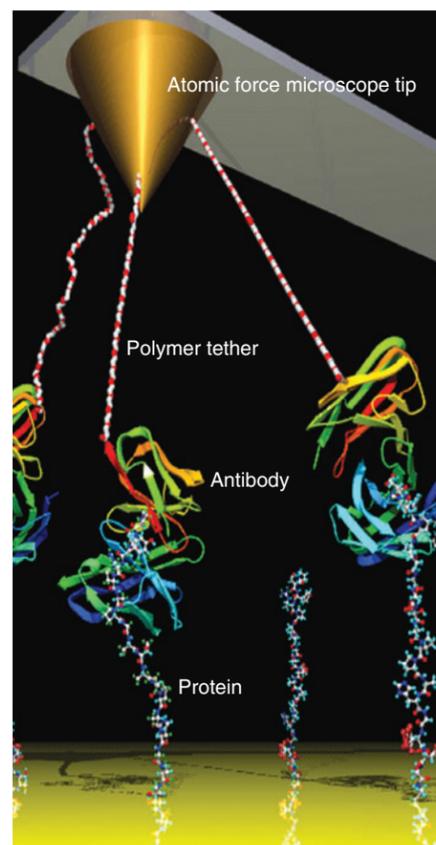
Many cellular processes in the body, including immune reactions, require multiple molecules combined to perform important tasks—a function called multivalent interaction. We are studying these multivalent interactions to improve immunotherapeutics for cancer treatment. This area of medicine connects cytotoxic drugs with antibodies that target and bind cancer cells so that the toxicity is localized on the tumor, and healthy areas of the body are spared. However, single antibodies bind to their protein target for only a few minutes, whereas cytotoxic drugs require many hours to do their work.

To solve this problem, drug developers are using multiple connected antibodies to extend drug-binding time to cancer cells. Unfortunately, when these larger, multivalent molecules are used, there may be less penetration into targeted tissues and greater accumulation in the liver. Our goal is to determine the binding time of multivalent binders to optimize efficacy so we can develop better immunotherapeutics.

## Relevance to CMS Research Themes

We are examining multivalent interactions to provide information that can be used to better deliver anticancer drugs to targeted cells. Because multivalency significantly alters molecular-binding kinetics, an understanding of this interplay may help further efforts for a variety of CMS research at the intersection of chemistry, materials science, and biology.

**Figure 1.** This illustration shows polymer tethers extending from the tip of an atomic force microscope, linking antibodies (colored ribbons) to the surface of a protein. We then measure the antibody and protein molecules connected to each tether independently to determine the binding strength and duration.



For example, increasing the collection rate of ultrasensitive biological detectors requires that analyte binding become specific and irreversible, which cannot be achieved with single antibody bonds. Infectious agents such as viruses use multivalent binding to circumvent the body's defenses. Understanding these mechanisms may lead to more potent countermeasures that can affect efforts in biological, chemical, and materials science and technology for national-security applications.

## Major Accomplishments in 2005

Techniques to directly measure the binding time of multivalent binders have been limited because they measure binding of a collection of molecules to

provide an average binding profile. This method works if all of the molecules are identical, as in the case of a single antibody. However, a collection of multivalent molecules can each bind with a range of valencies simultaneously, and there is no effective way to extract the binding time of a particular valency from an average binding profile.

By combining the atomic force microscope (AFM)—a highly sensitive tool—with the method of dynamic force spectroscopy (DFS), we can for the first time accurately characterize binding time for a range of valencies, from single bonds to three bonds. AFM allows us to measure the force required to pull apart a molecular complex composed of multiple antibodies and protein targets. Using DFS, we can then simultaneously measure both bond strength and valency to elucidate the unresolved relationship between the two (Figure 1).

In collaboration with UC Davis, we were the first to simultaneously measure bond strength and bond number independently using DFS. We measured the rupture force of a single complex formed by MUC1 protein, an indicator for breast and prostate cancer, and the therapeutic antibody that targets MUC1.

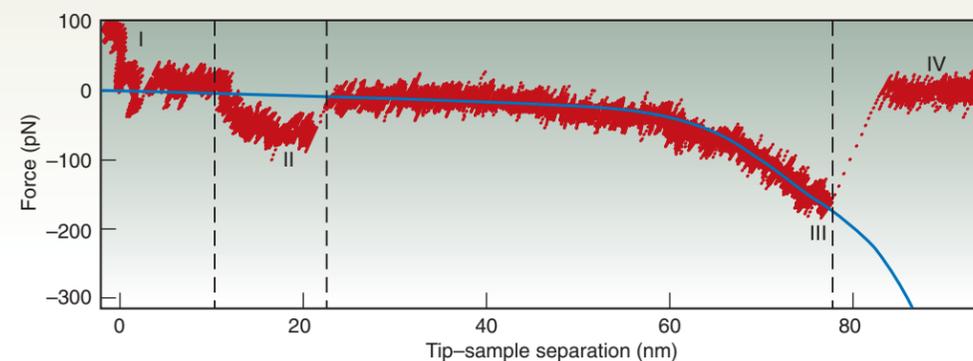
A key feature of our measurements is that we isolate interacting biomolecules on polymer tethers. We identify the number of interacting molecules by measuring the unique force extension signature that results from stretching multiple polymer tethers. The bond number, determined from measuring the number of tethers, is then correlated with the measured bond rupture force (Figure 2).

The bond lifetimes for one-, two-, and three-valent binders are determined from the dynamic force—that is, how the rupture force varies as a function of force pulling rate (Figure 3). Extrapolating this data provides an estimate for the bond

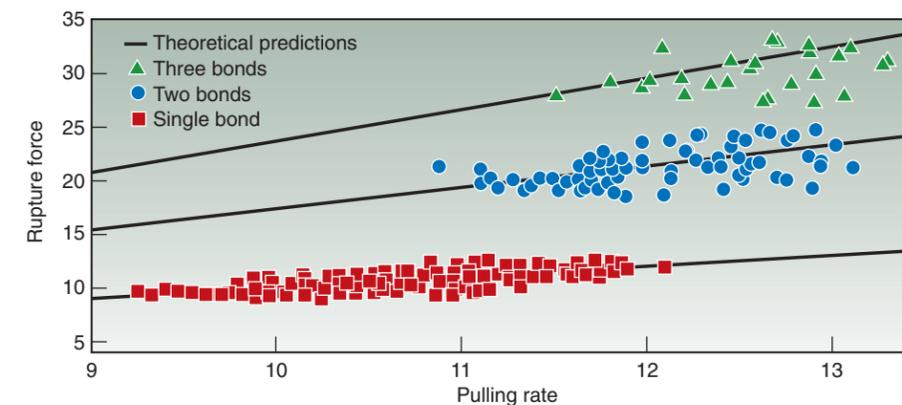
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**Figure 2.** Dynamic force spectroscopy (DFS) measures the rupture force of a single molecular complex formed by a MUC1 protein and the antibody that targets the protein. In DFS, the tip of a cantilever touches the protein's surface in region I, pulls away from the surface at region II, ruptures the antibody-protein bond at III, and returns to the relaxed state at IV.



**Figure 3.** The dynamic force spectra of one-, two-, and three-valent bond-rupture event plots illustrate rupture force versus the normalized pulling rate. These measurements offer the first-ever support for the theoretical prediction of Markovian dissociation dynamics of multivalent bonds.

lifetime under thermodynamic conditions. The effective bond time rises dramatically with the number of bonds. For one, two, and three bonds, the measured bond times were 384 seconds, 3.8 hours, and many days, respectively. These results provide the first-ever support for the theoretical prediction of Markovian dissociation dynamics of multivalent bonds.

## Scientific Impact

Multivalent binding is a promising tool for molecular targeting that will enable more accurate delivery of therapeutic drugs to targeted cells. We have demonstrated that DFS provides accurate kinetic measurements for

molecular systems. These results provide a direct measure of the effective lifetimes of multivalent bonds. The ability to resolve individual and multiple bond ruptures circumvents the problem of averaging from ensembles of molecules. In addition to drug design, the results of our studies will also provide opportunities for research in other areas such as biophysics.

## Related Publications

T. Sulchek et al., "Dynamic Force Spectroscopy of Parallel Individual Mucin1-Antibody Bonds," *Proc. Natl. Acad. Sci.* **102**, 16638 (2005).

T. Sulchek et al., "Strength of Multiple Parallel Biological Bonds," *Biophys. J.*, in press.

## NEW FRONTIERS

Directly measuring multivalent bond lifetimes is an effective method to screen and optimize therapeutic agents. By using atomic force measurements, it may become possible to map cellular surfaces for potential drug targets and quantify binding kinetics. Single-molecule force spectroscopy can be used to determine the binding efficiency of various configurations of multivalent binders, which will help researchers design better therapeutic agents. By combining these high-resolution techniques, we will for the first time be able to characterize very strong protein-antibody interactions that could be difficult to perform experimentally at relevant timescales.

# Probing Proteins and Nucleic Acids

Proteins, like shoelaces, fold and unfold in a variety of ways. By learning how and why a protein occasionally folds incorrectly, researchers may be able to better treat victims of Alzheimer's, Mad Cow, and other neurodegenerative diseases.

The ability to gain such an understanding of protein folding and misfolding requires measurements of fluctuating distance distributions occurring over nanoscale distances (0.1–100 nm) and many timescales (picoseconds to minutes). Folded, unfolded, and partially folded species may be simultaneously present and rapidly interconverting, obscuring the properties of individual species. As a result, we needed an experimental method to unravel distance distributions and fast conformational fluctuations.

Using a technique called fluorescence resonance energy transfer, or FRET, we are able to measure the distances between two specific points on a protein. We use highly sensitive microscopes, which allow us to detect FRET signals from individual molecules with a time resolution of approximately 100  $\mu$ s. The time resolution is limited by the strength of single-molecule signals.

Previously, we measured FRET for single proteins, distinguishing folded and unfolded proteins one at a time. We have now extended single-molecule methods to

measure distance distributions that fluctuate on timescales longer than 1 ns.

## Relevance to CMS Research Themes

In this research, we are using methods from the physical sciences that have been adapted and then applied to areas of high biological importance, such as protein folding. Our goal is to develop a quantitative description of heteropolymers, such as DNA (deoxyribonucleic acid) and proteins with strong charge and/or specific intrachain interactions.

Our work will eventually lead to a deeper understanding of disease mechanisms and contribute to national security through improved human health. Single-molecule methods related to this work may, in the future, provide bio-warfare agent detection with the ultimate sensitivity—detecting pathogens one molecule at a time.

## Major Accomplishments in 2005

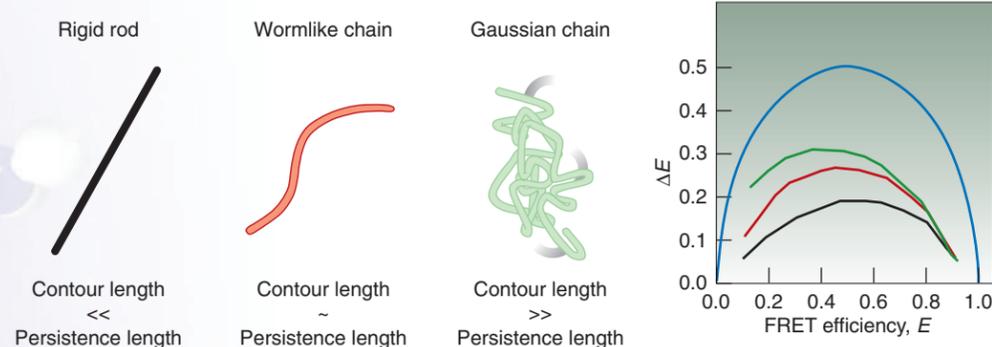
Combining the strengths of single-molecule as well as ensemble-level approaches, we introduced a new technique that interlaced picosecond pulses from two synchronized pulsed lasers to perform alternating laser excitation (ALEX) experiments on single molecules in conjunction with time-resolved FRET measurements. We sorted the molecules into subpopulations (such as folded and unfolded proteins) based on

single-molecule signals detected within 0.1–1 ms. Within these subpopulations, we studied distance distributions fluctuating faster than 100  $\mu$ s using fluorescence lifetime analysis. Even when folded proteins were present, we successfully studied the nanosecond timescale fluctuations of only unfolded proteins, made possible by excluding signals from the folded proteins.

Distance distributions of energy transfer efficiency depend on the stiffness of the polymer, which depends on the contour length and the persistence length (Figure 1). The contour length is the length of the polymer when it is fully extended or stretched out. The persistence length is the length over which the polymer naturally stays straight. If the contour length is much less than the persistence length, then the polymer is a rigid rod (black line). If the contour length is much greater than the persistence length, then the polymer is a very flexible Gaussian chain (green line) with maximal distribution in distances, denoted as  $\Delta E$  FRET efficiency. In between, the polymer is a wormlike chain (red line).

In our studies of unfolded protein behavior in the presence of folded protein, we looked at double-stranded and single-stranded DNA as well as the unfolded states of two well-studied proteins—CI2 (chymotrypsin inhibitor 2) and ACBP (acyl-CoA binding protein).

Figure 1. FRET, or fluorescence resonance energy transfer, reveals distance distributions related to a polymer's flexibility. The more flexible the polymer is, the higher the distance distributions of energy transfer efficiency, as illustrated in the plot based on computational predictions.



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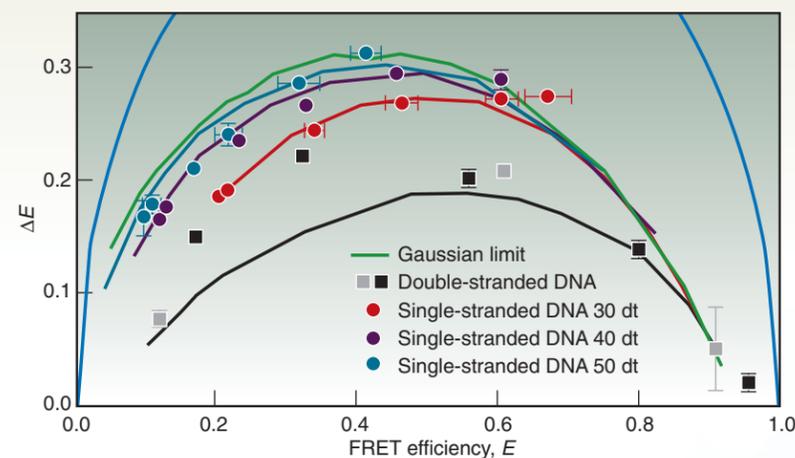


Figure 2. Using a nanosecond alternating laser excitation technique, we can measure both single- and double-stranded fluorescent-labeled DNA. All DNA data points lie between the rigid rod limit (black line) and the Gaussian chain limit (green line). Single-stranded DNA has a distance distribution closer to the Gaussian chain limit. Data are shown as symbols, and simulations are shown as lines.

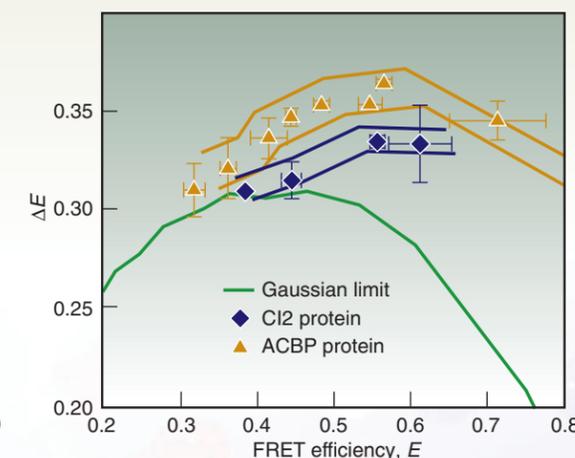


Figure 3. All of the CI2 and ACBP protein measurements are at or above the Gaussian chain limit (green line). For each data set, lowering the denaturant concentration results in measurements moving toward the upper-right, indicating more compact states with increasing fluctuations.

As illustrated in Figure 2, all of the DNA measurements of distance distributions lie between the rigid rod limit (black line) and the Gaussian chain limit (green line), exhibiting varying effects in a generally unstructured complex.

However, the unfolded CI2 and ACBP proteins exhibit fluctuations above the Gaussian chain limit (Figure 3). Nanosecond ALEX-based single-molecule sorting allows the exclusion of signal from folded CI2 and ACBP. These extra large fluctuations become more pronounced at lower denaturant concentrations (higher mean  $E$ ), as the solution conditions become closer to natural conditions. Our observations can be explained by transient formation of structures, caused by protein denaturation, which constantly changes the effective contour length and persistence length. Such measurements of unfolded proteins in native-like conditions will improve our understanding of the starting point of the protein-folding process. Questions regarding protein misfolding will be more easily addressed in the context of these experiments.

## Scientific Impact

Our understanding of biopolymers in general, and polyelectrolytes and protein folding in particular, will benefit from our ability to sort molecules into subpopulations and probe their distance distributions. We can gain new insights into fast conformational dynamics involved in protein machines, cell-signaling, and other biological processes. The quantitative information obtained from these new biophysical methods promises to revolutionize our basic understanding of life at the molecular level. For example, we can gain a better understanding of how pathogens hijack cellular networks, providing targets for drug development, as well as ways to detect emerging natural and engineered threats.

## Related Publications

T. A. Laurence et al., "Probing Structural Heterogeneities and Conformational Fluctuations of Biopolymers," *Proc. Natl. Acad. Sci.* **102**(48): 17348–17353 (2005).

A. N. Kapanidis, T. A. Laurence, et al., "Alternating-Laser Excitation of Single Biomolecules," *Acc. Chem. Res.* **38**(7): 523–533 (2005).

## NEW FRONTIERS

The next step in gaining a better understanding of how proteins fold is to extend our techniques so that we can compare how proteins fold into their native and functional structures in vitro and within living cells. We are now testing our hypothesis that the large  $\Delta E$  FRET efficiency is due to transient residual structure. By measuring the dependence of  $\Delta E$  FRET efficiency on the position along the protein chain and on side chain truncations (removal of sections of the protein that form structure), we hope to elucidate how protein denaturation affects the transient formation of protein structures.

# Solving a Nitrogen Fixation Conundrum with NanoSIMS

Largely responsible for the oxygen in our atmosphere, cyanobacteria have been a dominant mechanism for converting—or fixing—carbon from carbon dioxide, making life as we know it possible. Today, these microorganisms are still important to the global carbon cycle because, in addition to fixing carbon, they also fix large quantities of nitrogen. Yet, we still do not fully understand how these organisms perform this critical function of nitrogen fixation.

In collaboration with the University of Southern California, we are studying nitrogen fixation and photosynthesis in the marine cyanobacteria that play a critical role in global carbon cycling. By enhancing our understanding of microbial metabolism and the roles of individual microbial species, ecosystem researchers will be able to improve predictions of how these processes respond to and affect climate change.

Our approach is to expose the bacteria to stable isotope tracers and then map the

tracer distribution in individual bacterial cells with the nanoscale secondary ion mass spectrometer (NanoSIMS)—an ultrahigh-resolution ion microprobe. Using cells labeled with stable isotopes of carbon and/or nitrogen, NanoSIMS imaging reveals locations of active growth and allows us to follow nutrient fluxes between cells.

## Relevance to CMS Research Themes

Chemical imaging of biological materials is advancing our understanding of biochemical processes and the role of microbes in energy production, environmental remediation, and carbon sequestration. With the NanoSIMS, we aim to link microbial metabolism to molecular structures and produce a detailed view of how isotopically marked species propagate throughout individual cells.

These research areas are central to Livermore's role in the Genomics: GTL (previously known as Genomes-to-Life)

program for the Department of Energy, which seeks to provide a system-level understanding of microbial processes essential to carbon cycling and the cycling of such other elements as nitrogen, phosphorous, sulfur, oxygen, and metals.

Furthermore, our efforts to quantitatively measure biochemical systems at subcellular scales have direct benefits in the forensic characterization of biological weapons materials.

## Major Accomplishments in 2005

One particular cyanobacteria, *Trichodesmium* (sea sawdust), may account for up to half of the N<sub>2</sub> fixation in the North Atlantic Ocean. However, it is unclear how *Trichodesmium* simultaneously fixes both carbon and nitrogen because nitrogenase enzymes used in N<sub>2</sub> fixation are strongly inhibited by the O<sub>2</sub> produced during photosynthesis. Thus, these two critical processes must be either spatially or temporally isolated.

Another genus of cyanobacteria, *Anabaena*, solves the incompatibility problem by isolating nitrogen fixation in specialized cells called heterocysts (Figure 1a). While these specialized cells are easily identified in *Anabaena*, specialized nitrogen-fixing cells have been suspected but never identified in *Trichodesmium*.

Combining transmission electron microscopy and NanoSIMS, we tracked uptake and redistribution of nitrogen and carbon at the cellular and subcellular level. We identified the exact sites where newly fixed carbon and nitrogen were allocated in cells grown in a <sup>13</sup>C- and <sup>15</sup>N-enriched environment. In the model organism *Anabaena*, newly fixed carbon is significantly lower in nitrogen-fixing heterocyst cells (Figure 1b), while neighboring vegetative cells are dramatically enriched because of their

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photosynthetic activity. Corresponding images indicate that, after being fixed in heterocysts, nitrogen is rapidly allocated to locations of new biomass growth in neighboring cell walls (Figure 1c).

In contrast, in experiments involving *Trichodesmium*, our analyses indicated few cell-to-cell differences in concentrations of newly fixed carbon, nitrogen, or phosphorus (Figure 2). A large portion of this newly fixed nitrogen was immediately confined to localized subcellular regions. These regions, called cyanophycin granules, are thought to be storage structures and temporary holding sites for nitrogen. In samples collected after 24 hours, these regions were less distinct and overall cell enrichment had risen dramatically. In conclusion, unlike *Anabaena*, which uses specialized nitrogen-fixing cells, *Trichodesmium*

uses temporary nitrogen storage at the subcellular level as a primary mechanism of metabolic segregation. It also processes carbon and nitrogen at different times in the same cells.

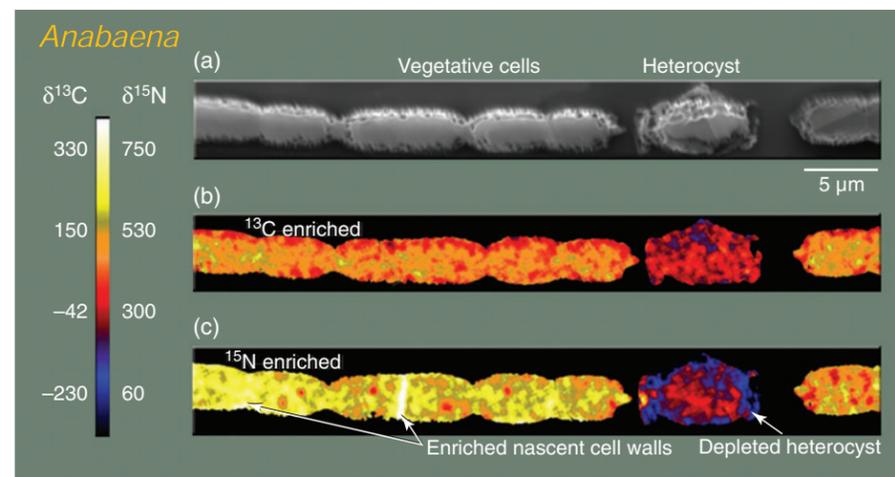
## Scientific Impact

Marine microbiologists have long sought to explain the paradoxical behavior of *Trichodesmium*—a nonheterocystous cyanobacteria that is able to fix both CO<sub>2</sub> and N<sub>2</sub> concurrently during the day. Several competing hypotheses have been proposed that support either temporal and spatial segregation mechanisms; however, our analyses with the NanoSIMS presented the first direct imaging of nitrogen and carbon behavior at the subcellular level. In general, these results support the temporal segregation model for *Trichodesmium*.

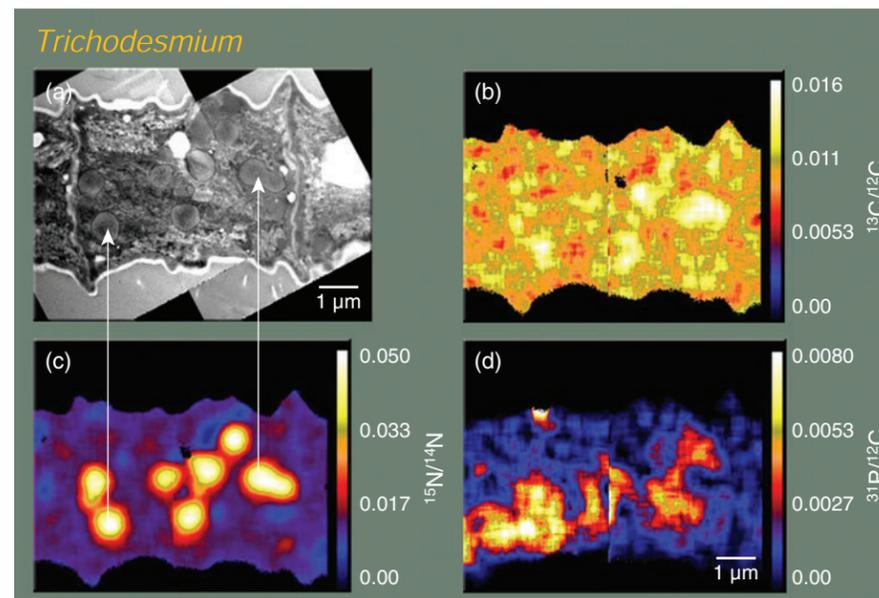
Our experiments clearly illustrate how the NanoSIMS and stable isotope tracers can be used to track nutrient allocation at the individual cell and subcellular levels. This capability can be used to study a wide range of topics in the emerging fields of microbial proteomics and metabolomics, allowing us to shed light on critical functions of environmental microbes. This knowledge will be critical to modeling and bioengineering efforts in topics ranging from environmental cleanup to carbon sequestration and energy generation.

## Related Publications

C. G. Marxer et al., "Supported Membrane Composition Analysis by Secondary Ion Mass Spectrometry with High Lateral Resolution," *Biophys. J.* **88**: 2965–2975 (2005).



**Figure 1.** Using NanoSIMS, we have analyzed a chain of seven cells from a filament of *Anabaena* after four hours of incubation with carbon and nitrogen isotopic tracers. The secondary electron image (a) identifies the vegetative cells and specialized nitrogen-fixing cells, known as heterocysts. The enrichment of carbon (b) and nitrogen (c) is much lower in the heterocyst, confirming that the heterocyst is not fixing new carbon and is rapidly disbursing newly fixed nitrogen to neighboring cells.



**Figure 2.** Unlike *Anabaena*, *Trichodesmium* does not isolate nitrogen fixation in specialized cells. Instead, it uses subcellular storage as indicated in these corresponding NanoSIMS and transmission electron microscope images. The micrograph (a) shows two *Trichodesmium* cells after eight hours of incubation with carbon and nitrogen. In images showing (b) carbon isotope, (c) nitrogen isotope, and (d) phosphorus-to-<sup>12</sup>C ratios, respectively, the cyanophycin granules, which are thought to store nitrogen, are clearly visible and are indicated by arrows.

## NEW FRONTIERS

Several nitrogen- and carbon-fixing marine cyanobacteria genomes have recently been fully sequenced, providing unprecedented opportunities to link genes, proteins, and metabolic activities. Using NanoSIMS, we will study these organisms and genetically modified strains with one or more genes that have been made inoperative in critical functional processes. Once we understand the gene encoding for specific proteins, we will study the spatial location of these proteins and their movements within the cell during critical functions such as DNA replication, mitosis, and biomass growth. By linking the power of NanoSIMS and molecular genomic approaches, we hope to increase the speed with which we can discern microbial metabolic strategies in uncultured and novel organisms.

# Reducing Nuclear Threats with Better Radiation Detectors

One of the outstanding challenges in homeland security is to detect materials associated with potential nuclear threats, even when they have weak radiation emissions, while effectively filtering out the many legitimate radioactive objects commonly found in commerce and the environment.

Using a Compton scattering approach, we are developing a compact, portable gamma-ray detector that can efficiently and accurately detect, identify, and localize radioactive sources with unsurpassed sensitivity. Our system can identify the path of gamma rays in the detector regardless of the direction of the source, effectively addressing the deficiencies of current detection systems. Using three-dimensional position-sensitive silicon and germanium detectors, the detection system can localize gamma rays in the energy range of 150 to 2600 keV.

In addition to building advanced prototype detectors for homeland security, we are evaluating the feasibility of Compton imaging and gamma-ray tracking for other applications ranging from fundamental physics to biomedical imaging.

## Relevance to CMS Research Themes

Our work supports the applied nuclear science theme, with the goal of improving national security and human health. Our current focus is on homeland security and the development of measures to counter the proliferation of nuclear materials. However, the underlying technologies and concepts also apply to biomedical imaging and may lead to significantly improved tools for developing and evaluating new drugs, better detection of the early stages of breast cancer, and improved cancer treatment.

## Major Accomplishments in 2005

Our first hybrid Compton gamma-ray imager can measure the location and shapes of gamma-ray sources without a collimator. It consists of high-resolution and two-dimensionally segmented silicon and germanium detectors, which are read out by a fully digital data-acquisition system.

Using gamma-ray tracking algorithms, the imager determines the scattering sequence of the interactions. It can uniquely define the source location in three dimensions as multiple gamma rays interact with the detector through Compton scattering.

Our system is mounted on a cart to allow transport and operation at different locations (Figure 1). The Compton imager has excellent energy and angular resolution for a range of energies and source locations. We have

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achieved angular resolution values of 1–3 degrees for energies ranging from 244 to 1408 keV (Figure 2).

We also developed and implemented new signal- and event-processing algorithms, which allow us to reconstruct an event with up to 80% efficiency, maintaining the intrinsic high efficiency of the detectors. Because of the improved signal processing, we can now get excellent position resolution of about 0.5 mm throughout the sensitive volumes of the detectors.

One of the remaining challenges for us is to improve sensitivity when gamma-ray interactions occur close to each other. By calculating complete pulse shapes throughout the detector volume, we will be able to fit measured signals with calculated signals. These signal decomposition calculations will allow us to identify and measure multiple interactions even if they occur in close vicinity.

While image reconstruction algorithms have been evolving in conventional imaging for decades, reconstruction for Compton-scattering imaging is still in its infancy. To improve resolution and contrast in the images, we developed new and fast-filtered projection algorithms specifically for Compton imagers and successfully demonstrated it for our system.

For applications in nuclear safeguard and in nuclear-fuel reprocessing, our gamma-ray detector offers the unique ability to easily visualize extended radiation sources. Our detector can now render tomographic images of radioactive sources from our measurements and overlay them with photographic images (Figure 3). By comparing the images, we can identify deviation from installation designs of nuclear facilities or potential diversion of nuclear materials.

## Scientific Impact

The technology we are developing for the Department of Homeland Security

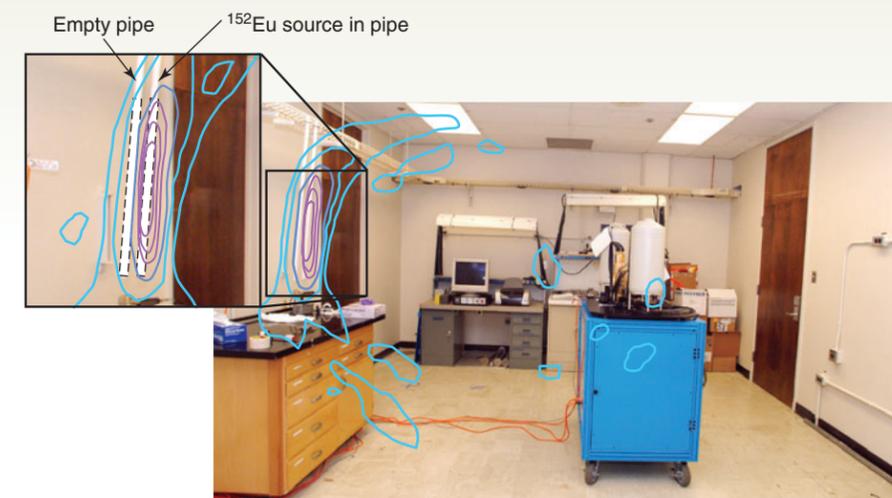


Figure 3. An extended  $^{152}\text{Eu}$  source is hidden in one of two visible pipes. Not only is our Compton imaging system able to identify the source through the characteristic gamma-ray energies (purple), it is also able to determine the location and extent of the source.

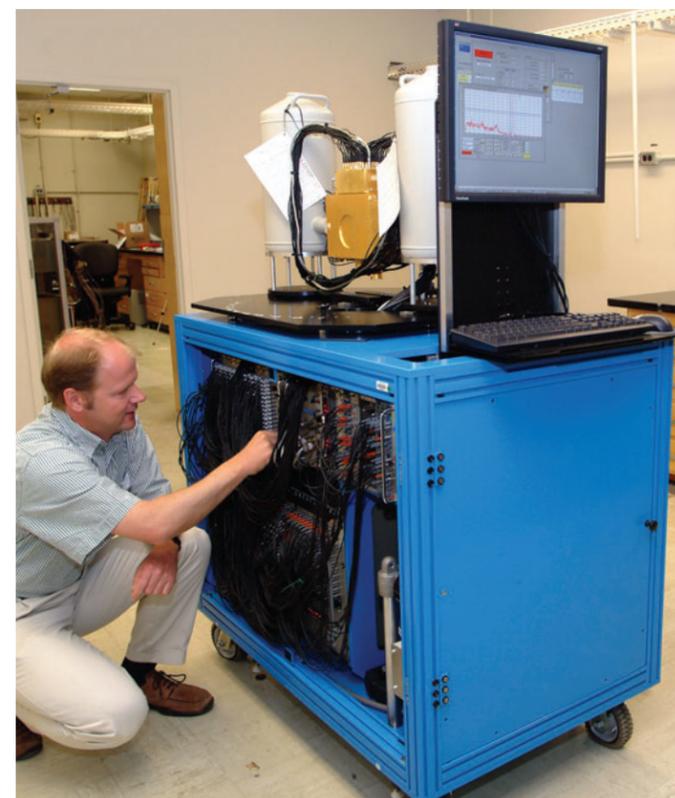


Figure 1. Our first transportable, hybrid Compton imaging system has a large silicon detector and a large germanium detector mounted on the top. The fully digital acquisition system includes a computer and a monitor to control the system and to display histograms.

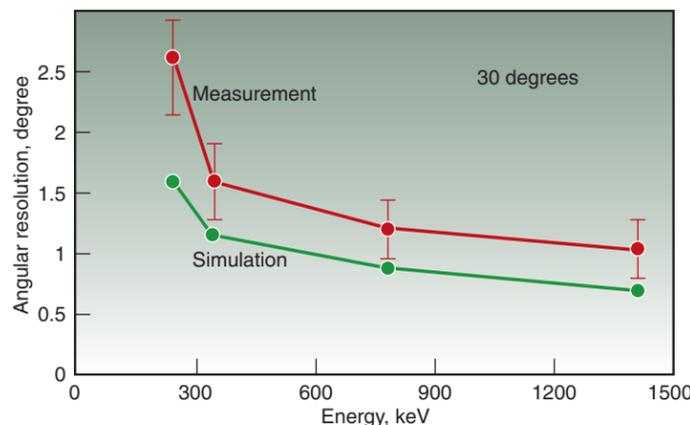


Figure 2. We have achieved angular resolution values of 1–3 degrees for energies ranging from 244 to 1408 keV. This plot illustrates measured (red) and calculated (green) angular resolution for different gamma-ray energies at a source location of 30 degrees.

## NEW FRONTIERS

The technologies we are developing will help address some of the outstanding questions in fundamental physics and biomedical research. One of these questions in physics relates to the mass and characteristic of neutrinos—fundamental particles that exist in our world in large numbers. By measuring the mass of the neutrino, we may prove that a neutrino is its own antiparticle. We can accomplish this by observing the so-called neutrinoless double decay—an extremely rare process, in which a nucleus undergoes two simultaneous beta decays without emitting a neutrino. The challenge in such experiments is to suppress background events, which can be very effectively done by employing the same gamma-ray tracking concept needed for Compton imaging.

The high efficiency and high position resolution of this detector could also enable imaging of small animals with unprecedented sensitivity.

will potentially help detect nuclear threats at U.S. borders, in transit to potential targets, or in place prior to a terrorist attack. However, there is a wide range of applications for our imager. We are exploring ways to increase the sensitivity over state-of-the-art systems in other areas such as biomedical research, where we could perform small-animal imaging with position-emission tomography or single-photon-emission tomography.

## Related Publications

T. Niedermayr, K. Vetter, et al., "Gamma-Ray Imaging with a Coaxial HPGe Detector," *Nucl. Instr. Meth. A* **553**, 501 (2005).

K. Vetter et al., "Gamma-Ray Imaging with Position-Sensitive HPGe Detectors," *Nucl. Instr. Meth. A* **525**, 322 (2004).

K. Vetter, "Recent Developments in the Fabrication and Operation of Germanium Detectors," *Annu. Rev. Nucl. Part. Sci.*, in press.

# CHEMISTRY AND MATERIALS SCIENCE

# *Dynamic Teams*

*Our researchers combine science with a dynamic organizational structure. We have three divisions that maintain a close relationship with Laboratory programs, working with directorate and program leaders to ensure an effective response to programmatic needs. This section of our annual report describes our divisions, the laboratories, and facilities where our scientists work; our postdoctoral program; and the awards and recognition that CMS has won in 2005.*

- **Chemical Biology and Nuclear Science Division**
- **Chemistry and Chemical Engineering Division**
- **Materials Science and Technology Division**
- **Postdoctoral Fellows**
- **Awards and Recognition**

# Chemical Biology and Nuclear Science Division

*To provide unique and integrated solutions to issues at the intersection of chemical, biological, and nuclear science and to sustain a strong and viable life-sciences expertise*

**C**hemical Biology and Nuclear Science Division (CBND) core competencies include radio- and isotopic chemistry, radiation measurements, forensic and analytical chemistry, and bionanoscience, which includes biophysical chemistry and protein engineering. The division supports programs throughout the Laboratory, primarily the Stockpile Stewardship Program, counterterrorism and nonproliferation, and energy and environment.

## Strategic Theme-Related Accomplishments in 2005

CBND strengths are strongly aligned with the CMS research themes of science in support of national objectives at the

intersection of chemistry, materials science, and biology; and applied nuclear science for human health and national security. Our accomplishments in this thematic area during 2005 are described in the following sections.

**New Bioimaging Tools.** CBND is using chemical imaging of biological materials to advance our understanding of biochemical processes relevant to our biosecurity mission as well as the energy and environment area. Using atomic force microscopy (AFM), we have systematically studied the molecular architecture and structural variability of pathogen surfaces in vitro to determine spatial, temporal, developmental, and environmental organizational scales. We

were the first to observe that spore coat architecture and topology are environmentally influenced, and that AFM analysis can be used to help reconstruct the environmental conditions present during spore formation and processing. This methodology is now being implemented to support several bioweapons attribution efforts.

We have also developed new imaging methodologies that can be applied to many areas, including noninvasive understanding of host-pathogen interactions, growth and function of microbial communities, and human health. In one of these methodologies, we showed the

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feasibility of using nanoparticle-based probes for in situ monitoring of biological processes. In another, we applied high-sensitivity, high-resolution, molecular-resonance imaging and spectroscopy to understand the initiation stages of biofilm formation.

**New Chemical and Biological Weapon Detection Platforms.** This year, CBND was very successful in exploiting our dual expertise in materials science and analytical methods to develop platforms for chemical and bioagent detection. In partnership with the University of Washington, and Honeywell, we successfully created advanced gas chromatography separation

columns with the stationary phase constructed from carbon nanotubes. Our team demonstrated the fastest separation by gas chromatography to date using on-chip temperature programming and carbon nanotubes. This accomplishment represents a significant advance in the field of gas chromatography. Our bioaerosol mass spectrometry team exceeded their remarkable successes of the last few years by winning a 2005 R&D 100 Award for their analytical system, which can identify dilute aerosolized biothreat agents in seconds with minimal false positives.

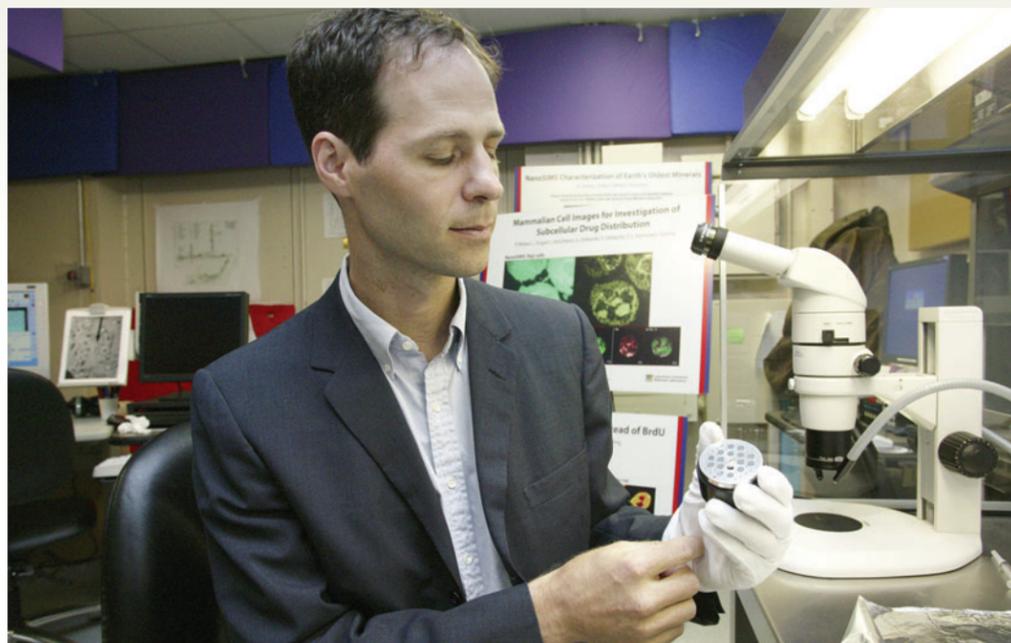


Through the effective deployment of mobile systems such as a Department of Homeland Security van shown here, Livermore is providing expertise in radiation detection to support our nation's counterterrorism efforts.



Screening at U.S. ports of entry requires a broad-based approach in technology development. CMS scientists rely on our enduring capabilities in radiation measurements and isotopic chemistry to develop new tools for radiation detection.

We use nanoSIMS, a secondary-ion mass spectrometer with nanometer-scale resolution, for biological and nuclear forensics. The nanoSIMS allows us to investigate biological samples such as bioagents or cancer at the subcellular level.



**Nuclear Nonproliferation and Counterterrorism.** CBND continues to successfully deliver services to LLNL nuclear nonproliferation and counterterrorism programs. Our radiation measurements group worked for the Department of Homeland Security's Countermeasures Test Bed Program and received the Undersecretary for Science and Technologies Award last year. Our scientists continue to maintain world-class analytical capabilities that support LLNL's programs in the weapons of mass destruction attribution area.

CBND also participated in the 18th official proficiency test by the International Organization for the

Prohibition of Chemical Weapons in 2005 and received an "A" grade, maintaining certification with this important international treaty-implementing body. We also successfully completed a national validation exercise to test our responses to potential post-detonation nuclear events. More recently, we began a new nonproliferation project funded by NNSA to develop methods to detect diversion of nuclear materials from spent-fuel ponds.

#### State-of-the-Art Technologies

CBND applies its unique expertise toward a wide range of analytical chemistry disciplines. For example, our support for homeland security takes

advantage of parallel expertise in actinide chemistry (nuclear attribution), analytical chemistry (chemical agent detection), and molecular recognition chemistry (bioagent detection). We apply these areas of expertise through our scientific centers, which house state-of-the-art facilities, including one of 10 nanoSIMS instruments in the United States. The nanoSIMS is a secondary-ion mass spectrometer that combines nanometer-scale spatial resolution with part-per-million ( $\mu\text{g/g}$ ) sensitivity. Our scientific centers also house mass-spectrometry and nuclear magnetic resonance facilities and AFM laboratories.

## LABORATORIES AND SCIENTIFIC FACILITIES

**BioSecurity and Nanosciences Laboratory.** The BioSecurity and Nanosciences Laboratory (BSNL) is a multidisciplinary, multiprogrammatic initiative at LLNL whose mission is to provide the nation with scientific expertise and capabilities to protect the nation against biological threats and natural disease outbreaks. CBND uses the BSNL to conduct research in proteomic analysis, bioaerosol science, pathogen signatures, bioorganic synthesis, nanofabrication of device platforms, and cellular- and molecular-scale measurements. The BSNL has brought together a unique suite of analytical tools that provide advanced characterization capabilities at the molecular to single organism level. The BSNL AFM laboratories, for example, can determine structure with single-protein spatial resolution, measure interaction forces at the single-molecule level, and determine the chemical pattern of surfaces at the 10-nm length scale.

**Forensic Science Center.** The Forensic Science Center (FSC) provides advanced analysis for LLNL's national-security programs in chemical, nuclear, and biological counterterrorism. While serving immediate, short-term needs in these areas, the center also developed a technology portfolio to support long-term missions.

The FSC is recognized as a critical center and scientific asset by a variety of federal agencies, including the Federal Bureau of Investigation, The Department of Homeland Security, and the Food and Drug Administration. The FSC has also been named a member of the Food Emergency Response Network, a national sentinel laboratory system that monitors and analyzes potential threats to the national food supply. The FSC receives, analyzes, and identifies unknown samples for all types of threats. We leverage this expertise in a number of ways to support established collaborations and provide leadership to emerging national and interagency efforts in the areas of national security, nonproliferation, and intelligence support.



Through the Laboratory's Student Employee Graduate Research Fellowship Program, a University of Davis student works on a bioaerosol mass spectrometer at LLNL. This instrument can detect and identify spores at low concentrations in less than a minute.

# Chemistry and Chemical Engineering Division

*Science and engineering for investigating the chemical properties, reactivity, and synthesis of energetic and optical materials*

The Chemistry and Chemical Engineering Division (CChED) conducts research and development in the areas of chemistry and chemical engineering in support of LLNL's programmatic missions. Many of the chemical processes of interest to these programs occur under conditions of very high temperatures and pressures. Such extreme conditions are relevant, for instance, to nuclear weapons performance, chemical explosive formulation and testing, and laser fusion experiments at the National Ignition Facility (NIF).

## Strategic Theme-Related Accomplishments in 2005

CChED's strengths are strongly aligned with the CMS research theme of chemistry under extreme conditions and chemical engineering in support of national-security programs.

Our accomplishments in this thematic area during 2005 are described in the following sections.

**Chemistry under Extreme Conditions.** We recently confirmed the existence of superionic water, a unique, nonmolecular form of water predicted to exist under very high pressure (500,000 bars) and temperature (>1200 K) conditions.

Under these conditions, the oxygen atoms form a relatively fixed lattice, while the hydrogen atoms diffuse at a rate similar to the molecules in an ordinary liquid. The existence of superionic water demonstrates that

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common materials can take on exotic forms under extreme conditions. The confirmation involved a combination of high-pressure Raman-scattering experiments, conducted in a diamond anvil cell, and first-principles molecular dynamics (MD) simulations using LLNL's Thunder supercomputer.

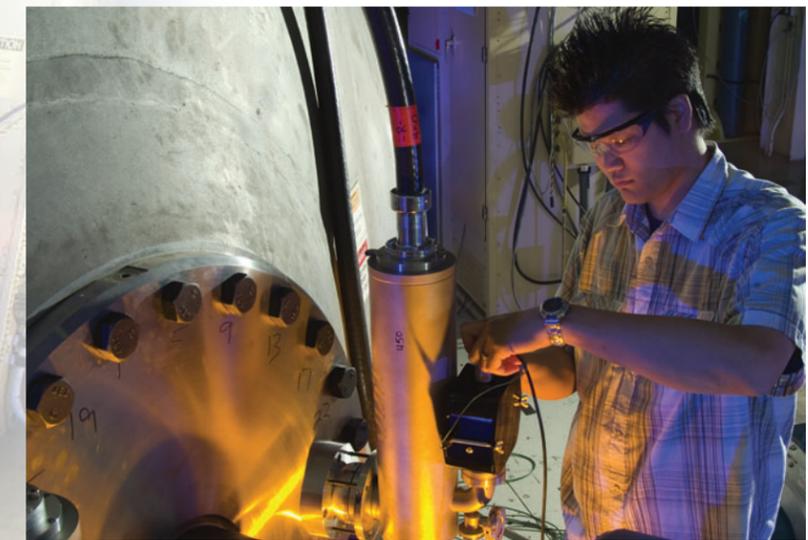
We also demonstrated the existence of a novel polymeric form of formic acid, the simplest carboxylic acid, which is

relevant to numerous fields that range from biology to combustion to cosmochemistry. We found that formic acid links into hydrogen-bonded chains at pressures above 130,000 bars. At pressures above 300,000 bars, the chains themselves cross-link.

**Support to Defense Programs.** Using the capabilities of the High Explosives Applications Facility (HEAF), we showed that a mixture of single-walled carbon

nanotubes and high explosives can be detonated by ordinary light. In the past, optical ignition and initiation of energetic materials could only be accomplished using high-power lasers with a very specific pulse length, wavelength, and spot size. Our new results show that optical initiation of energetic materials is possible using ordinary light sources with milliwatt power, leading to new uses such as explosively operated safety systems on space shuttle rockets or aircraft exit doors.

At Livermore's High Explosives Application Facility, scientists conduct hydrotests and other shock experiments in the spherical firing tank. By conducting high-explosives detonations, we improve our understanding of how steel and other materials fail.



A scientist adjusts diagnostics outside the High Explosives Application Facility's spherical firing tank. We use dynamic x-ray imaging with diagnostics such as fast framing cameras, spectroscopy, velocimetry, and embedded fibers to gather data on the processes occurring in our experiments.

In other explosives-related work, we used the Hydra x-ray system in HEAF's Energetic Materials Center to investigate the shock response, deformation, failure, fragmentation, and spallation of metals to validate hydrocodes. These experiments produced very detailed, real-time radiographs that identified features not predicted by the codes and greatly increased our understanding of material response to intense shock.

We developed the offline solid-phase microextraction technique to nondestructively assess the internal chemistry of the nation's nuclear stockpile. This technique allows us to evaluate a weapon's health and will help us develop life-performance predictions for materials and assemblies.

As part of our efforts to model the chemistry of detonations, we validated the Cheetah thermochemical code with equation-of-state data derived from first-principles simulations of water. These

simulations showed the importance of including ions in a treatment of high-pressure chemistry, so we are modifying the Cheetah code to take ions into account. This will substantially improve our ability to predict how energetic materials perform.

**Advanced Materials Synthesis.** We have been improving the sol-gel process to tailor aerogel properties for specific applications. In one example, we developed ultralow-density, high-surface-area nanoporous  $\text{GeO}_2$ , which is of interest for optical systems, for charge-storage elements in memory devices, and for an easily removable/dissolvable template for the synthesis of other nanoporous solids. We also improved the techniques to prepare nanostructured  $\text{SnO}_2$  for use in new high-performance devices, such as gas sensors, biosensors, batteries, and catalysts. Our sol-gel method is a great improvement on the traditional process, which required highly

reactive precursors, complex solvent systems, and/or elevated temperatures. Nanoporous metals also hold great promise for NIF laser fusion targets, as well as a wide range of other applications, such as catalysis, energy storage and conversion, sensors/detectors, and nanoelectronics.

**Support to NIF.** CChED's work for NIF includes developing novel materials for use in laser targets and production of large optics. This year, we repeatedly broke our own records for the largest, rapidly grown potassium dihydrogen phosphate (KDP) crystal. These advances were possible because of new research on how the characteristics of the seed crystal affect the characteristics of the final product crystal. In addition, we optimized the operating conditions for producing crystals with favorable aspect ratios, thereby increasing the yield.

Livermore scientists use the Laboratory's supercomputers to perform molecular dynamics (MD) simulations. Recent MD experiments helped confirm the existence of superionic water and a new mechanism for the production of coherent radiation.



## LABORATORIES AND SCIENTIFIC FACILITIES

**Advanced Chemical Synthesis and Processing Laboratories.** CChED has more than 3000 ft<sup>2</sup> of chemistry laboratory space with equipment for synthesizing and purifying reagents and other products. These laboratories house special autoclaves and supercritical solvent extractors for making large monoliths of aerogels, as well as vacuum and controlled-atmosphere ovens and furnaces for thermal treatments such as sintering and pyrolysis. We maintain an in-house suite of spectroscopic and characterization tools and make extensive use of the other characterization facilities within CMS and around LLNL.

**Energetic Materials Center (EMC).** The EMC uses the capabilities of HEAF and Site 300 to gain a

detailed understanding of the chemistry and physics of energetic materials in support of their many applications to national defense. HEAF and Site 300 house unique facilities for the synthesis, characterization, and testing of high explosives and other energetic materials. In addition, HEAF and Site 300 are equipped with extensive, high-fidelity, high-speed diagnostic capabilities, including x-ray radiography, high-speed photography, laser velocimetry, and embedded particle velocity and pressure measurements. We conduct experiments at these facilities to develop and test new explosive formulations, study how aging affects the properties of explosives, understand how materials deform under shock loading, and characterize the basic chemistry and physics of detonations.



We are working to improve the performance of optical systems by identifying the structure of the defect precursors leading to damage in optical materials. Our research will enable material improvements to crystals used in the National Ignition Facility.

# Materials Science and Technology Division

*Providing a fundamental scientific capability for predicting the properties and performance of materials under extreme conditions*

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The Materials Science and Technology Division (MSTD) supports major Laboratory programs and executes world-class research and development in a wide range of disciplines. Our program is aligned with specific projects supporting the U.S. Stockpile Stewardship Program, the National Ignition Facility (NIF), the Yucca Mountain Project, and the nation's counterproliferation efforts.

## Strategic Theme-Related Accomplishments in 2005

MSTD's strengths are strongly aligned with the CMS research theme of materials properties and performance under extreme conditions. Our accomplishments in this thematic area during 2005 are described in the following sections.

**Materials Dynamics.** MSTD applies multiple approaches—including time-resolved dynamic observations, recovery-

based observations, and large-scale computational modeling—to better understand how extreme dynamic stress affects a material's phase, strength, and damage evolution.

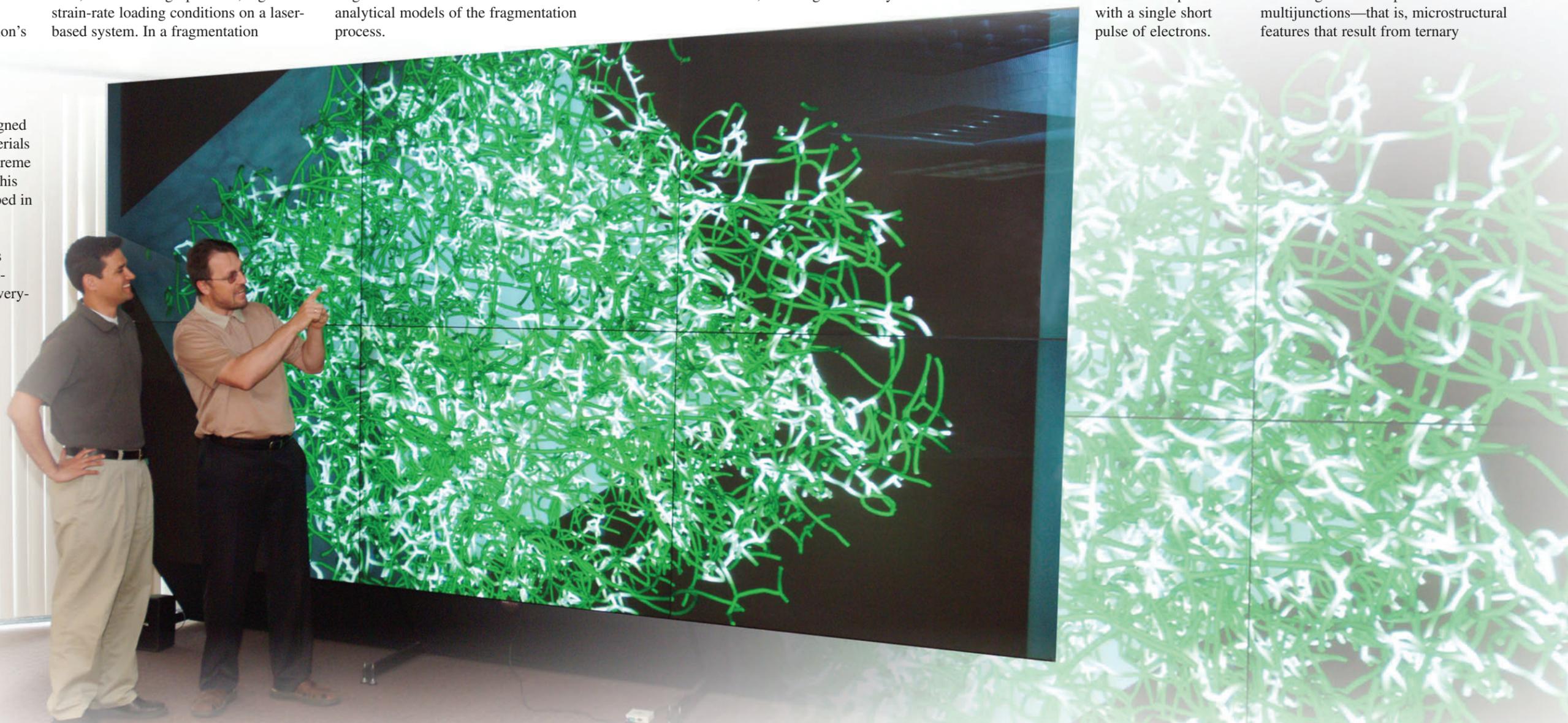
Our studies of material deformation mechanisms demonstrated, for the first time, control of high-pressure, high-strain-rate loading conditions on a laser-based system. In a fragmentation

experiment on stainless steel at Site 300, we loaded a stainless steel spherical cap with high explosives. Using high-speed optics and soft recovery of the fragments, we were able to calculate the uniform strain before failure and the failure time. The measurements of the recovered fragments were also used to calibrate analytical models of the fragmentation process.

**Ultrafast Science.** In addition to x-ray and optical techniques, we are using electrons as an ultrafast probe of dynamic processes in both our transmission electron microscope (TEM) and dynamic TEM (DTEM). The TEM captures images at high spatial resolution, allowing us to study the

defects in materials that often control material behavior. Our DTEM, a modified TEM, has high temporal resolution in addition to high spatial resolution. This spatial resolution is significantly better than that achieved previously and demonstrates that high resolution is possible with a single short pulse of electrons.

**Computational Materials Science.** MSTD simulates the dynamic behavior of materials across multiple length and time scales on the world's largest parallel computers. This year, in the Parallel Dislocation Simulator (ParaDiS) project, we uncovered a new mechanism for strain hardening due to the proliferation of multijunctions—that is, microstructural features that result from ternary



Livermore scientists Tom Arsenlis (left) and Vasily Bulatov (right) are gaining new insight on dislocation dynamics and how materials deform and fail by combining advances in supercomputing and materials experiments and characterization. This simulation, done as part of the ParaDiS project, shows the formation of multijunctions, which tie together three or more dislocation lines into tight knots.

dislocation reactions. We used large-scale molecular dynamic (MD) simulations to study the strength and ductility of nanocrystalline metals at high pressures under shock conditions. Our results showed that the strength of these materials is enhanced at these conditions as compared to ambient pressures. Other large-scale MD simulations on the dynamic loading of irradiated materials have shown that the nanoscale voids that remain from the annealing of displacement cascades can affect a

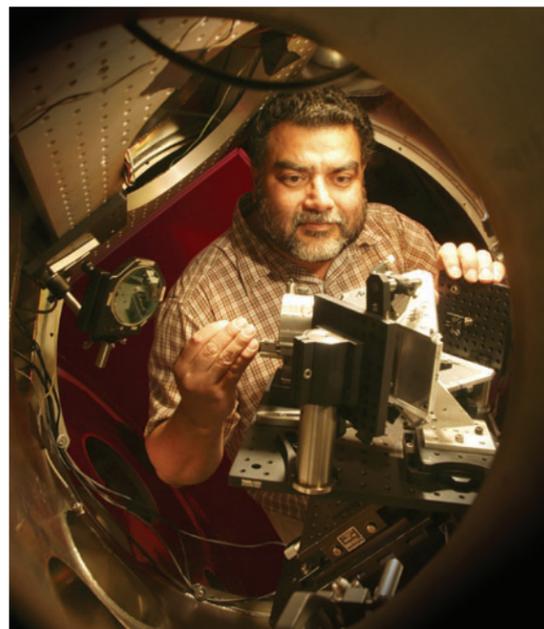
material's equation of state under dynamic loading conditions.

**Nanoporous Metals.** We are working to clarify the high strength and failure mechanism of nanoporous foams under compression/tension using nanomechanical testing and MD simulations on LLNL's massively parallel Thunder supercomputer. Micrometer-sized pillars of nanoporous gold were fabricated by focused ion beam (FIB) and tested under compression in collaboration with Forschungszentrum

Karlsruhe in Germany. Based on the nanomechanical tests (nanoindentation and pillar compression), we were able to study nanoporous gold foam ranging from 60–80% porosity and with pore sizes ranging from 5–900 nm. This has allowed us to calculate new scaling equations for open-cell nanoporous foams based on foam porosity and pore size. We compared the new scaling equations to experimental results on nanoporous platinum and copper and have accurately predicted their mechanical behavior.



Warren Moberlychan (left) and Nick Teslich (right) use focused ion beam (FIB) technology to fabricate materials with tolerances as fine as 10 nm and to characterize material with resolutions as fine as 2 nm. FIB technology is being used to modify NIF targets, prepare and analyze biological samples, and to create ion-beam rippling of surfaces.



Using ultrabright, ultrafast x-ray sources at high-energy laser and accelerator facilities, CMS scientists are directly probing the lattice of the shocked solid to better understand how extreme dynamic stress affects a material's phase, strength, and damage evolution. In this photo, Hector Lorenzana checks target and detector alignment in the vacuum chamber of the LLNL Janus Laser.

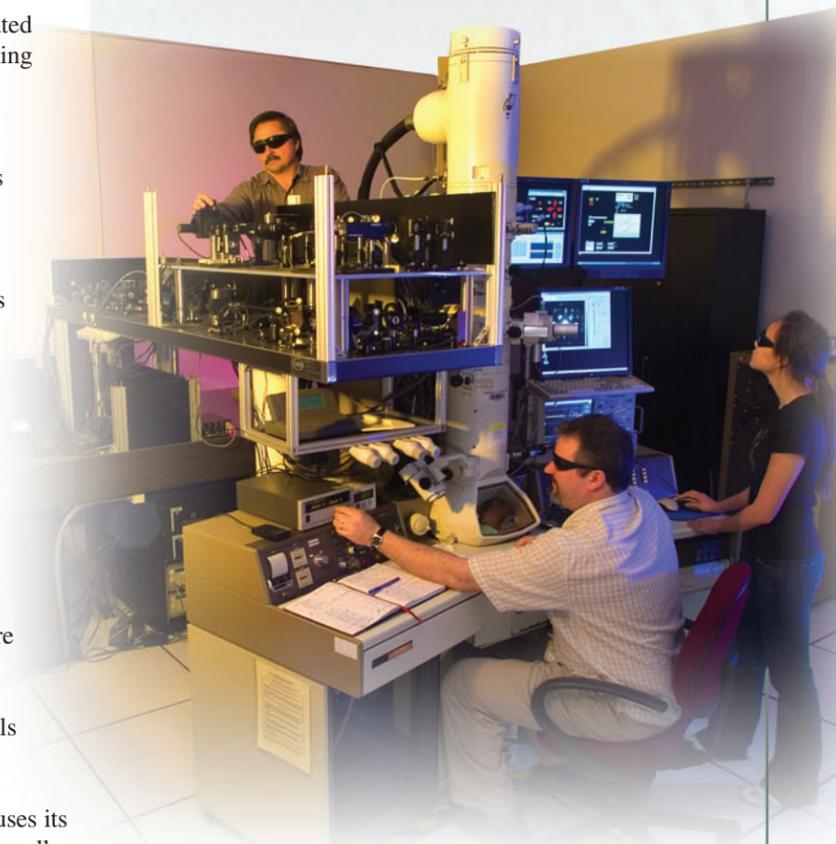
## LABORATORIES AND SCIENTIFIC FACILITIES

**Dynamic Transmission Electron Microscope.** MSTD uses the DTEM, which provides high-resolution imaging and diffraction, to study material properties. The DTEM is a modified TEM that provides high time resolution by creating short, intense electron pulses to illuminate the specimen. These pulses are created by striking a photocathode with an ultraviolet laser pulse, which stimulates photoemission from a large quantity of electrons. The electrons are accelerated and focused onto the specimen and then magnified to produce the image. The image is formed when the electrons strike a scintillator that converts the energetic electrons to photons that are then brought to a charge-coupled device. A second laser strikes the specimen, stimulating the response that is to be investigated in situ during the experiment. The relative timing of the two lasers sets the timing of the observation.

**Site 300.** Another facility essential to MSTD's work with materials performance under extreme conditions is Site 300, Livermore's high explosives testing site. Applying a sophisticated soft recovery procedure that uses deceleration through materials of steadily increasing densities to capture the fragments undamaged, a crew of experts uses a suite of diagnostics to analyze the shot. Site 300 has outdoor firing facilities with specialty diagnostic equipment, such as line velocity interferometry system for any reflector or low-energy x-ray radiography, as well as complementary experimental capabilities, such as the Contained Firing Facility (CFF). The CFF has high-speed optics and can acquire multibeam Fabry-Perot velocimetry and high-energy flash x-ray radiography, all in a contained setting to prevent release of materials to the environment.

**Radiological Materials Area.** MSTD also uses its radiological materials area (RMA) to conduct small-scale experiments on actinides—which include the nuclear weapon metals uranium and plutonium. The RMA has two dry-train glove boxes used to prepare actinide samples for a variety of onsite and offsite

experiments, including TEM, optical microscopy, resistometry, x-ray diffraction, magnetic property measurements, differential scanning calorimetry, extended x-ray absorption fine structure, and phonon dispersion studies. In these experiments, we seek to provide greater insight about an atom's inner 5f electron bands or shells, which can move about, resulting in changes in material properties and molecular structures. By connecting the 5f electronic structure to observed chemical reactions and structural phase transformations, we gain a fuller understanding of extreme materials in support of our stockpile stewardship work.



Livermore scientists conduct research on the dynamic transmission electron microscope, which uses electrons as an ultrafast probe of dynamic processes, yielding images at high spatial and high temporal resolution.

# Postdoctoral Fellows and Graduate Students

The CMS Postdoctoral Program continues to attract excellent young scientists to LLNL. They come from top universities around the world, bringing fresh ideas and leading-edge skills to our community. Recently the CMS Postdoctoral Program joined the Glenn T. Seaborg Institute to expand and make education even more central within CMS. The program has grown to include more than 50 postdoctoral researchers who are making significant contributions to key Laboratory programs and carrying out excellent basic science research, while still maintaining close ties to external collaborators. There are also about 20 graduate students pursuing degrees within CMS, each under the joint supervision of a CMS scientist and a faculty thesis advisor. The postdoctoral and graduate students, grouped according to our current strategic research areas, include the following:

## Ultrafast Materials Science

**Michael Armstrong** (University of Rochester) is working on applications of the dynamic transmission electron

microscopy (DTEM) for ultrafast analysis of phase transition kinetics. **Thomas LaGrange** (Swiss Federal Institute of Technology) is also using the DTEM to investigate thermally driven phase transformations in materials relevant to high-energy-density physics.

## Nanoscale Materials Science and Technology

**Robert Meulenberg** (UC Santa Barbara) is studying materials that are highly luminescent in the infrared range by using rare-earth (lanthanide) doping on group IV nanocrystals. **Raluca Negres** (Central Florida) is studying defect reactions associated with laser-induced damage in nonlinear optical crystals. **Yinmin "Morris" Wang** (Johns Hopkins) is working on deformation mechanisms of nanocrystalline materials and synthesis techniques for fabricating high-energy-density experimental targets for the National Ignition Facility. **Trevor Willey** (UC Davis) is using small-angle x-ray scattering to determine nanostructures in explosives and aerogels and the electronic structure in subnanometer diamondoids.

## Nuclear Materials Stewardship

**Bassem El-Dasher** (Carnegie Mellon) is studying the phase stability and crystalline interface behavior of the welds that will be used in the outer barrier of the Yucca Mountain waste containment. **Jeremy Gray** (UC Davis) is using atomic force microscopy (AFM) to understand shape control of nanoparticles and to characterize the corrosion properties of nuclear waste containment material.

## Correlated Electron Systems and Alloy Properties

**Sung Woo Yu** (Universität Bielefeld, Germany) is using spin-resolved photoemission spectroscopy to investigate electron correlations in complex systems. **David Clatterbuck** (UC Berkeley) contributed to measurements of the phonon dispersion curves and studying phase transformation behavior of plutonium using synchrotron radiation-based methods. **Martin Butterfield** (Loughborough, U.K.) has been carrying out spectroscopic studies of actinides, and **Scott McCall** (Florida State University) has been searching for a quantum critical

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Keith Coffee was part of the team that won an R&D 100 Award for work on the bio-aerosol mass spectrometer (BAMS), an instrument that can detect and identify pathogens at low concentrations in less than 1 minute.



point in plutonium/ americium alloys with low-temperature experiments on physical properties such as magnetization, resistivity, and specific heat. **Benoit Oudot** (Université de Franche-Comté, France) is investigating the stability of the high-temperature  $\delta$  phase and the kinetics of the  $\delta$ -to- $\alpha'$  transformation in plutonium-gallium alloys.

## High-Performance Computing

**Masato Hiratani** (Michigan Tech) carried out stochastic computer simulations of dislocation dynamics under various extreme conditions such as irradiation and annealing and incorporated analysis tools such as pattern analysis and chaos and fractal theory.

## Stockpile Metallurgy and Joining

**Jikou (James) Zhou** (Princeton) is using his background in functionalized magnetic nanoparticles to investigate structure-property relationships in stockpile-related materials.

## Extreme Chemistry

**Nir Goldman** (UC Berkeley) has used first-principles molecular dynamics to study superionic phases of simple molecules, including water. Lawrence Fellow **Evan Reed** (MIT) is using computational and theoretical techniques to study optical emissions from shock waves in crystals and is developing multiscale simulation methods for shock waves. **Naida Lacevic** (Johns Hopkins) is modeling polymeric crystallization and

using course-grained atomistic models of polymer composites to provide crucial information about structure-property relationships of polymeric systems. **Thaddeus Norman** (UC Santa Cruz) is characterizing the time-dependent photo- and radio-luminescent properties of transparent ceramic scintillator materials prepared from nanoparticle precursors.

## Advanced Material Synthesis

**Yong Han** (UC Santa Barbara) is applying his background in interfacial chemistry to develop bio-inspired synthetic routes for novel inorganic materials. **Joshua Kuntz** (UC Davis) is employing consolidation techniques such as spark plasma sintering to synthesize low-density aerogels.

### Environmental Radiochemistry and Radiation Measurements

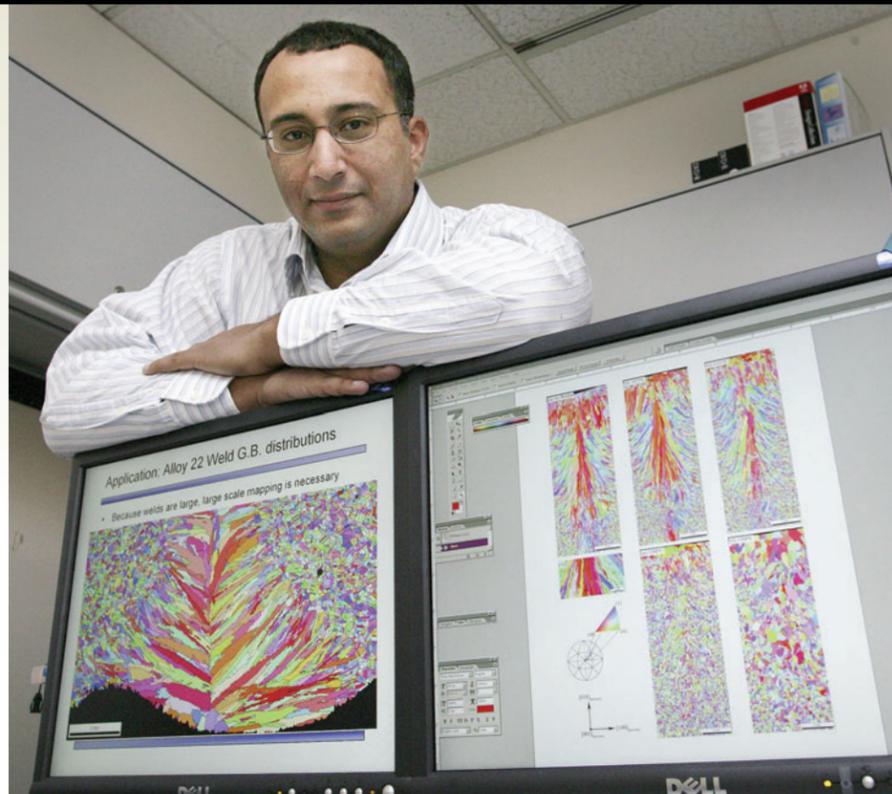
**Michael Singleton** (Washington University) is working on groundwater contamination by nitrates in California. **David Campbell** (Florida State) is examining mobile radiation detection systems for homeland-security applications and refining pulse-shape analysis algorithms for segmented high-purity germanium detectors.

### Chemical and Isotopic Signatures

**Jerome Aleon** (Institut National Polytechnique de Lorraine, France) is performing isotope analysis of interplanetary materials such as zircons and cometary samples returned from the Stardust mission. **Sutapa Ghosal** (UC Irvine) is using nanoSIMS to investigate detection of biological weapon agents, and **Jennifer Pett-Ridge** (UC Berkeley) is using the instrument for studies on nanoscale patterns of nitrogen and carbon fixation in marine cyanobacteria.

### Bioorganic Synthesis and Protein Chemistry

**Richard Kimura** (UC Davis) is developing methods with protein-splicing tools for biosynthesis of cyclic peptides containing cysteine knots. **Youngeun Kwon** (University of Chicago) is developing protein microarrays by using



Bassem El-Dasher received ASM International's 2005 Henry Marion Howe Medal for his contribution to a project that creates 3D models of materials. The new method saves an enormous amount of time compared to older methods, and is now being applied to the Yucca Mountain project.

chemical synthesis of proteins and engineering of biologically expressed proteins. **Saphon Hok** (UC Davis) is using dynamic combinatorial chemistry for target-driven ligand development to identify synthetic high-affinity ligands for tetanus toxin C fragments. **John LaTour** (Princeton) is using organic synthesis techniques to functionalize biosensors. **Youn-hi Woo** (Oregon State University) is working on traceless in vivo cell labeling, using protein transplicing intein chemistry, to explore DNA-protein interactions. **Nicholas Fischer** (University of Massachusetts, Amherst) is synthesizing a peptide combinatorial library against protein targets to explore novel biodetection technologies using gold nanocrystals. **David Cordes** (UC Santa Cruz) is developing several sets of new reagents, including recombinant antibodies and synthetic

molecules that bind selectively to unique protein signatures of biotoxins.

### Molecular Biophysics and Functional Nanostructures

**Michael Stadermann** (University of North Carolina) is investigating the use of carbon nanotubes in gas chromatography and as transducer elements in chemical sensors. **Jason Holt** (California Institute of Technology) is studying nanoscale fluid mechanics and developing carbon-nanotube-based permeable membranes for separation processes such as desalination and dialysis. **Tim Ratto** (UC Davis) is using molecular recognition force spectroscopy to investigate the adhesive properties of bacterial spores to decontamination materials, and designing fluidic membranes for protein production and analysis. **Shuhuai Yao** (Stanford) is developing ultrafast microfluidic mixers for the study of protein-folding reactions.



Livermore's dynamic transmission electron microscope uses electrons as an ultrafast probe of dynamic processes, yielding images at high spatial and high temporal resolution. The image shows alternating gold and carbon layers in which the fine structure around 30 nm is discernable.

### Biomaterials Sciences and Molecular Imaging

**Jonathan Lee** (Cambridge, U.K.) is using x-ray absorption spectroscopy for structural studies of biomimetic inorganic crystal growth on organic templates. **Jennifer Giocondi** (Carnegie Mellon) is conducting experiments to determine the modulation of the calcium phosphate biominerals crystal growth by ionic and organic modifiers. **Marco Plomp** (University of Nijmegen, The Netherlands) is using AFM to study the nanoscale structure of viruses and spores. **Sung Wook Chung** (UCLA) is investigating the macromolecular assemblies on surfaces using scanned probe microscopy. Lawrence Fellow **Yu Huang** (Harvard) is identifying biomolecules that bind to specific substrates and investigating the assembly kinetics they use to control inorganic minerals.

### Physical Biosciences

**Amy Hiddessen** (University of Pennsylvania) is developing bioengineered tools to understand the mechanisms of cellular response to chemical signals. **Chris Jeans** (Imperial College, U.K.) is employing single molecule AFM techniques to determine the nature of packing interactions in chromatin. **Ted Laurence** (UCLA) uses surface-enhanced Raman scattering for intracellular chemical measurements. **Nan Shen** (Harvard) is developing optical techniques to investigate spatially distinctive subcellular structures. **Todd Sulchek** (Stanford) has performed force measurements to measure binding interactions of cancer cell antibodies. **Jianhua Xing** (UC Berkeley) is a theoretical biophysicist whose research focuses on modeling how protein motors convert chemical energy into mechanical work.

### Bio Mass Spectrometry

**Keith Coffee** (UC Riverside) is part of the bioaerosol mass spectrometry (BAMS) group where he is studying the feasibility of combining aerosol particle size, fluorescence, and mass-spectrum signatures to detect and identify harmful biological particles such as bacterial cells and spores, viruses, or chemical toxins. **George Farquar** (Louisiana State University) is using aerosol mass spectroscopy to detect uranium isotopes and explosives.

### CMS Postdoc Symposium

The 2005 CMS Postdoc Symposium featured more than 40 oral and poster presentations showcasing the outstanding research performed in the last year by CMS postdoctoral staff members. **Nir Goldman** was awarded the Hal C. Graboske Jr. Postdoc Award for his outstanding achievements over the last year and his talk entitled, "Simulations of Water in Giant Planets: Discovery of Symmetric H-Bonding in the Superionic Phase." **Naida Laceyvic** won the Best Poster Award for her poster entitled, "Molecular Dynamics Simulations of Spinodal-Assisted Crystallization of Polymer Melts."

# Awards and Recognition in 2005

**R&D 100 AWARDS**

Each year, R&D Magazine recognizes the 100 most technologically significant products of the year. CMS scientists played significant roles in the four R&D 100 awards that Livermore won in 2005 for developing advanced technologies with commercial potential

## Soldering with Localized Heat Source

Nearly every product, from computer chips to airplanes, requires a number of joining steps during manufacturing to form strong and durable metallic bonds without damaging the materials being bonded.

NanoFoil<sup>®</sup>, an outgrowth of the technology used to fabricate multilayer x-ray and extreme ultraviolet optics, is a nanoengineered material that can deliver a rapid and local heat source, replacing the furnaces and torches used in conventional soldering.

The salient intellectual property for NanoFoil<sup>®</sup> was created in work on reactive nanolaminate materials initiated and performed in the laboratory of Troy Barbee Jr., a CMS senior scientist. Now

manufactured and sold exclusively by Reactive NanoTechnologies, Inc., NanoFoil<sup>®</sup> can be used to bond metals, ceramics, semiconductors, and polymers.

NanoFoil<sup>®</sup> delivers just enough heat to melt the solder but not enough to damage a chip. When one end of the foil is pulsed with energy, NanoFoil's thousands of nanolayers of nickel and aluminum begin to chemically react and release heat into the surrounding solder material. This reaction front propagates across the foil, causing the temperature of the reacted area to leap to more than 1500°C while the remainder of the foil is still at room temperature. NanoFoil<sup>®</sup> enables lead-free soldering and brazing of materials at room temperature, making such applications predictable, controllable, and far more affordable.



## Protecting Against Bioterrorism

The release of an airborne pathogen such as anthrax is a significant threat to our national security. Because of the potential damage to human health, experts need to identify the pathogens and take action within minutes. Unfortunately, many commercial systems that can identify airborne pathogenic microbes may take days or, at best, hours to produce results.

Combining laser-induced fluorescence and mass spectrometry, the bioaerosol mass spectrometer (BAMS) is a prototype that can rapidly detect and differentiate a broad range of biothreat agents in real time and without any sample preparation. It is the only instrument that can identify spores at low concentrations in less than 1 minute with almost no false positives.



Currently employed at California borders, the Adaptable Radiation Area Monitor can detect small amounts of radioactive material hidden in a vehicle moving at highway speeds.

## Detecting Radiation and Nuclear Threats

Developed by a team of Livermore researchers, the adaptable radiation area monitor (ARAM) is a unique radiation detector that can pinpoint very small quantities of radioactive materials moving as fast as 60 miles per hour.

ARAM can achieve the highest signal-to-noise ratio to date among comparable detector systems by employing a thallium-doped sodium iodide crystal to detect even very small amounts of radiation. The crystal detects full spectral data and counts single photons, producing large quantities of raw, time-stamped data that can be analyzed in a number of ways.

Already deployed at border crossings, ARAM can also be used as a portable detector or a fixed detector to monitor slow-moving objects, such as packages, luggage, or pedestrians. This system can serve as a stand-alone radiation monitor, or it can be networked into a system of monitors to cover a large area.

The ARAM team shares the R&D 100 Award with Innovative Survivability Technologies of Goleta, California, which licensed the technology in 2004.

## A Better Look at Heart Disease

For more than half a century, three classes of standard tests that measure levels of total cholesterol have been used to assess the risk of heart disease: low-density lipoproteins, high-density lipoproteins, and triglycerides. Unfortunately, these tests cannot precisely measure how many and what type of lipoproteins are pulsing through a person's blood stream.

In collaboration with the Lawrence Berkeley National Laboratory, CMS scientist Henry Benner is developing an easier and more exact means of evaluating the risk of heart disease by accounting for the size, quantity, and distribution of the lipoproteins that carry cholesterol.

This system, known as ion mobility analysis, measures the drift of lipoproteins as they are dragged through air by the force of an electric field. Charge and drift velocity separate the particles by weight and size. The sorted particles are then counted through a detector. Ion mobility analysis is faster and potentially less expensive than current technologies and is likely to be used more frequently in the evaluation and management of risk for cardiovascular disease.

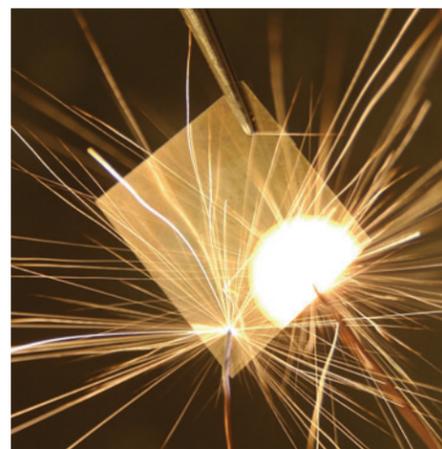


Image courtesy of Reactive NanoTechnologies.



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When a NanoFoil<sup>®</sup> is soldered, the reaction propagates outward at about 5 meters per second. In the reaction region (white area), the temperature has jumped to 1500°C, while the remainder of the foil is still at room temperature.



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# Excellence

## Professional Society Honors

Two CMS scientists were elected fellows of the American Physical Society (APS) in 2005, an honor given to no more than 0.5% of the APS membership:

- **Vasily V. Bulatov** was nominated by APS's Division of Computational Physics for his "outstanding contributions to computational materials science, particularly in the areas of dislocation dynamics and crystal plasticity."

- **Joe Wong** was nominated by APS's Division of Materials Physics for his "innovative and significant contributions to experimental materials physics, particularly for contributions to x-ray absorption fine-structure and x-ray absorption near edge structure, and for the first measurements of phonon dispersion in plutonium."

**Bryan Balazs**, Deputy Enhanced Surveillance Campaign Leader, was appointed to the Board of Trustees of the California Section of the American Chemical Society. The trustees manage the section's trust fund, which supports programs in education, public outreach, and career development.

**Patrice Turchi** was elected 2005 Division Chair of the Electronic, Magnetic, and Photonic Materials Division of the Minerals, Metals & Materials Society.

## Scientific Achievements

**Bassem El-Dasher**, along with a team of Carnegie Mellon colleagues, is a recipient of the ASM International's 2005 Henry Marion Howe Medal for a paper entitled, "Statistically Representative Three-Dimensional Microstructures Based on Orthogonal Observation Sections." This work highlights a revolutionary approach to model three-dimensional microstructures.



Vasily V. Bulatov



Joe Wong



Jeff Kass



Tom Parham



Bryan Balazs



Patrice Turchi



Russ Wallace



Patrick Gallagher



Bassem El-Dasher



Keith Coffee



David Ferguson



Herbert Tobias

The Henry Marion Howe Medal recognizes the authors of the best paper of those published in a given year in a specific volume of *Metallurgical and Materials Transactions*.

CMS scientists were among the recipients of the Laboratory's Science and Technology Award. This award is the highest honor granted by the Laboratory for science and technology accomplishments.

**Eric Gard** led the team that developed the bioaerosol mass spectrometer (BAMS). The BAMS team also won a 2004 R&D 100 Award. Other CMS employees on the team include **Keith Coffee**, **David Ferguson**, and **Herbert Tobias**.

**Jeff Kass** was a member of the National Ignition Facility (NIF) Early Light team that successfully

# Dedication

demonstrated the individual beam performance of the NIF laser and its utility to perform experiments. Other CMS employees on the team include **Tom Parham** and **Russ Wallace**.

## National Recognition

Two CMS projects received the "Best in Class" award, given annually by the Department of Energy's Office of Science. **Reginald Gaylord** and **Patrick Gallagher** are among the recipients who received the award for significantly reducing mixed to low-level waste. **Karen Dodson** led a second team that won an award for the Plutonium Facility tilt-pour furnace process described below.

Livermore's Tilt-Pour Furnace Development Team was recognized by the National Nuclear Security Administration (NNSA) with a Weapons Award of Excellence for developing a new approach for key plutonium pyrochemical operations that can significantly reduce transuranic waste by about 70 percent and plutonium purification time by at least 50 percent. CMS team members include **Karen Dodson** (leader), **Michael Blau**, **Robert Klatt**, **Doug McAvoy**, and **Michael West**.

**Bill McLean** received the Technical Excellence in Weapons Design and Engineering Award from NNSA for developing time-, temperature-, and pressure-dependent models for corrosion in nuclear weapons pits and secondary assemblies. These predictive models were validated against laboratory tests and stockpile surveillance observations and have been applied to all LLNL nuclear weapons systems.

## Leadership Positions

**Wayne King**, Division Leader for Materials Science and Technology Division, was a key organizer for the Forum on High-Energy-Density Science and Ultrafast Science that was sponsored by the University of California (UC) Office of the President.

## Editorships

Many CMS scientists play important roles in their respective professional societies, with about 22 CMS researchers serving as editors or on the editorial boards of technical journals. These scientists provide a valuable connection between CMS and researchers at universities, other national laboratories, and important industries.

## Patents and Licenses

CMS scientists and engineers participated in groundbreaking research that resulted in the following patents in 2005:

Invention Disclosures	34
Patent Applications	10
Patents Issued	8
Licenses Executed	4



Karen Dodson



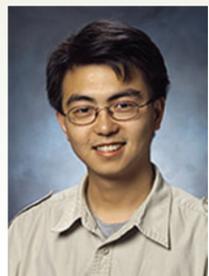
Bill McLean



Wayne King



# Teamwork



Wei Cai



Mike Fluss



Charlie Westbrook



Christian Mailhiot



Joe Satcher



Olgica Bakajin

## Postdoctoral Fellows and Interns

Former Lawrence Fellow **Wei Cai** received the prestigious Presidential Early Career Award for Scientists and Engineers in a White House ceremony for groundbreaking accomplishments early in his career and for his potential for future leadership.

**Molly Darragh** received a National Science Foundation graduate student fellowship. She is now a UC San Francisco graduate student.

## Other Recognition

The *CMS 2004 Annual Report* received an International Award of Excellence in Technical Communications from the Society of Technical Communications. In addition to highlights and accomplishments by more than 30 authors, a team of production staff—including **Mike Fluss**, **Charlie Westbrook**, **George Kitrinis**, **Gabriele Rennie**, and **Stephanie Shang**—contributed to the consistently high quality of the annual report.

## University Collaborations

The research activities of CMS members frequently include technical interactions with leading groups and individuals at universities in the United

States and other countries. Some of these interactions with university research programs are particularly desirable and valuable, and CMS has provided funding to these programs to facilitate interactions (e.g., by granting graduate students and faculty special access to the Laboratory). There were several such active collaborations in 2005:

- Dr. Brian Wirth of UC Berkeley partnered with **Christian Mailhiot** to investigate material degradation and deformation.
- Dr. Mildred Dresselhaus of Massachusetts Institute of Technology partnered with **Joe Satcher** to study carbon aerogels.
- Dr. Shimon Weiss of UC Santa Barbara partnered with **Olgica Bakajin** on microfluidics technology.
- Dr. Todd Ditmire of UC Davis partnered with **Jeff Colvin** to study optical diagnostic techniques.
- Dr. Brenda Anderson of State University of New York, Stony Brook, partnered with **Ian Hutcheon** to investigate imaging methods using the nanoSIMS.
- Dr. Steven Yalisove of University of Michigan partnered with **George Gilmer** to implement characterization tools for ultrafast laser-material interaction.



Jeff Colvin



Ian Hutcheon



George Gilmer

# Pride