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SANDIA TECHNOLOGY

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New avenue to the 5th phase of matter

Sandia National Laboratories

What is LDRD

Sandia's world-class science, technology, and engineering work define the Labs' value to the nation. These capabilities must remain on the cutting edge, because the security of the U.S. depends directly upon them. Sandia's Laboratory Directed Research and Development (LDRD) Program provides the flexibility to invest in long-term, high-risk, and potentially high-pay-off research and development that stretches the Labs' science and technology capabilities.

LDRD supports four primary strategic business objectives: nuclear weapons; nonproliferation and materials assessment; energy and infrastructure assurance; and military technologies and applications; and an emerging strategic objective in homeland security. LDRD also promotes creative and innovative research and development by funding projects that are discretionary, short term, and often high risk, attracting exceptional research talent from across many disciplines.

When the LDRD symbol appears in this issue, it indicates that at some state in the history of the technology or program, LDRD funding played a critical role.

On the Cover:

Sandia Senior Scientist Dave Chandler aligns mirrors used to direct laser beams into an apparatus that generates very cold molecules and measures their velocity. The device causes molecules to collide with atoms to slow them dramatically, cooling them down. The technique may become a first step in efforts to more easily create Bose-Einstein condensates, a phase of matter that is of much interest to scientists. Story on page 8. (Photo by Daniel Strong)

Sandia Technology (ISSN: 1547-5190) is a quarterly journal published by Sandia National Laboratories. Sandia is a multiprogram engineering and science laboratory operated by Sandia Corporation, a Lockheed Martin company, for the Department of Energy. With main facilities in Albuquerque, New Mexico, and Livermore, California, Sandia has broad-based research and development responsibilities for nuclear competitiveness and other areas of importance to the needs of the nation. The Laboratories' principal mission is to support national defense policies by ensuring that the nuclear weapon stockpile meets the highest standards of performance. For more information on Sandia, see our Web site at *http://www.sandia.gov*

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Summer Issue 2004

FROM THE Editor

Dear Readers,

One respected observer of nanotechnology has portrayed present manufacturing as pushing around massive piles of Lego™ blocks with boxing gloves on. We cast, grind, mill and otherwise shuffle giant piles of atoms to create products. The perfection of nanotechnology, the observer explains, will allow us to take off the gloves and snap the building blocks together into smaller, stronger, cheaper, more precise products.

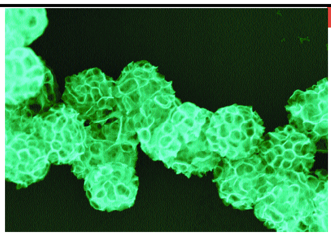
To that end, a large number of Sandia researchers are busy working to understand how to "take off the gloves." Redesigning platinum molecules; creating durable and useful nanocrystal arrays, or quantum dots; and measuring the sometimes counter-intuitive levels of friction in microelectromechanical systems (snapped together from those nanomaterials) are three examples of current Sandia work.

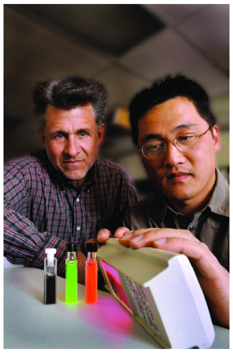
Our cover story looks at Sandia research into slow (cold) molecules as a first step in creating Bose-Einstein condensates, a phase of matter predicted long before science was able to create it. And a DOE announcement naming Sandia to lead a Center of Excellence to investigate hydrogen storage materials as part of the FreedomCAR initiative confirms the Labs' role as an important player in this research field.

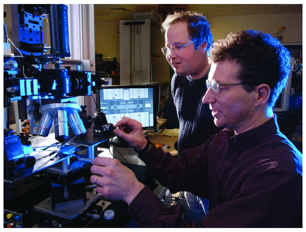
Sandia's Combustion Research Facility (CRF) in Livermore, California, is celebrating its 25th anniversary. Recent research on real-time particulate emissions testing and an alternative piston-engine combustion process shows that the CRF is just as relevant today as it was a quarter-century ago.

Last but not least, Bill Kirchhoff, former program manager for chemical physics in the DOE's Office of Basic Energy Sciences, provides a perspective on CRF's contributions with his "Insights" column.

Will Keener
Editor







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Platinum technology

Researchers "redesigning" platinum

New strides in nanotechnology hold the promise of redesigning platinum so that it can be used in many new applications, including catalysts, sensors, and optoelectronic and magnetic devices.

Researchers have developed a way of changing the properties of platinum by manipulating the metal at the nanoscale. The method mimics the action of photosynthetic proteins.

As a result, the future may see the development of smaller and/or more sensitive catalysts, sensors, and other devices.

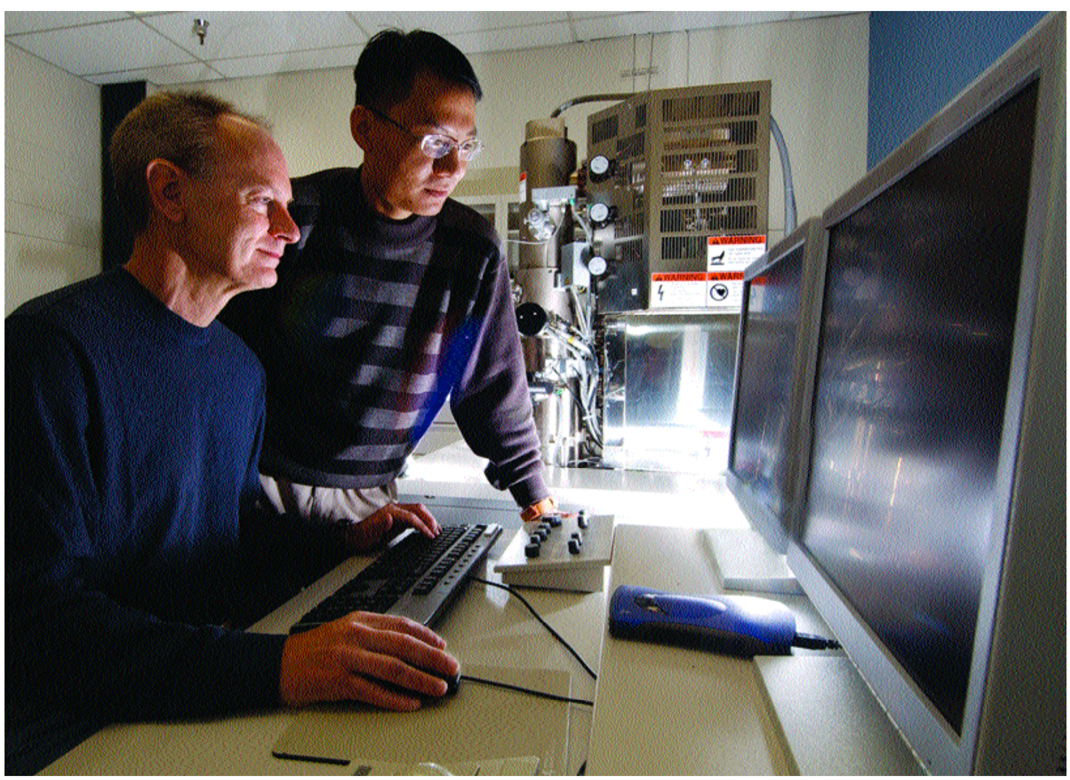
Investigations of the new technique are continuing at Sandia and the University of New Mexico.

"We see the possibility of manipulating the nanoscale structure of platinum so that we can have control over the size, porosity, composition, surface species, solubility, stability, and other functional properties of these metal nanostructures," says Sandia's John Shelnutt.

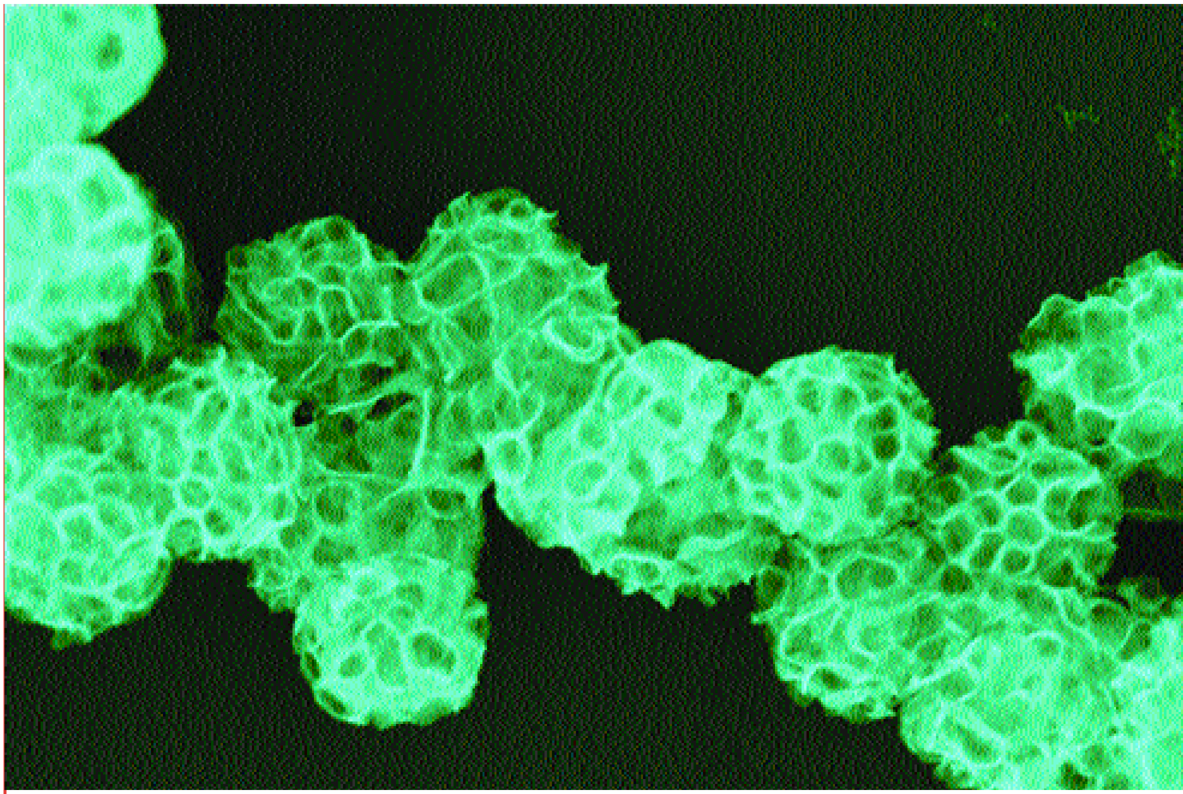
He adds that while research groups have reported a few platinum nano-structures — including nanoparticles, nanowires, nanosheets, and others — the addition of new types of nanostructures is "highly desirable and potentially technologically important."

Like photosynthesis

The idea for the technique is similar to photosynthesis, a process in which plants use the energy from sunlight to produce sugar. But instead of manu-facturing sugar, the new method changes a platinum ion to neutral metal atoms. Certain molecules mimic these photosynthetic proteins, repeatedly converting metal ions each time light is



Sandia researcher John Shelnutt and University of New Mexico Ph.D. student Yujiang Song examine platinum at the nanoscale, using new scanning electron microscope. (Photo by Randy Montoya)



A scanning microscope image of platinum-lace nanoballs. Liposomes aggregate, providing a foam-like template for a platinum sheet to grow.

Platinum nanostructures take on a different form when they are prepared under different conditions.

absorbed and depositing the metal atoms as desired at the nanoscale.

The method involves putting porphyrin molecules — the active part of photosynthetic proteins — along with the platinum salt in an aqueous solution of ascorbic acid at room temperature. When light is shined on the solution, the porphyrins excite, becoming catalysts for platinum reduction and deposition. As this occurs, the metal grows onto the surfaces of the surfactant structures as a thin sheet or in other ways.

For the metals platinum and palladium that form these nanostructures, it is enough for the porphyrin molecule to grow only a small metal "seed" particle composed of about 500 atoms. When it reaches this size, the seed starts to catalyze its own rapid growth (by oxidation of ascorbic acid), budding off arms in all directions and creating the "Koosh™"-ball-like nanostructures.

The platinum nanostructures take on a different form when they are prepared under different conditions — for example they may look like three-dimensional Koosh™ balls or lace-like sheets. Under some solution conditions, growth can give platinum foam-like materials and foam nanoballs.

Since the porphyrin remains attached to the platinum nanostructure and active in the presence of light, it can also perform other functions besides growing itself. For example when illuminated with light, the platinum nanostructure evolves hydrogen from water. This reaction is similar to one of interest to car manufacturers looking for new ways to build automobiles powered by hydrogen fuel cells.

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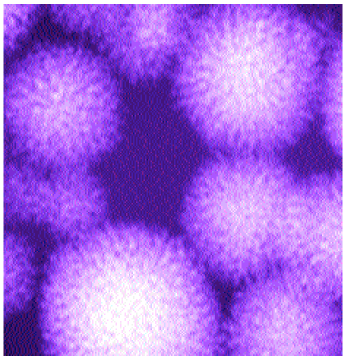
Platinum nanoballs reminiscent of Koosh™ ball toys are captured in scanning and transmission microscope images. Sandia researchers use porphyrin molecules and light to grow these nanoballs.



Nanotools

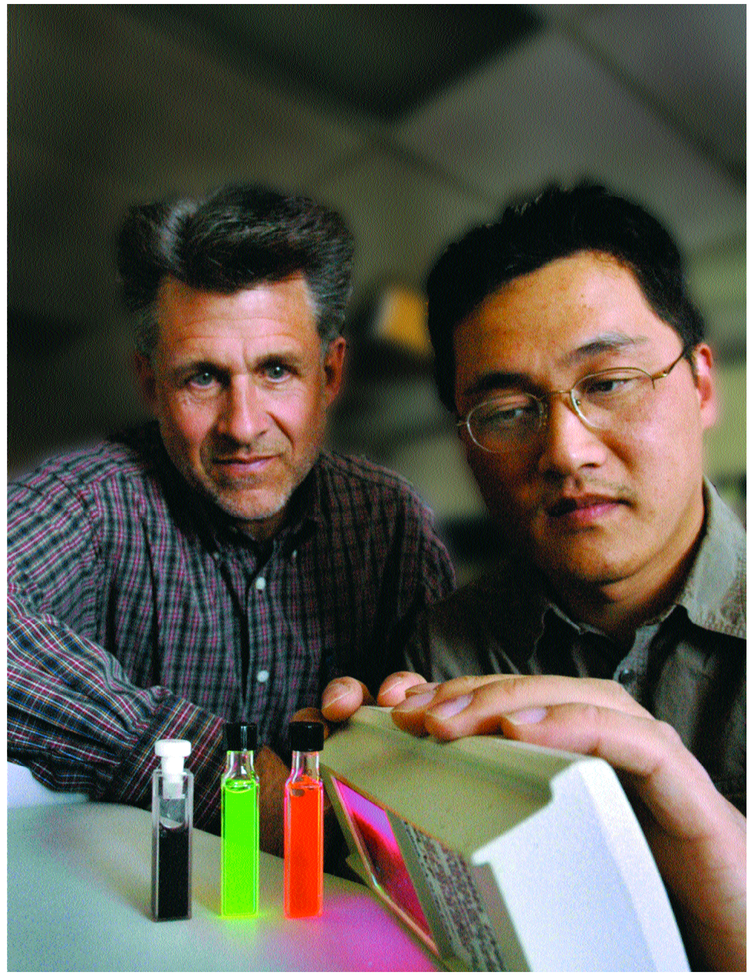
Self-assembling durable nanocrystal arrays

A wish list for nanotechnologists would likely include a simple, inexpensive means of self-assembling nanocrystals into robust, orderly arrangements, like soup cans on a shelf or bricks in a wall, each separated from the next by an insulating layer of silicon dioxide.

The silica matrix could be linked to compatible semi-conductor devices. The trapped nanocrystals might function as a lasing medium, their frequency dependent on their size, or as a very fine catalyst with unusually large surface area, or perhaps a memory device tunable by particle size and composition.

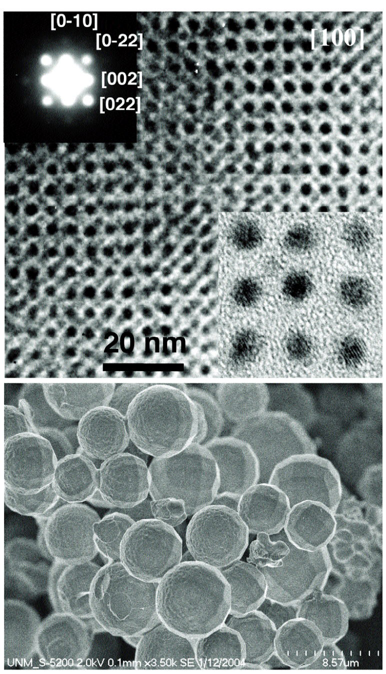
Or perhaps the technologist might want to stop nanocrystals from clumping. Agglom-eration prevents them from being used as light-emitting tagging mechanisms to locate cancer cells in the body and from being used in light-emitting devices needed for solid-state lighting.

A simple, commercially feasible method for doing both these things was described in the April 23, 2004, issue of *Science* magazine, in an article titled "Self-Assembly of Ordered, Robust, Three-Dimensional Gold Nanocrystal/ Silica Arrays."



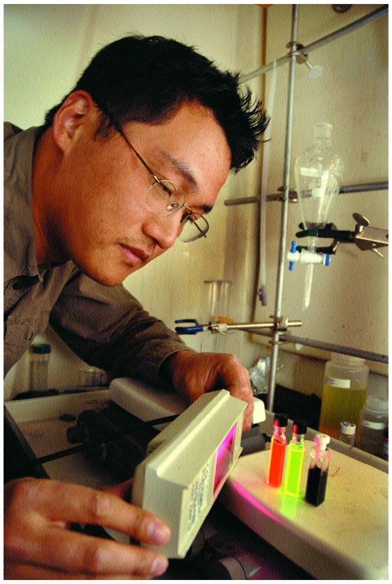
Sandia's Jeff Brinker (left) and Hongyou Fan observe satisfactory fluorescence by their well-trained nanocrystals in water solution. The dark vial holds gold nanocrystals; the orange and green hold semiconductor nanocrystals. (Photo by Randy Montoya)

"The question in nanotechnology isn't 'where's the beef," says Jeff Brinker, Sandia Fellow and University of New Mexico (UNM) chemical engineering professor. Brinker, with Sandia's Hongyou Fan, led the self-assembly effort. "It's 'where are the connectors?' How does one make connections from the macroscale to the nanoscale? This question lies at the heart of nanotechnology."



Top: ordered gold nanocrystal packed inside silica. Electron diffraction pattern (left corner) and high-resolution image (right corner) confirmed the nanostructure and gold nanocrystals. Bottom: self-assembled, well-shaped gold nanocrystal/silica arrays.

Innovation shows a way forward for harnessing the intriguing nanocrystal. It may help open the door to improved cancer tracking, solid-state lasers, catalysts, lighting devices, and memory storage.



Hongyou Fan observes the new materials. (Photo by Randy Montoya)

Bridging huge gaps

The Sandia/UNM self-assembly approach allows nanocrystal arrays to be integrated into devices using standard microelectronic processing techniques, bridging huge gaps in scale.

"One thing that's nice is that these are hard materials," says IBM staff researcher Chuck Black of T. J. Watson Research Center in Yorktown Heights, NY. "Often they come with an organic surfactant layer that makes it difficult to process materials, like a kind of grease." The Sandia/UNM approach scrubs the surfactants with an ozone compound. "This material is embedded in oxide. It sounds like a neat thing and a new approach."

"Quantum dots (another term for nanocrystals) can also be important for bio-labeling and bio-sensing," says Fan, who initiated the effort to use the nanocrystals for those purposes. "Our approach makes quantum dots both water-soluble and bio-compatible, which are two essential qualities for *in-vivo* imaging. The functional organic groups on the quantum dots can link with a variety of peptides, proteins, DNA, antibodies, etc., so that the dots can bind to and help locate targets like cancer cells."

Sandia has applied for a patent on this approach, which should aid attempts to identify individual cancer cells before they increase in number. Researchers have found that, at the nanoscopic realm, changing the size of a material changes the frequency it emits when "pumped" by outside energy. Thus, quantum dots of particular sizes and material will emit at predictable frequencies, which makes them useful adjuncts when bound to particular cancer molecules.

The process uses a simple surfactant similar to dishwashing soap to surround the nanocrystals — in this case, made of gold — to make them water soluble. Further processing involving silica causes the gold nanocrystals to arrange themselves within a silica matrix in a lattice with adjustable properties.

Physicists' dream

A further use allows physicists to go beyond computer modeling. "Previously," says Brinker, "there was no way to make precisely ordered 3-D nanocrystalline solids, integrate them in devices, and characterize their behavior. There was no theoretical model."

The new material can be used as an artificial solid to test out theories. "It should be a dream for physicists," says Brinker.

A kind of choreographed transmission possibility exists with the so-called "Coulomb blockade," Brinker says. No current is passed at low voltages because each crystal is separated by a thin (several nanometer-thick) layer of silica dioxide. This creates an insulator between the stored charges and each nanocrystal charges separately. "This could be configured into a flash memory with a huge number of charges stored in an array of nodes," says Brinker.

Researchers at UNM's Center for High Technology Materials performed experiments to establish the current/voltage-scaling characteristics of the gold/silica arrays as a function of temperature. Sandia researcher Tim Boyle made and provided nanocrystal semiconductor (cadmium selenide) quantum dots.

The full-text *Science* article is posted at http://www.sciencemag.org/cgi/content/full/304/5670/567

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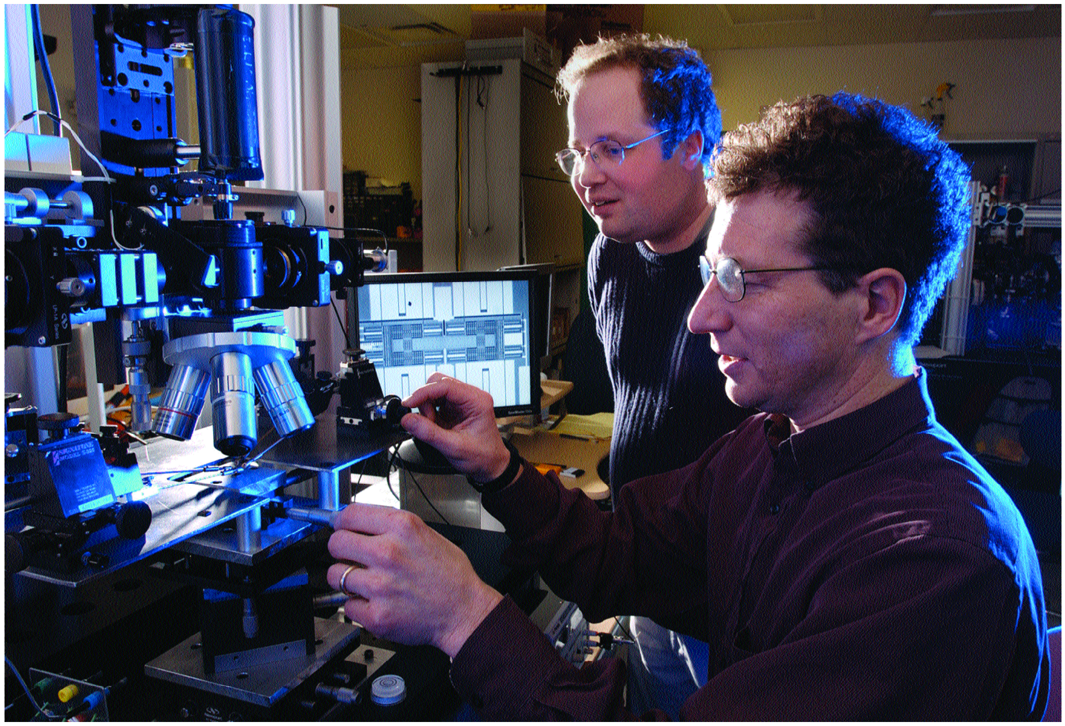
Stiction

‘Nanotractor’ studies microscale friction

A Sandia study shows that adhesive forces can cause micromachines to defy 300-year-old Amontons’ law governing static friction.



Sandia’s Maarten de Boer (right) and Alex Corwin investigate friction at the microscale. (Photo by Randy Montoya)

Interest in the development of MEMS (microelectromechanical systems) has grown steadily during the past decade. These tiny devices, now used in such applications as auto airbag systems, inkjet printers, and display units, are attractive because they take up little space and require little or no assembly. They also are cheap to produce in batch quantities because they are made with a technology that is already mature — the microlithography used to make silicon chips.

Arguably, MEMS could prove to be a ubiquitous “disruptive technology” that transforms a variety of engineering disciplines just as the silicon chip transformed electronics engineering. Yet the process of integrating MEMS into new systems has been slow. An overarching reason is that physics — especially the effects of adhesion and friction — sometimes works differently at the microscale.

Some assumptions seem intuitively correct because they apply to conventional machines. For example, Amontons’ law, first stated 300 years ago, says friction is proportional to force applied normal to (perpendicular to) a surface. Yet relying on this assertion could prove disastrous when applied to devices the size of a pinhead.

At Sandia, where engineers are eager to pack increased capability into very small spaces, the development of tools to manipulate microdevices — one example is a microtweezers — has been in high gear for over a decade. More recently, research has turned to the use of nanotechnology as an “enabling technology” to make better MEMS devices.

But creating a device small enough to measure friction on a MEMS device is no easy task, for the tool must be about the width of a human hair.

Stiction

Friction or "stiction" — the tendency of small parts to adhere to one another — has proven a significant hindrance to MEMS development. Treating the touching or sliding surfaces of a micromachine with a slippery molecular monolayer can reduce friction. However, there remains the need for a tool to measure the friction between two MEMS surfaces accurately to determine exactly what conditions are most effective in reducing it. With this information in hand, engineers will gain an extremely important tool in modeling MEMS devices prior to their actual manufacture.

But creating a device small enough to measure friction on a MEMS device is no easy task, for the tool must be about the width of a human hair.

In order to study friction at the micro-scale, Sandia's Maarten de Boer and coworkers set about building a polysilicon actuator that would controllably and accurately generate both very low and very high forces, and apply them both perpendicularly and tangentially.

The resulting "nanotractor" design incorporates an actuation plate in its central section and frictional clamps on its two ends. In the clamps, load is applied electrostatically but borne mechanically to develop friction forces. To obtain motion, the leading clamp is fixed in place with a large voltage. The plate is then actuated by attracting it toward the substrate.

Because the actuation plate is now bending, the trailing clamp, which is not loaded, slides a short distance (about 40 nanometers) toward the leading clamp. The trailing clamp is now held fixed with a large voltage, and the voltages on the leading clamp and plate are turned off. The leading clamp then slips forward. This stepping cycle is applied repeatedly to obtain large-scale motion with very high precision.

De Boer and postdoctoral researcher Alex Corwin determined that this nanotractor operates at up to 80,000 cycles a second, with a velocity of up to 3 millimeters per second. A maximum force of 2.5 millinewtons is achieved when the nanotractor stalls out, about 250 times more force than a comb drive.

Defying the law

Working with Corwin, de Boer found that the coefficient of static friction began to increase at low normal loads (below 50 micronewtons). De Boer attributes this deviation from Amontons' law to adhesive forces. They also observed sliding of up to 200 nanometers before the static friction event. This means Amontons' law is also not valid over short sliding distances.

Besides serving as a test structure for model friction studies, the nanotractor actuator is attractive for other uses. Marc Polosky, a Sandia staff member, has demonstrated its use in a MEMS system that performs mechanical logic functions. It also may prove useful for the precise positioning and control of micro-optical elements.

"Modelers are excited by the nanotractor test results, and now face the challenge of understanding and modeling newly observed phenomena such as gross slip prior to sliding," says Sandia staff member Dave Reedy. "Our goal is to develop a capability to perform simulations of MEMS components that accurately predict response in the presence of adhesion and friction."

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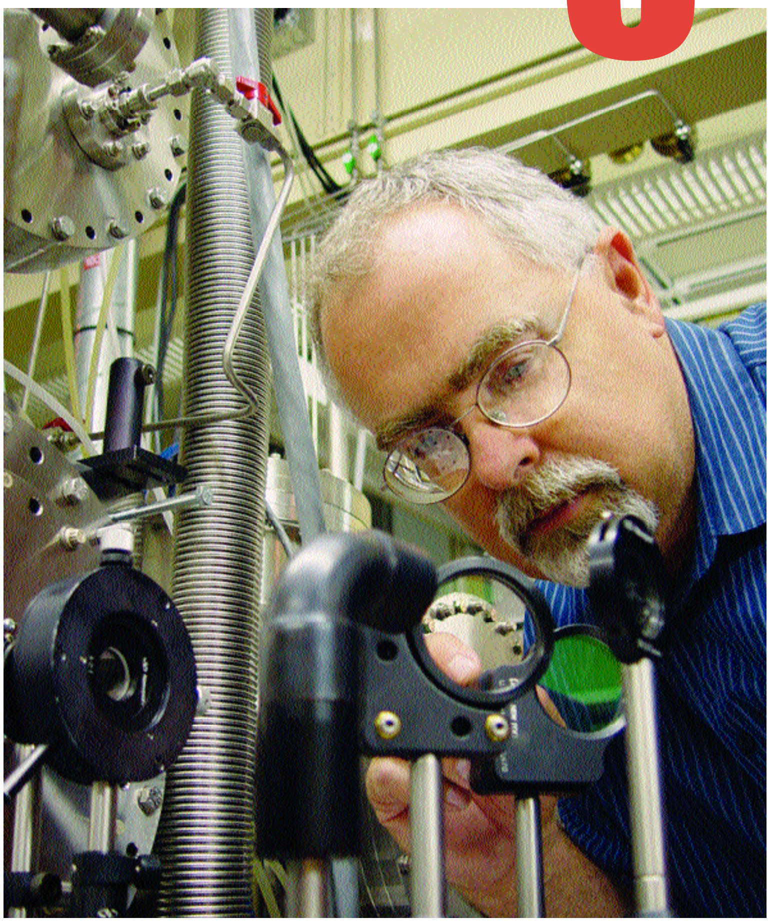
Cold Molecules

New avenue to the 5th phase of matter



Sandia's Dave Chandler aligning mirrors on apperatus to generate cold molecules. (Photo by Daniel Strong)

LDRD

Using a method usually more suitable to billiards than atomic physics, researchers from Sandia and Columbia University have created extremely cold molecules that could be used as an improved first step in creating molecular Bose-Einstein condensates (BECs).

BECs, predicted in the 1920s but not actually made until 1995, represent a special fifth phase of matter — like liquids, solids, gases, and plasmas — but can only exist at extremely low temperature. Their existence was first proposed by Satayendra Nath Bose, then formalized by Albert Einstein.

Future applications, assuming BECs can be usefully harnessed, range from improved atomic clocks to individual yes/no switches (Q-bits) in computers; from precision gravity detectors that could perhaps locate underground caverns to a model black hole in which light can enter, but cannot escape.

Researchers from Sandia and Columbia made a serendipitous discovery while studying collisional energy transfer between a beam of atoms intersecting a beam of molecules. They noted that some collisions occurred — as they might between two billiard balls — at exactly the right velocity for molecules to become motionless.

Zero Kelvin

The definition of a cold molecule is one that is moving slowly, and this experiment produced some very slow-moving molecules. (Zero Kelvin, or absolute zero, is defined as a molecule or atom being stationary.)

The study led to a new technique for cooling molecules to tens of milliKelvin temperatures — tens of thousandth of a Kelvin. In a paper, the team reported that single collisions among molecules in two beams of nitric oxide molecules with argon atoms can produce nitric oxide molecules with speeds no greater than 15 meters per second, equal to a maximum temperature of 0.4 degrees Kelvin.

"Our technique has promise to be developed into a first step in the cooling process needed for a molecular Bose-Einstein condensate," says Sandia researcher and principal investigator Dave Chandler. The work is co-authored by Sandia post-doctorate Mike Elioff and James Valentini of Columbia University.

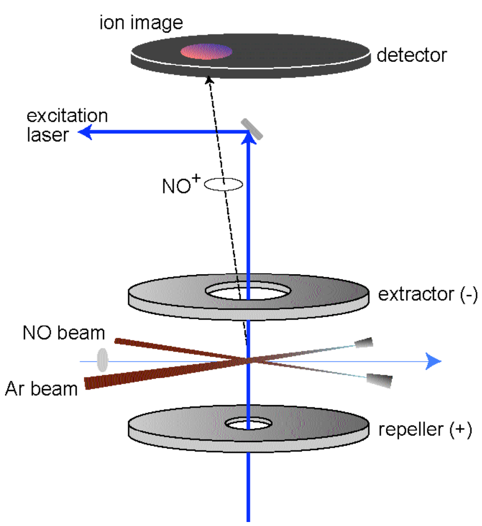


Diagram shows how nitric oxide and argon beams are collided to produce nitric oxide molecules moving at speeds slower than 15 meters per second.

The main method used to achieve atomic ultra-cooling to the microKelvin temperature range — the same preliminary cooling range as the Sandia technique — makes use of laser beams that intersect at a point. An atom, possessing the appropriate absorption characteristics, passing through that point in effect stands still, like a kid in a dodgeball game struck from all sides with balls. Transfixed by pressure from the beams, the atom becomes almost motionless.

The problem in cooling molecules by the laser method is that while some atoms possess characteristics that can be harmonically matched by a laser frequency, like the same note played by two pianos, molecular energy frequencies are more complex. This complexity makes them unsuitable for this type of laser cooling.

This leaves the field open for other techniques to be developed for the preliminary cooling of molecules. Four or five other techniques, published recently, had some level of success at cooling molecules. The most successful method to date has been the welding of ultracold atoms together to make ultracold molecules.

An open field

"We only manage to cool one molecule in a million," says Chandler. "But — inefficient or efficient — we generate cold molecules. With some improvements, we hope to be able to make substantial numbers of them." Molecules are cheap, he says, so getting one in a million cooling collisions out of a quadrillion total collisions per second the molecules undergo in the beams doesn't bother him.

This first-step method — the only one to rely solely on the masses of the atoms and molecules involved — could be useful in slowing down the speed of a variety of molecules sufficiently such that magnetic or electrical traps can be used to cool molecules further. Without prior slow-down, molecules would escape these relatively weak traps, like molecules of water rising from the surface of hot coffee.

Instruments in Chandler's lab, working at their resolution limit, show selected molecules in the intersecting beams slowing from 600 meters/second to 15 meters/second. The group's calculations indicate an average speed to be on the order of 4 meters/second. This average speed is equivalent to a temperature in the milliKelvin range, still several thousandths of a degree above the universe's absolute zero of -273 Celsius.

The last 99 yards, so to speak, are the hardest: Bose-Einstein condensates exist in the nanoKelvin range, still six orders of magnitude colder.

The work, funded by DOE's Basic Energy Sciences, focuses on understanding how energy flows between molecules for a better understanding of heat transfer.

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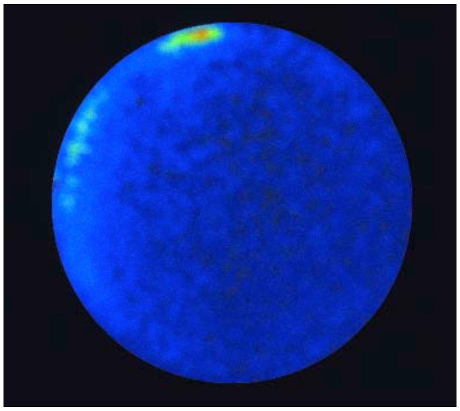
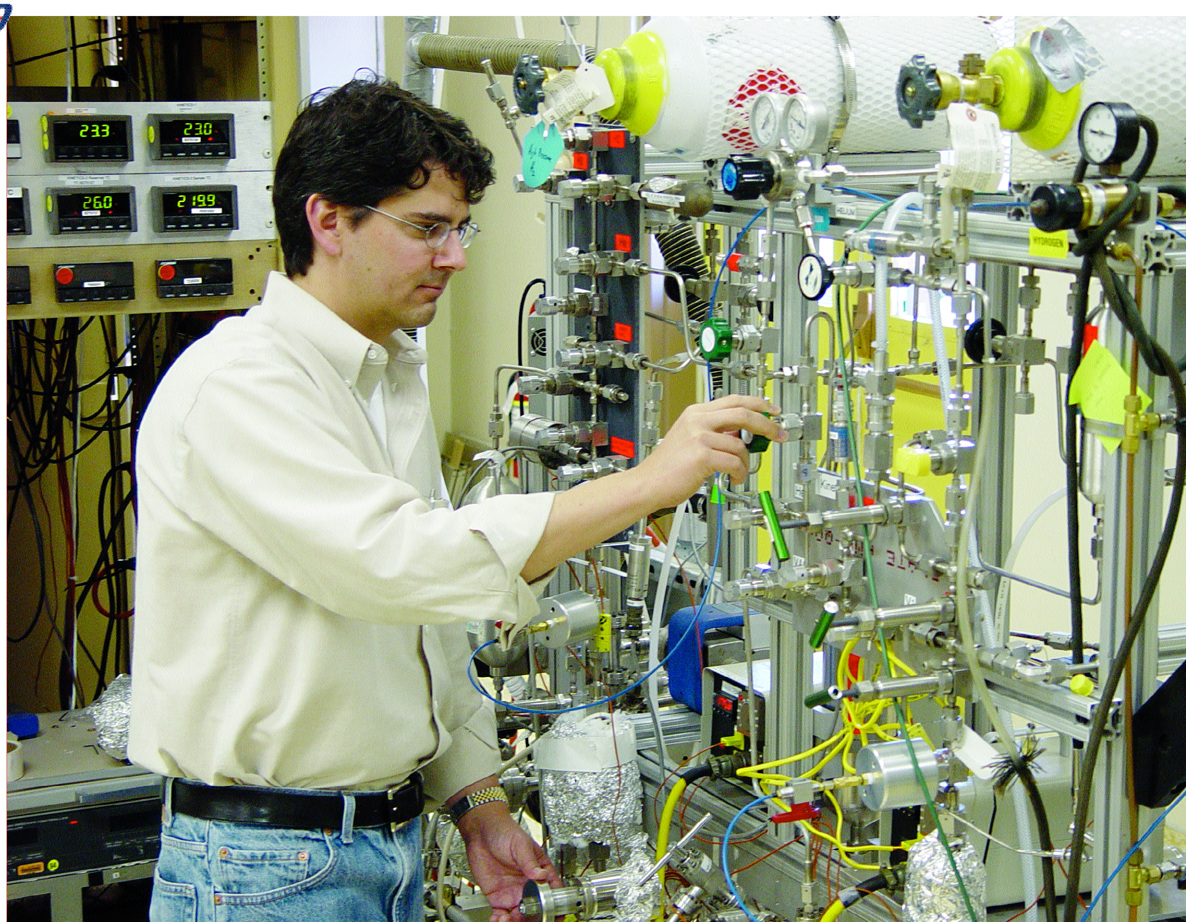
Colors of the ball indicate the number of molecules at a given velocity.



Metal Hydrides

Sandia to lead Center of Excellence



Sandia's Eric Majzoub conducting research in reversible metal hydrides. (Photo by Bud Pelletier)

Jim Wang, director of the Center of Excellence.

The Department of Energy has selected Sandia to lead a Center of Excellence for the development of reversible metal hydrides materials. A key objective will be to develop materials capable of storing hydrogen safely and economically in a vehicle that can run for at least 300 miles before refueling.

The center consists of eight universities, three other national laboratories, and three industrial companies, with Sandia serving as laboratory lead and coordinator of research and development. It will undertake $30 million of research and development over the next five years.

Sandia takes the lead

Sandia's winning proposal is in response to a "Grand Challenge" issued by the DOE last year. The center will be established at Sandia California in October. Jim Wang, manager of Analytical Materials Science Department, will serve as director.

The study of a promising class of hydrides, complex metal hydrides, is a key stepping stone in clearing the hydrogen storage riddle, says Jay Keller, manager of Sandia's Hydrogen and Combustion Technology Department. Currently, no material exists that can be

With Sandia at the lead, a consortium of national laboratories, university research departments, and private companies is taking on the task of finding a metal hydride material that will meet the demands of the coming hydrogen economy for an automobile fuel tank with a 300-mile range.

used to construct a fuel tank for safely and efficiently storing hydrogen fuel.

Hydrides are metallic alloys that absorb and then release hydrogen. They operate at pressures and temperatures close to ambient conditions, making them highly promising for future on-board hydrogen storage systems.

Sandia's 40 years of hydrogen science and engineering expertise leaves the group well positioned to lead the research effort, says Wang.

"Achieving or exceeding"

"Our approach will be to focus on achieving or exceeding the hydrogen storage targets through novel materials development, supported by our strengths in fundamental and applied materials science," says Wang

"Our plan is to coordinate, support, stimulate, and focus complementary expertise in chemistry, materials sciences, modeling, and synthesis and characterization with other national lab partners, universities, and industries to achieve the storage goals."

The FreedomCAR initiative, announced by Secretary of Energy Spencer Abraham in 2001, promotes the use of hydrogen as a primary fuel. The effort targets initial hydrogen storage to allow roughly a 300-mile driving range per vehicle fill-up.

"No material provides that yet," says Wang. "Our research for the past few years has been on the leading edge of hydride development, however, and has identified the class of material that appears to come the closest to that goal."

Hydrogen's advantages over fossil fuels include its lack of polluting emissions and the fact that it can be produced anywhere from renewable energy resources, such as solar electricity or biomass. Proponents of a hydrogen economy point to the potential to improve urban air quality, decrease greenhouse gases (released by burning fossil fuels), and gain independence from foreign oil.

Sandia researchers in the Labs' Combustion Research Facility (CRF) in California have also been building on Sandia's long-standing strengths in the study of metal-hydrogen interactions and engine studies to explore hydrogen use for electrical production by stationary power sources — turbines in particular.

CRF researchers are involved in the International Energy Agency's efforts to create next-generation models for turbines that can burn hydrogen. The CRF is also seeking funding to demonstrate use of hydrogen fuel, with its near-zero emissions of smog-producing oxides of nitrogen, in an internal combustion engine.

Although one of the biggest impacts of switching to hydrogen from fossil fuel will be seen in transportation, its use in stationary power generation will also help to develop an infrastructure for hydrogen distribution and use.

The center, says Wang, will bring together scientists and institutions with strong and focused capabilities in several research areas. Partnering with Sandia on the Metal Hydride Center of Excellence are: Brookhaven National Laboratory, Oak Ridge National Laboratory, Jet Propulsion Laboratory, and the National Institute of Standards and Technology; the University of Hawaii, University of Pittsburgh, Carnegie Mellon University, University of Nevada-Reno, University of Illinois-Urbana-Champaign, University of Utah, California Institute of Technology, and Stanford University; and General Electric Company-Global Research, HRL Laboratories, and Intematix.

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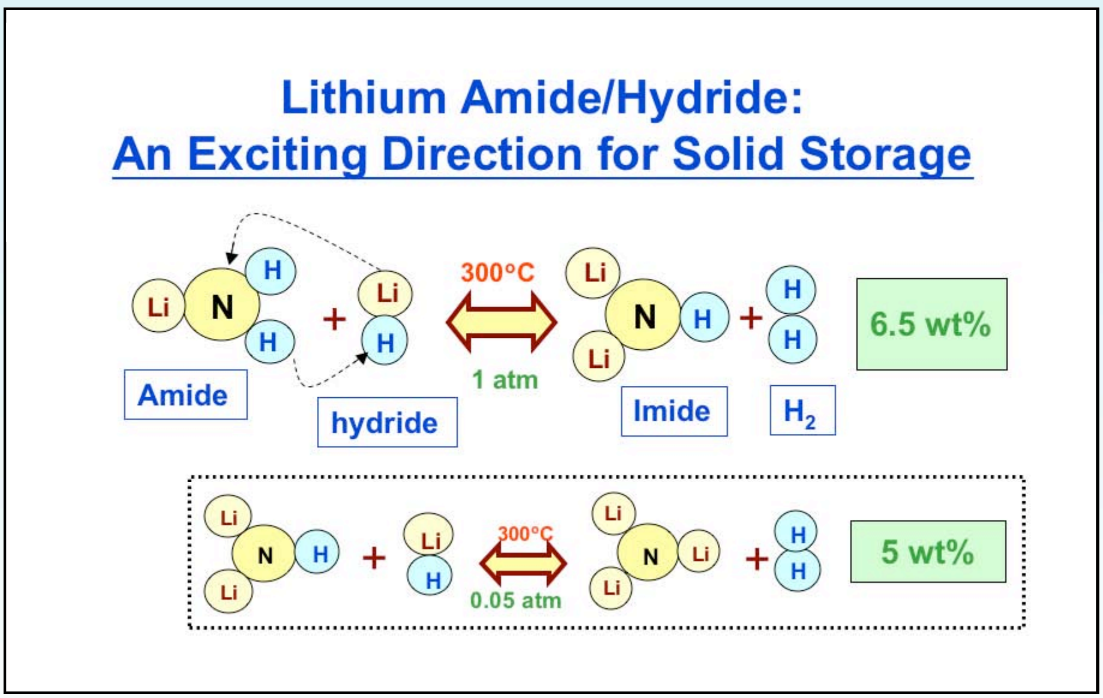
Hydrogen storage — a critical energy issue

Storage is widely considered one of the most important hurdles for the commercial success of hydrogen as a clean fuel. This is especially true in the case of vehicles because of weight, volume, and cost constraints. Sandia's storage work with hydrogen dates back 10 years and has included system design and fabrication, fundamental modeling, and fuel cell and storage integration.

- Researchers have studied complex hydrides with high capacities. The hydrogen absorption properties of a new sodium alanate material last year were termed "astonishing" and Sandia scientists continue to study the material.
- Sandia researchers recently improved the operating conditions of lithium imides for hydrogen storage. This new class of materials absorbs hydrogen reversibly in two steps (see diagram below), providing a total theoretical capacity of 10.8 percent storage by weight.

A patent application has been filed on the synthesis of the imides material. Jim Wang says his team is exploring further improvements on similar materials for hydrogen storage capacity.

In 1997, Sandia initiated a collaborative alanate program through the DOE with the University of Hawaii. Other current partnerships include those with the University of Geneva, University of Alaska-Fairbanks, and others. Wang says that collaborative efforts will expand substantially with the Center of Excellence.



This diagram shows a two-step process for the absorption and release of hydrogen from Lithium Amide/Hydride compounds. At 300 degrees Celsius, Lithium Amide reacts with Lithium Hydride and releases hydrogen at a pressure of 1 atmosphere (top reaction). Lithium Imide reacts with Lithium Hydride to release more hydrogen at lower pressure, 0.05 atmosphere (reaction inside dotted box). Lithium Amide/Hydride can release hydrogen at 11.5 percent by weight with the two steps.

Real-time emissions

Measuring particulate emissions

A unique laser-based technique for measuring real world emissions is seen as key to validating federal vehicle compliance procedures and may alter the way in which the automotive industry gauges particulate emissions.

Using a unique laser-based, soot heating technique, a team led by researchers at Sandia National Laboratories' Combustion Research Facility (CRF) has demonstrated the ability to measure real-world particulate emissions from a vehicle under actual driving conditions.

While on-board measurements of gaseous emissions are routine, real-time particulate measurements have been far more elusive. Yet they are essential for validating federal emissions guidelines for vehicle compliance.

Pete Witze, an engineer in Sandia's CRF engine combustion department, recently collaborated with Artium Technologies, Chevron Oronite, and the National Research Council (NRC) Canada to demonstrate the feasibility of obtaining on-board measurements of vehicle particulate emissions using a technology called "laser-induced incandescence," or LII. It is a non-intrusive diagnostic technology that can perform real-time measurements of particulate emissions produced by internal combustion engines.

New emission gauge

Sandia, Artium Technologies, and the NRC worked together to develop the portable version of LII instrumentation that was successfully applied during a recent trial. Consequently, this new method may alter the way the automotive industry effectively gauges particulate emissions.

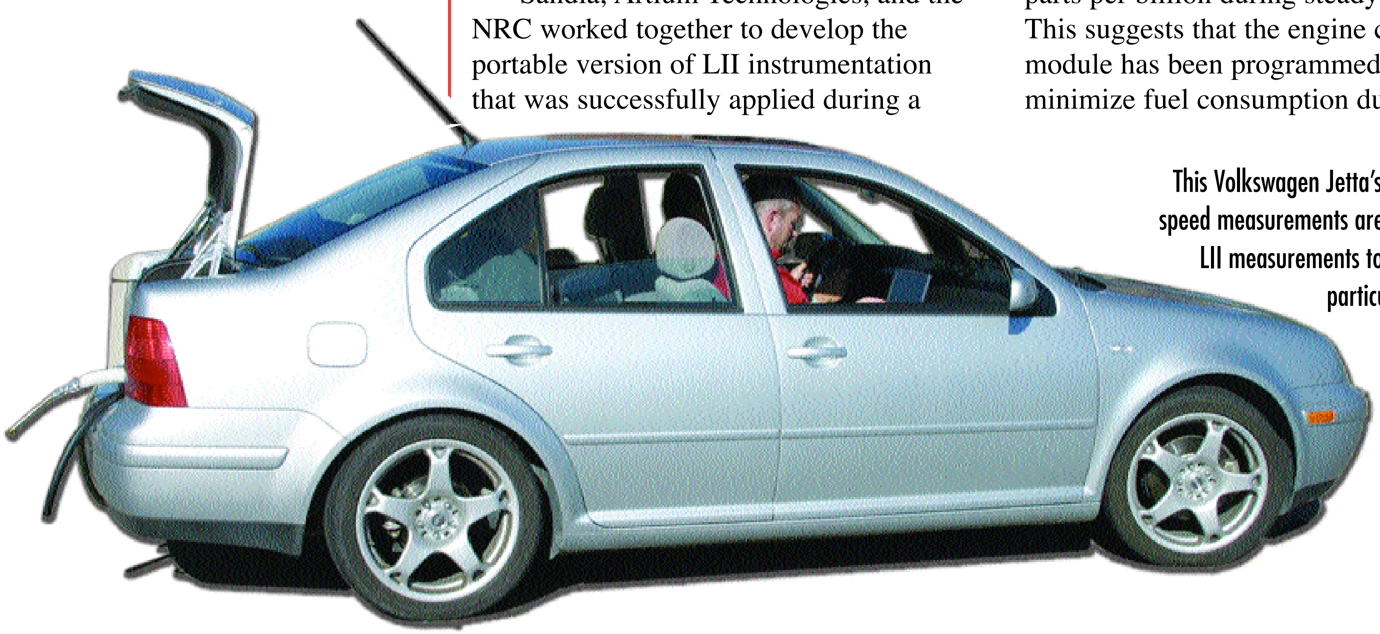
During the past decade, CRF and NRC researchers honed the LII technique, discovered in the 1970s, with the NRC securing an important temperature-measurement patent that is key to the current measurement capability.

Most notable

The most notable result during the recent tests, says Witze, was obtained during the coasting descent. "Although the vehicle speed and engine rpm were reasonably steady for a period of 470 to 600 seconds, the particulate emissions suggest that fuel injection cycled on and off intermittently," says Witze. (See graph on page 14.)

While the researchers believe the ideal fueling strategy would be to turn off injection for the entire descent, the vehicle is equipped with a catalyst that needs to be kept at its operating temperature.

The average particulate emissions measured by LII during this period were 8.4 parts per billion, as compared to 10-11 parts per billion during steady-state idle. This suggests that the engine control module has been programmed to minimize fuel consumption during a



This Volkswagen Jetta's vehicle and engine speed measurements are time-matched with LII measurements to correlate real-time particulate emissions with driving variables.

descent while maintaining idle-like particulate emission levels and an active catalyst.

The ability to measure on-board particulate tailpipe emissions is of growing environmental interest because of the desire to validate current U.S. Environmental Protection Agency (EPA) vehicle certification procedures. These procedures, which have been the industry standard for more than 30 years, measure emissions using a chassis dynamometer and specify engine speed to be applied during testing.

On- and off-road

Because such tests do not replicate variables, such as grade changes and weather encountered under actual driving conditions, the automotive industry expects dynamometer emissions testing to be supplemented with on-road measurements in the future.

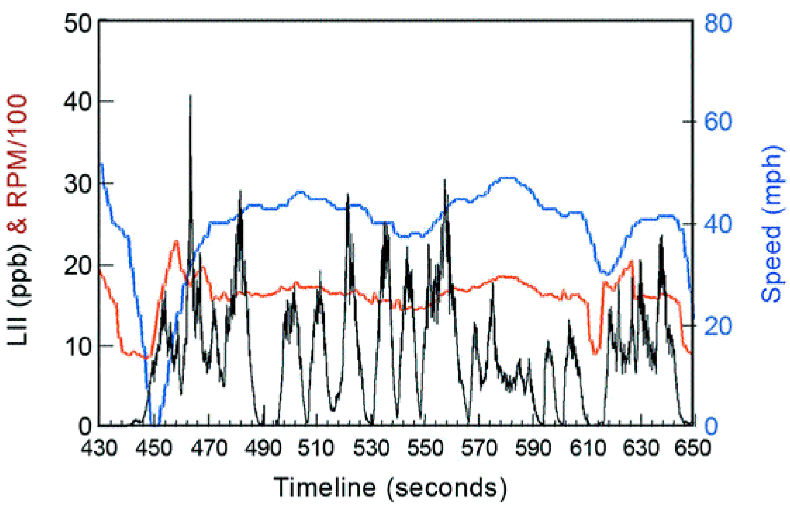
In general, innovative new methods are needed to evaluate the effects of mobile source emissions — both from on- and off-road sources — on air quality.

The research team with the test vehicle.

In conducting the tests, Artium's commercially available LII instrument and ancillary equipment was placed in the trunk and on one side of the rear seat of a 2002 Volkswagen Jetta with automatic transmission and a turbocharged direct-injection diesel engine. An on-board diagnostics tool was used to access the vehicle and engine speeds for recording while the vehicle was driven on a test route in northern California.

These measurements were then time-matched with the LII measurements to obtain a synchronized data set correlating particulate emissions with a variety of vehicle operating conditions, including city driving, freeway driving with entrance-acceleration, hill ascent, and coasting descent on a rural road.

Sandia's Witze said another unique aspect of the LII measurement technique is that, unlike other systems, it does not require an operator to conduct the tests. For this and other reasons, he said engine manufacturers have proven to be "extremely interested" in LII.



LII compared to engine (red) and vehicle speed (blue) measurements for the coasting descent show that fuel injection cycled on and off.

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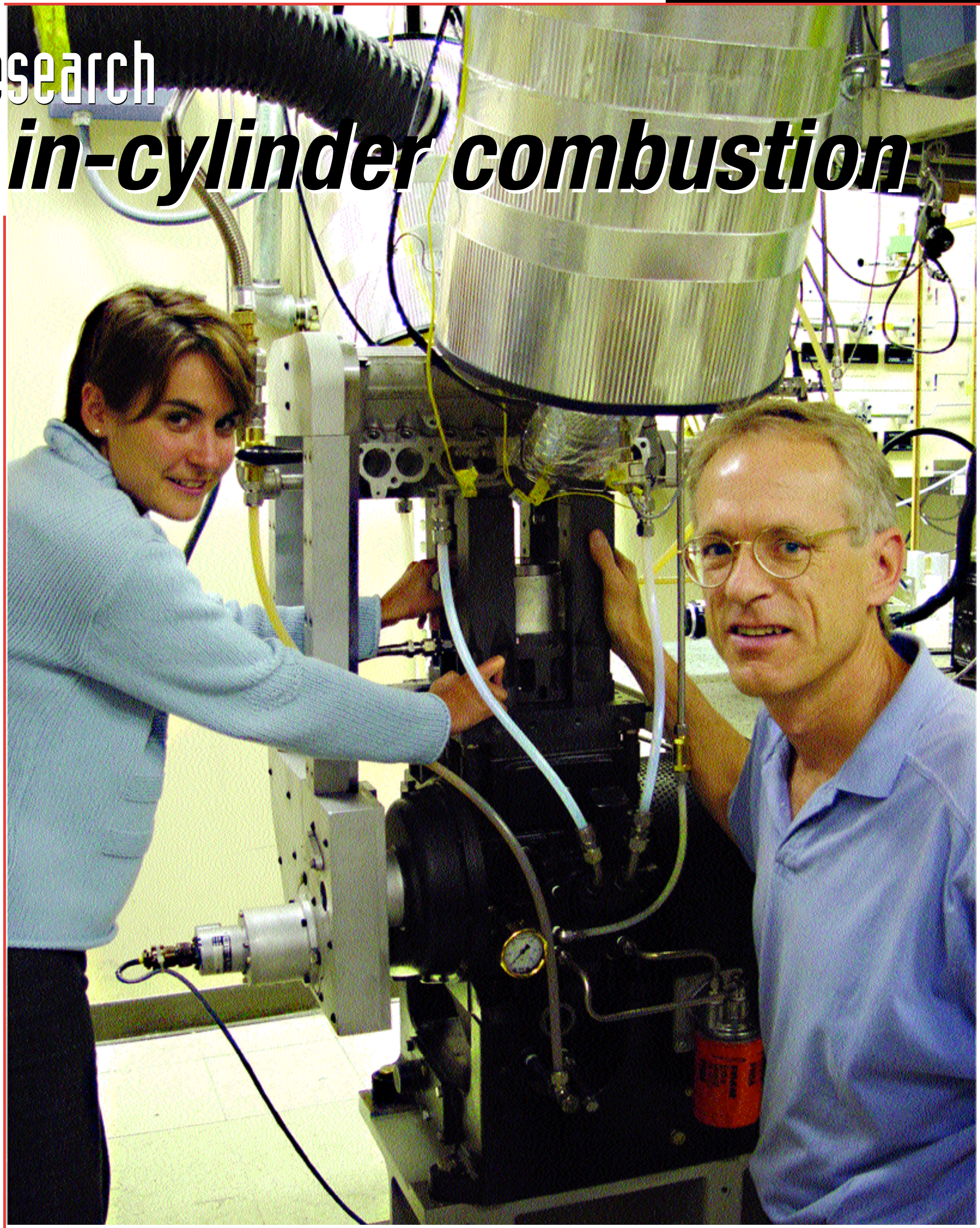
Combustion Research

Studying *in-cylinder combustion*

Scientists are using an all-new lab to look into the merits of a new-type engine for low-emission, high-efficiency operation.



Richard Steeper (right) oversees the CRF's new HCCI Laboratory. Here he works with Amelia Fayoux, a doctoral student and employee of Peugeot-Citroen, at the facility's optically accessible single-cylinder HCCI engine. (Photo by Bud Pelletier)

A new laboratory for the study of ultra low-emission, high-efficiency combustion engines has begun operation at Sandia's Combustion Research Facility (CRF) in Livermore, California. Dubbed the HCCI Lab (Automotive Homogeneous Charge Compression Ignition Laboratory), it is funded by the U.S. Department of Energy's FreedomCAR and Vehicle Technologies Program.

Lab researchers are using advanced optical diagnostics to study and characterize combustion occurring inside an alternative piston-engine combustion process that potentially can rival the high efficiency of diesel engines while minimizing NO_x (nitrogen oxides) and particulate emissions.

The HCCI lab features a single-cylinder, automotive-scale engine that has

Using or matching industry prototypes assures experimental results from the labs are relevant to industry's current HCCI development needs.

a high temperature and pressure intake air supply and a 12:1 compression ratio, enabling operation over a wide range of conditions. An HCCI engine could use a variety of fuels.

Worldwide attention

The technique's potential has caught the attention of automotive and diesel engine manufacturers worldwide.

However, researchers must overcome several technical barriers, such as controlling ignition timing, reducing unburned hydrocarbon and carbon monoxide emissions, extending operation to higher loads, and maintaining combustion stability.

Key engine components were either supplied by auto industry partners or designed to match industry prototypes.

"This assures that experimental results coming out of the lab are relevant to industry's current HCCI development needs," says scientist Richard Steeper, who oversees the lab.

CRF researchers are currently using the lab to achieve a better understanding of fuel injection strategies for controlling emissions during light-load HCCI operation and for extending the load range for high-efficiency operation.

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INSIGHTS

By Bill Kirchhoff

Bill Kirchhoff

Combustion Research Facility — 25 years of valuable service

The occasion of the 25th year of operation of the Combustion Research Facility naturally leads one to reflect on the influence the CRF has had on this oldest of technologies. To understand this influence, a few characteristics of combustion as a source of energy production need to be kept in mind. Whether it is providing electricity, heat, or transportation of a family to a soccer match or a team of astronauts beyond Earth's grasp, combustion produces nearly 85 percent of the nation's energy and is likely to do so for the foreseeable future. That this oldest of technologies still presents challenges for understanding and control is due to its inherent complexity.

The chemistry of combustion involves dozens of species and hundreds of reactions. Most of the species are unstable, transitory molecular fragments whose detection challenges, and usually defeats, the most advanced analytical techniques. The majority of these reactions will never be characterized experimentally and must therefore be determined through quantum chemistry.

Reaching the goal of developing computational models to design optimal combustion devices with maximum efficiency and minimum environmental impact requires a broad-based research program involving theoretical and experimental chemists, spectroscopists, engineers, mathematicians, and computer scientists.

Combustion is a process that will be understood and controlled only through incremental advancements in many interrelated fields by many, many more

Combustion Research Facility

scientists than those at the CRF alone.

While combustion diagnostics remain the CRF's primary area of recognition, its research and outreach activities have greatly expanded and its influence today derives in large measure from the breadth of its representation in combustion research and the excellence of its technical staff. CRF scientists use the most advanced techniques of measurement, theory and computational science to probe the extraordinary complexities that characterize all combustion phenomena.

- Theoretical chemists examine mechanisms for individual chemical reactions and for characterization of the elaborate networks of reactions that characterize combustion.
- Experimental chemists measure the rates of individual chemical reactions and study the details of molecular dynamics in the making and breaking of chemical bonds. CRF scientists and university collaborators developed the technique of ion imaging to characterize molecular collision dynamics, now used in dozens of laboratories around the world.
- Spectroscopists and physical chemists continue to develop new techniques for identifying and quantifying species in flames, working with colleagues to use synchrotron radiation at the Advanced Light Source at the E. O. Lawrence Berkeley National Laboratory to distinguish isomers of individual hydrocarbon radicals in flames. Scientists and engineers from all over the world now collaborate in a biennial International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames that has allowed for the first time meaningful comparison of well characterized and reproducible flames and their corresponding models.

CRF scientists use the most advanced techniques of measurement, theory and computational science to probe the extraordinary complexities that characterize all combustion phenomena.

Collaboration is the key

The list of individual accomplishments is too long and varied for an article such as this. The cumulative effect of this collaborative basic research program has led the CRF to the world-wide leadership role it now plays. Collaboration is the key because the diversity of scientific expertise that must be brought to bear on combustion problems. Collaborations are encouraged between basic and applied scientists and engineers and the research of each is enriched by the involvement of the other.

The collaborative environment of the CRF has led it to serve as the host institution for the Collaboratory for the Multiscale Chemical Science, which brings together leaders in scientific research and technological development across multiple DOE laboratories, other government laboratories, and academic institutions to develop an open "knowledge grid" for multiscale, informatics-based chemistry research.

While the DOE's Office of Basic Energy Sciences (BES) has supported research and operation of the CRF throughout its 25-year history, BES is no longer the primary sponsor. Indeed, many of CRF's better-known accomplishments have been those supported by other offices and programs. This is testimony to the CRF's success, of the excellence of its scientific staff, and of the fact that CRF continues to be a wise investment for the future.

Bill Kirchhoff is former program manager for chemical physics in the Department of Energy's Office of Basic Energy Sciences. Kirchhoff had oversight of the Combustion Research Facility's basic research program. He retired in January.

"The question in nanotechnology isn't 'where's the beef?' It's 'where are the connectors?' How does one make connections from the macroscale to the nanoscale? This question lies at the heart of nanotechnology."

Jeff Brinker,
Sandia Fellow and University of New Mexico Chemical Engineering Professor.

Sandia National Laboratories

LOCKHEED MARTIN

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000

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