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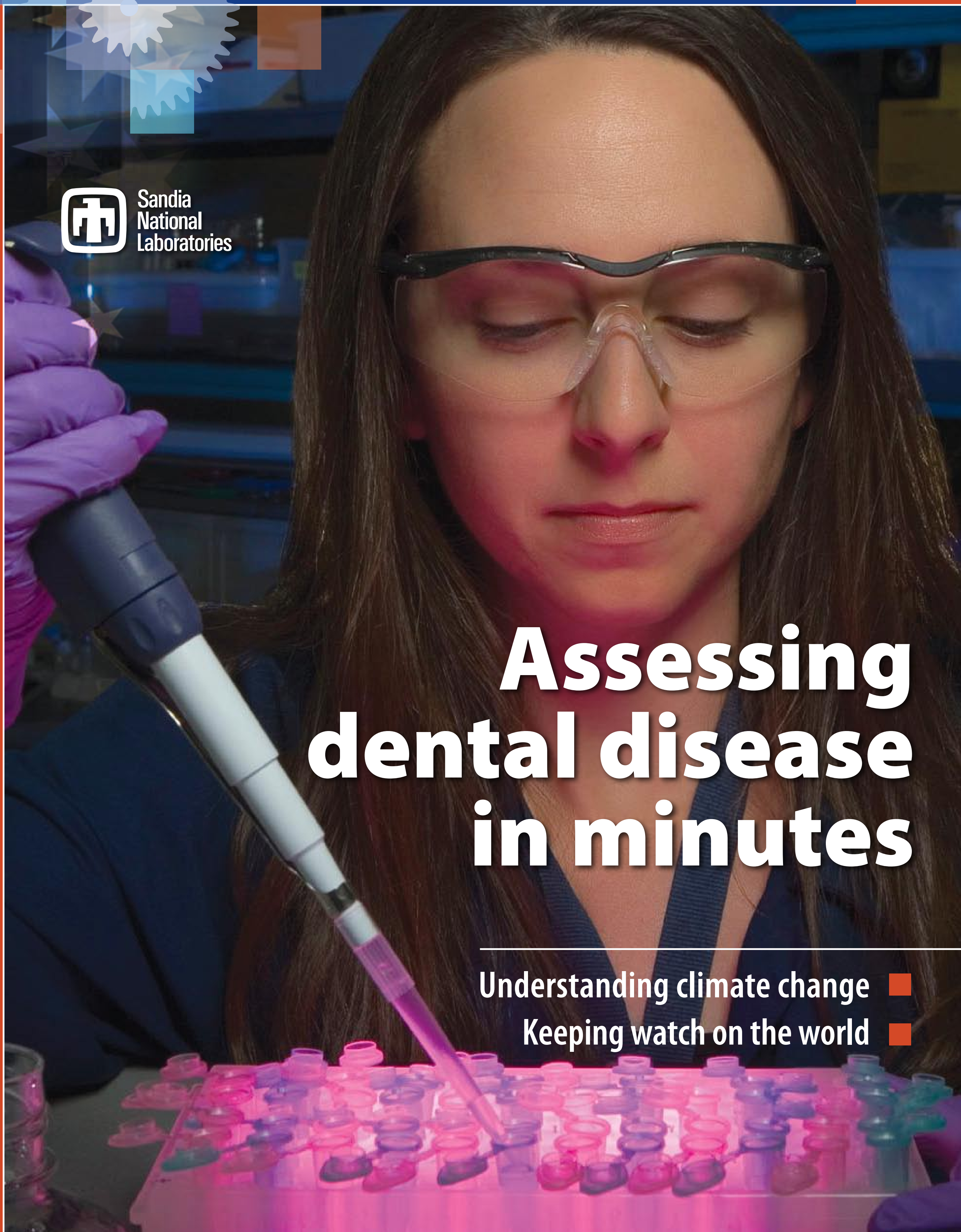

Assessing dental disease in minutes

Understanding climate change

Keeping watch on the world

Sandia Technology (ISSN: 1547-5190) is a quarterly magazine 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 weapons, arms control, energy, the environment, economic 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 safety, reliability, security, use control, and military performance. For more information on Sandia, see our website at **www.sandia.gov**

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What is LDRD

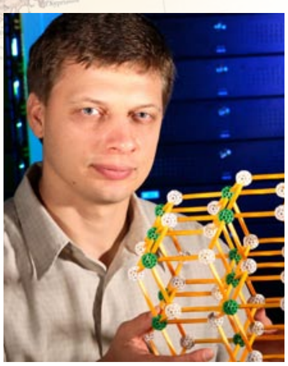
Sandia's world-class science, technology, and engineering work defines the Labs' value to the nation. These capabilities must remain on the cutting edge, because the security of the U.S. depends directly upon them. Sandia's Laboratory Directed Research and Development (LDRD) Program provides the flexibility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

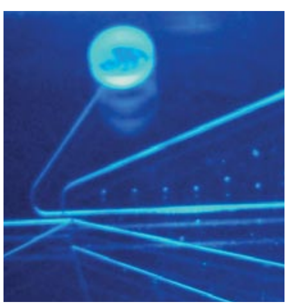
LDRD supports Sandia's four primary strategic business objectives: nuclear weapons; energy resources and nonproliferation; defense systems and assessments; and homeland security and defense. LDRD also promotes creative and innovative research and development by funding projects that are discretionary, short term, and often high risk, attracting exceptional research talent from across many disciplines.

When the LDRD logo 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's Amy Herr prepares human saliva samples for analysis that will be conducted using Sandia's lab-on-a-chip clinical diagnostic instruments. The tests can determine if a patient has gum disease and how advanced it is. (See story on page 10.)
Photo by Randy Wong





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FROM THE EDITOR

Dear Readers,

At Sandia, researchers often find themselves traveling to the far ends of the world to provide exceptional service and this issue of Sandia Technology provides an example. Over the years, our technical staff members have spent weeks — and months — away from home, living in remote locales.

Sandia's mission requires expertise across a wide range of disciplines and the nation continues to turn to the Labs to extend that expertise. For the past few years, a Sandia team has found itself doing vital work in the Arctic and elsewhere around the globe to better understand climate change issues.

Among the other highlights:

- Our cover story reveals how detecting dental disease is now as simple as taking a small sample of the patient's saliva and quickly analyzing it. The technology, which follows Sandia's lab-on-a-chip research, both detects disease and determines the extent of the disease's progress.

- Predicting the properties of materials by better understanding their electronic structure is the goal of several Sandia/California scientists and engineers. They are making a hard-to-use theoretical approach from 1965 amenable to computerization.

- Sandia's contributions to the U.S. Nuclear Detonation Detection System — a network of Global Positioning System and Defense Support Program satellites with multiple detectors and a handful of fixed and mobile ground stations — include the ICADS software system, which helps the U.S. Air Force quickly recognize nuclear detonations and other like-phenomena on a worldwide basis.

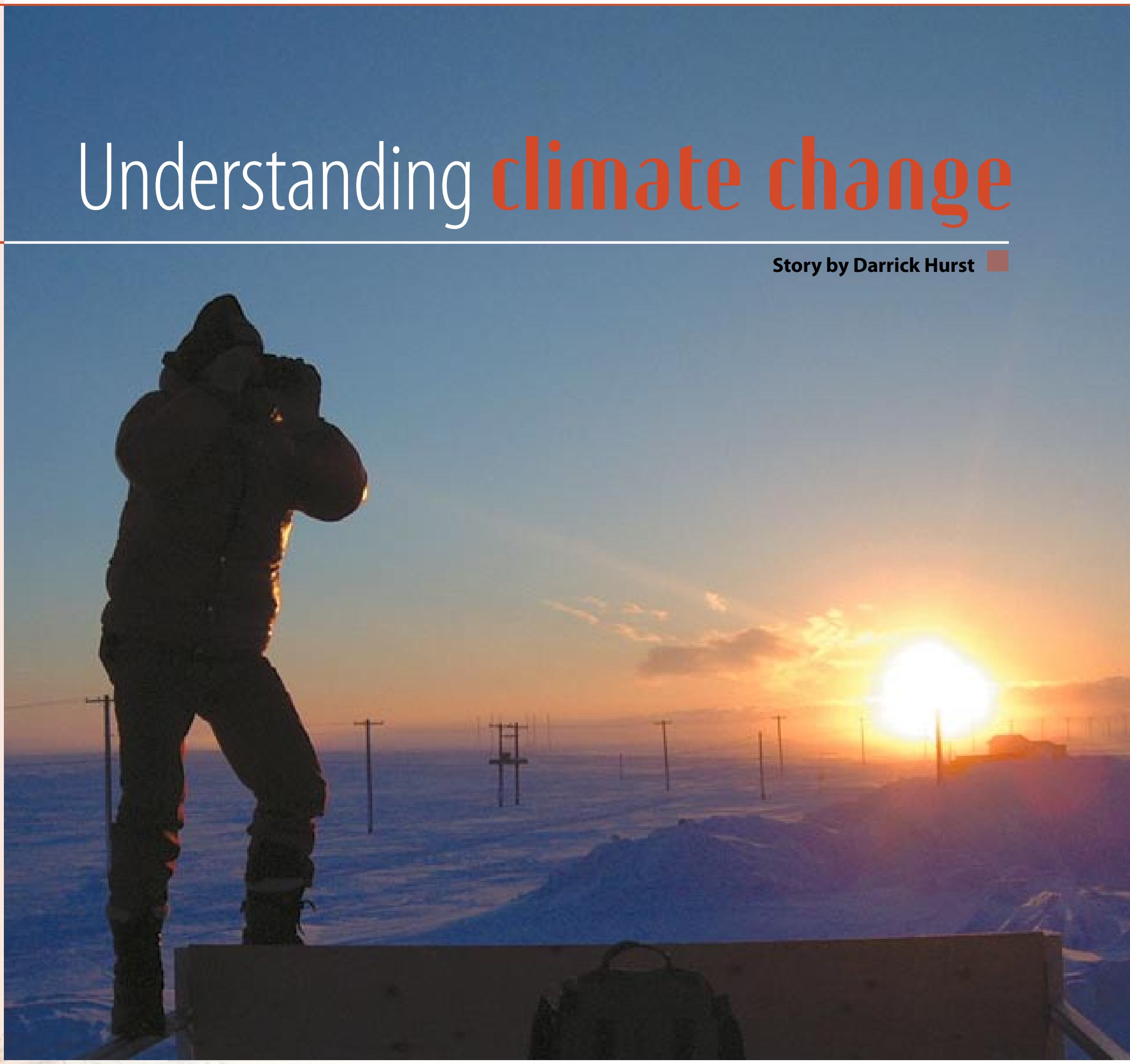
Finally, we take a look at the past, present, and possibly the future of microelectromechanical machines, or "small smart things" we call MEMS for short. Sandia has been at the forefront of MEMS development since the 1980s and this article takes stock of the successes and the problems inherent in the field.

Will Keener
Sandia Technology Editor

Understanding climate change

Story by Darrick Hurst

Climate researchers are focusing increased attention on high latitudes as they work to better understand the interactions of a complex atmosphere-land-ocean system. The Arctic is predicted to undergo more intense warming than any other region on earth because water undergoes a specific seasonal phase change there. Scientific evidence shows that this warming is already happening.



Above: High latitudes present a winter window into space. Photo captures a Barrow, Alaska, sunset.
Photo by Rune Storvold Geophysical Institute, University of Alaksa-Fairbanks

Sandia researchers Mark Ivey and Bernie Zak are members of a research team from around the world whose work on the cold tundra of northern Alaska is helping to transform scientific understanding of the Earth's future climate.

The North Slope of Alaska site covers the area just east of Barrow along the coast of the Chukchi Sea. The area provides researchers with a rare, ground-based window into the cloud and radiative processes that occur in the earth's atmosphere at high latitudes.

Sponsored by the DOE's offices of science and biological and environment research, the Atmospheric Radiation Measurement Climate Research Facility, or ACRF, operates two research sites at its North Slope locale – Barrow and Atqasuk. The research performed at these sites has made it one of today's most successful atmospheric programs.

The Barrow site in particular will serve as a center for atmospheric and ecological research as part of scientific activities taking place during the International Polar Year, 2007-2008. During this time, scientists from around the world will focus their research on the Arctic and the Antarctic.

Arid cold window

"The arid cold during winter at the North Slope provides a 'window' into space. Under these conditions, infrared radiant energy can escape more easily through the atmosphere — it's something that's part of the earth's natural energy balance," says Zak, Sandia science liaison for the site. "This is one of the ways that high latitudes are quite different from temperate or tropical regions, and reinforces the importance of our research here."

"Because the North Slope site is fairly cold year-round, we often observe clouds that are composed of ice or ice and water in mixed phases," says Ivey, the site manager. The value of these different regional factors is that the researchers have the chance to study how longwave energy gets trapped to varying degrees in the atmosphere by different chemical constituents and conditions. These include water vapor, carbon dioxide, methane, nitrous oxide, chlorofluorocarbons, and liquid water droplets that absorb the energy emitted by the surface of the Earth.

The site is a national user facility for interdisciplinary studies of earth systems operated by ACRF. Along with sites in the U.S. southern Great Plains and the tropical western Pacific, these primary, fixed locations are equipped with an extensive array of instruments for obtaining atmospheric data. In 2005, the ACRF added a mobile facility to its suite of research capabilities.

Using a closely integrated team of national laboratory partners, the ACRF provides the complex physical infrastructure and data systems needed for national and international research efforts related to global climate change, says Ivey. The North Slope site for ACRF provides the facilities, support, and atmospheric measurement data for an international group of scientists. "We've also been incredibly fortunate in receiving the support of native Inuit — what we call Eskimo — communities in the vicinity of the site," says Ivey.

Climate modeling

"Essentially, our work at these facilities enables us to contribute to improvements in climate models that simulate global climate change," Zak says. Such global climate models are tools for calculating atmospheric, land, and oceanic conditions all over the earth. By providing cloud and radiative transfer information to climate modelers, says Zak, the site's data will help to improve the performance of general-circulation and related models of the atmosphere as tools for predicting future global and regional climate changes.

Instrument cluster for guest researchers at ACRF research station.
Photo by Mark Ivey

Sandia's Jeff Zirzow checks Infrared and visible spectrum radiometers at North Slope site.
Photo by Larry Yellowhorse

A strong indicator of the value of the site's work is the number of researchers who make use of the data obtained there. Academic, foreign, domestic, and other researchers from many different areas of research use the data. Many also come to the site for field campaigns to temporarily add their own unique measurement capabilities to the existing instrumentation suite and study specific phenomena.

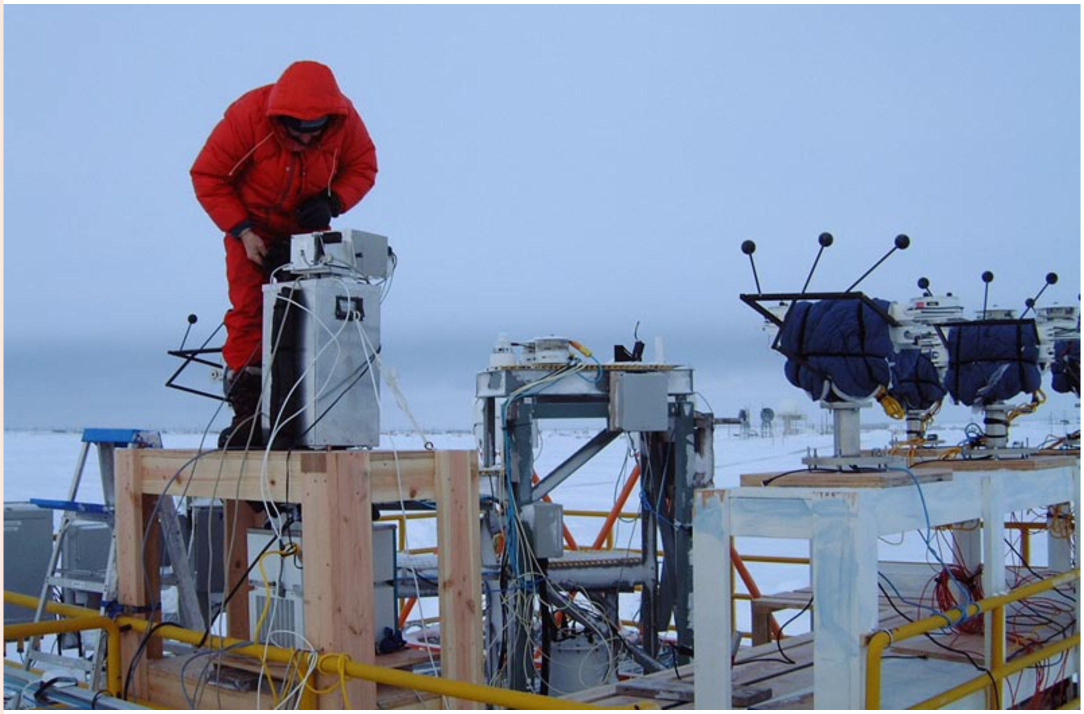
"People are still publishing peer-reviewed articles based on the 2004 data," says Zak. "We found far fewer ice nuclei than had been expected — that is, far fewer aerosol particles capable of nucleating ice crystals. This means that water was staying liquid even at very low temperatures. That has direct implications, not only for climate, but for the Federal Aviation Administration as well, because when this liquid water comes into contact with planes, it instantly converts to ice. These icing conditions can bring down an aircraft."

"Our work isn't just limited to climate research," says Ivey. "The Army has done research on the atmospheric phenomena that cause the twinkling of the night sky, and how distant objects can be seen more easily through the atmosphere at certain times of the day, under certain meteorological conditions. Our location and instruments at the North Slope provide data sets that are useful to a wide range of research interests. That is one of the reasons the locale was chosen."

Seeds of change

This year is also the 50th anniversary of the International Geophysical Year, an international scientific effort that initiated a comprehensive series of global geophysical activities spanning the period July 1957-December 1958. The seeds of the present concern about global climate change were planted during the International Geophysical Year. Prior to the 1957-58 effort, it was not known that the burning of fossil fuels was progressively changing the composition of the global atmosphere.

Site manager Mark Ivey at the North Slope site.
Photo by Eli Mlawer



Research scientist examines Absolute Skyscanning Radiometer at the North Slope site.
Photo courtesy U.S. DOE's Atmospheric Radiation Measurement Program

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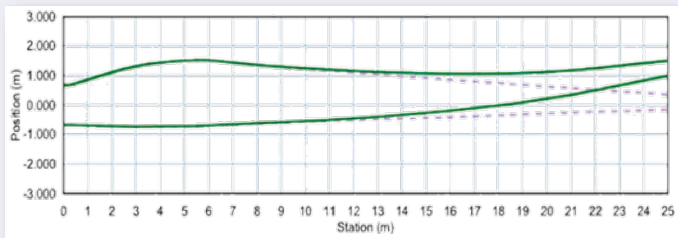
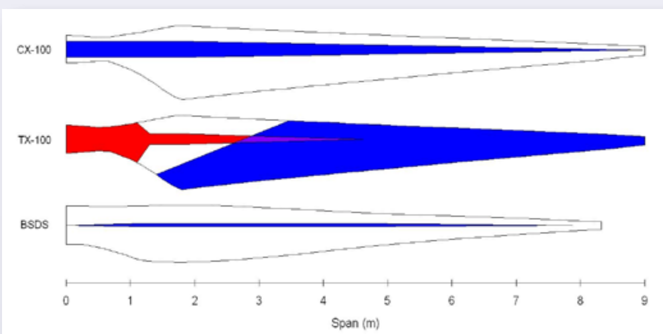
Sandia helps develop new wind turbine blade design

A new wind turbine blade design, developed by researchers at Sandia in partnership with Knight & Carver of San Diego, promises to be more efficient than current designs. It should significantly reduce the cost-of-energy of wind turbines at low-wind-speed sites.



Named "STAR" for Sweep Twist Adaptive Rotor, the blade is the first of its kind produced at a utility-grade size. Its most distinctive characteristic is a gently curved tip, or "sweep," which unlike the vast majority of blades in current use, is specially designed for low-wind-speed regions like the Midwest. The sites targeted by this effort have annual average wind speeds of 5.8 meters per second, measured at 10-meter height. Such sites are abundant in the U.S. and would increase by 20-fold the available land area that can be economically developed for wind energy.



At 27.1 meters — almost three meters longer than the baseline blade it will replace — STAR improves energy capture at lower wind speeds. The blade curves toward the trailing edge, which allows it to respond to turbulent gusts in a way that lowers fatigue to the blade. It is made of fiberglass and epoxy resin.

"This design allows the blade to twist more than traditional designs, thus relieving some of the effects of gusty turbulent wind on blade life," says Tom Ashwill, who leads Sandia's blade research efforts. "This then allows us to grow the blade length for the same rotor, providing for increased energy capture of 5 to 10 percent and yet retaining the same expected fatigue life."

The K&C contract is part of the Low Wind Speed Technology project that targets wind sites that are not the strongest but plentiful. In late 2005, DOE and Sandia awarded Knight & Carver the $2 million contract that includes $800,000 in K&C cost share. Sandia's role in the project has been in directing design and test planning. The K&C team provided the detailed design and blade fabrication. Four blades will be fabricated in the first quarter of 2007. Three will be flight-tested on a turbine in Iowa.

Other members of the design team are Dynamic Design of Davis, Calif.; MDZ Consulting of Clear Lake Shores, Texas; University of California, Davis; and NSE Composites of Seattle, Wash.

The first STAR blade (above) was tested in January at Knight & Carver's fabrication facility in San Diego.

Graphs (left) illustrate several innovative prototype blade designs for improved wind efficiency. Green outline shows curve, or sweep, in Knight & Carver design. Extra twist built into the blade reduces fatigue in high wind and allows longer blade length – resulting in 5-8 percent more energy generation. Red, white and blue blade drawings are of 9-meter prototypes, showing three innovations aimed at creating more design efficiencies.

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Describing fundamental properties of materials

Story by Nancy Garcia

Gold is shiny, diamonds are transparent, and iron is magnetic. Ever wonder why?

The answer lies with a material's electronic structure, which determines its electrical, optical, and magnetic properties. In a number of areas of engineering, including weapons, Sandia relies extensively on using and controlling such properties.

Predicting a material's properties by first calculating its electronic structure could cut down experimental time and lead researchers to uncover new materials with unexpected benefits. But commonly used simulations are often inaccurate. This is especially so for materials like silicon, whose strongly correlated electrons influence each other over a distance and make simple calculations difficult.

Theoretical innovations

Now a team of researchers at Sandia are looking at a solution that offers huge potential. Using LDRD and DOE Office of Science funding, Sergey Faleev and his colleagues have applied theoretical innovations and novel algorithms to make a hard-to-use theoretical approach from 1965 amenable to computation. The team's approach may open the door to discovering new phases of matter, creating new materials, or optimizing performance of compounds and devices, such as alloys and solar cells.

A paper on this subject, "Quasiparticle Self-Consistent GW Theory," appeared last year in *Physical Review Letters*. "GW" in the title refers to Lars Hedin's 1965 theory that elegantly predicts electronic energy for ground and excited states of materials. "G" stands for the Greens function — used to derive potential and kinetic energy. "W" is the screened Coulomb interaction, which represents electrostatic force acting on the electrons. "Quasiparticle" is used to describe particle-like behavior in a complex system of interacting particles. Self-consistent means the particle's motion and effective field, which determine each other, are iteratively solved, coming closer and closer to a solution until the result stops changing.

"Our code has no approximation except GW itself," said Faleev. "It's considered to be the most accurate of all GW implementations to date."

"It works well for everything in the periodic table," adds coauthor Mark van Schilfgaarde, a former Sandian now at Arizona State University. The paper reports results for diverse materials, whose properties cannot be consistently predicted by any other theory. The 32 examples include alkali metals, semiconductors, wide band-gap insulators, transition metals, transition metal oxides, magnetic insulators, and rare earth compounds.

Describing force

"Everything in solids is held together by electrostatic forces," says van Schilfgaarde. "You can think of this as a huge dance with an astronomically large number of particles that is essentially impossible to solve. The raw interactions among these particles are remarkably complex.

"Hedin replaced the raw interactions with 'dressing' the particle with a screened interaction," van Schilfgaarde continues, "so the effective charge is much smaller. It becomes much more tractable but the equations become more complicated — you have an infinite number of an infinite number of terms. The hope is that the higher-order terms die out quickly."

"We're pretty confident we got the approach right," he says. He now would like another group to independently verify this way of framing the task.

Challenges ahead

The researchers use a molecular dynamics code, VASP, to model equations of state in

Sandia's Sergey Faleev looks forward to unmet challenges, include predicting such properties as optical spectra or the behavior of solids with more than 10 atoms in a unit cell. *Photo by Jeff Shaw*

high-energy-density matter. These equations of state depend on quantities like electrical conductivity. Calculating this requires detailed knowledge of the electronic structure — a perfect application for Faleev's work. The researchers hope to describe optical spectra, calculate total energy, and account for more than 10 atoms in a unit cell at 100 times the current speed.

Accelerating the code would facilitate modeling in other research areas at Sandia, such as simulating titanium dioxide used in surface science, or aiding research into carbon nanotubes that might be used in electronic or optical devices.

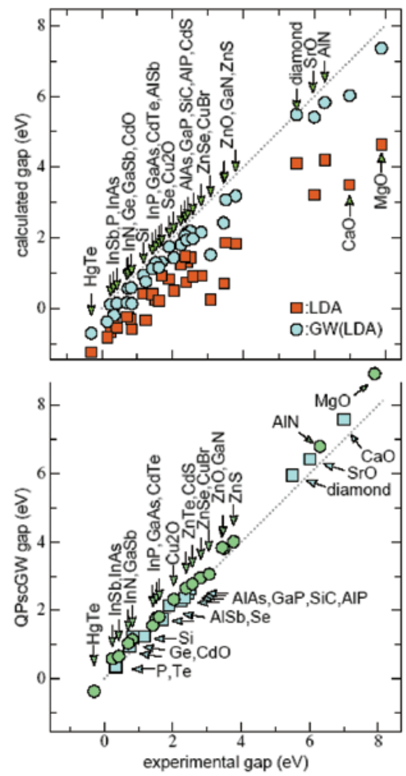
"To calculate absorption or optical spectra is a huge problem," Faleev says with anticipation. "To make it faster is a huge problem. To make it more accurate is a huge problem. To incorporate VASP is a huge problem."

Van Schilfgaarde agrees. "It's quite an accomplishment to do it at all. It takes someone who is very strong in math, and a clever programmer. We spent easily five to six man-years between us to make it work. If we can get the approach right, we can have a theory that's universally accurate for anything we want — that's really pretty neat, just requiring knowledge of where the atoms are.

Takao Kotani, of Arizona State University, is also an author on the *Physical Review Letters* paper.

Van Schilfgaarde believes the theory's advantage would be to offer true insight into material behavior. "It's kind of like adding night-vision goggles to soldiers working in the dark," he says. "Probably in 10 years, everyone will use this. "

Traditional (GW and LDA) calculation results (top graph) and deviations from an ideal (dotted line) are compared with calculations (bottom graph) using Sandia's quasiparticles GW method, which fall closer to the ideal line.



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Keeping watch on the world

Story by John German

"USNDS may be more important than ever to strategic national security. The threats are real, and USNDS provides critical global awareness."

— Jerry McDowell
Sandia Vice President for Defense Systems and Assessments

The next time a nuclear detonation occurs in space or in Earth's atmosphere, enlisted men and women in U.S. Air Force ground stations will be the first to know.

As data from dozens of satellites flood into their control rooms, it will be their jobs to decide quickly whether to refer the event to higher-ups as a violation of international law or to designate the event as something less nefarious — a lightning strike or, perhaps, a satellite sensor glitch.

The snap decisions they make could trigger an international diplomatic crisis or, if they are wrong, result in an embarrassing false alarm. Fortunately, the data will be processed, and their decisions simplified, by ICADS — the Integrated Correlation and Display System, created for the Air Force by Sandia.

ICADS is a key part of the U.S. Nuclear Detonation Detection System (USNDS), a network of Global Positioning System (GPS) and Defense Support Program (DSP) satellites, multiple detectors on board each satellite, and a handful of fixed and mobile ground stations.

"In some scenarios a nuclear proliferator or terrorist group might detonate a device in a way that makes it difficult to assign blame," says John Williams, Sandia senior manager for the USNDS program office. In that case, he says, U.S. policy makers would need accurate real-time information about the time, location, yield, and any other evidence available via USNDS.

With budding nuclear programs in at least two nations — Iran and North Korea — USNDS may be called on at any time to gather the facts about a modern nuclear detonation that could change the course of history.

"USNDS may be more important than ever to strategic national security," says Jerry McDowell, Sandia Vice President for Defense Systems and Assessments. "The threats are real, and USNDS provides critical global awareness."

Real-time reporting

ICADS includes the antennae, hardware, and software that help gather, correlate, and make sense of USNDS satellite data from multiple USNDS satellites.

The system allows operators to quickly compare live satellite signals with hundreds of event profiles in its event database. Certain atmospheric phenomena — lightning, solar storms, and even pings to a satellite by energetic micrometeorite particles — can cause

system was delivered fully qualified, under budget, and on time based on a delivery date set half a decade earlier — a rarity for a large military software development program, says Sandia ICADS project manager Don Rountree.

"A program this complex is almost expected to fall behind schedule," says McDowell. "To keep the promise we made back in 2000 required an incredible level of dedication by hundreds of people."

The program also required a broad spectrum of Sandia expertise, he says, from atmospheric phenomenology and high-energy physics to software development and systems engineering.

24/7 support

Sandians continue to support the USNDS

Sandia's Integrated Correlation and Display System (ICADS) helps the Air Force in its 24/7/365 mission to monitor the globe for nuclear detonations.
Photo by Randy Montoya

energy disturbances that register on the sensors.

"This is a complex, data-rich environment," says John. "It would take a very long time to integrate, correlate, and assess the signals from dozens of sensors. But U.S. decision makers need answers immediately. The analysis provided by ICADS before an operator ever sees the data makes real-time interpretation possible."

When a signal is verified by detectors aboard multiple satellites and bears the pulse waveform signature characteristic of a nuclear event, the operators refer the event up the national command structure, including the U.S. State Department.

Rare commitment

Last year Sandia delivered ICADS IIF, the latest USNDS military ground station system, including more than a million lines of custom software code and an emphasis on human-computer interface, which makes the job of interpreting ICADS data more intuitive. (IIF signifies the next generation of GPS satellites; the first GPS IIF bird is scheduled for launch in 2009.)

The $188 million Sandia ICADS IIF program was unusual in its size and complexity. The

A Sandia antenna field in New Mexico tracks GPS satellites carrying USNDS sensors.
Photo by David Kiffer

program. Technical experts at Sandia and Los Alamos national labs are on pager call around the clock to assist the Air Force with satellite and ground station troubleshooting.

They also provide second opinions regarding Air Force analysis of "zoo events" — unusual data signatures that don't match existing event profiles. And Sandians train the Air Force ICADS trainers, who in turn train the ICADS operators.

Under NNSA nonproliferation funding, Sandia is also working on the next generation of lighter-weight, smaller global burst detectors to fly aboard the GPS IIF and a planned new series of DSP and GPS III satellites. Continued ICADS development to support the new satellite systems is under way as well.

"USNDS is a long-term commitment for us," says Williams.

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Assessing dental disease **in minutes**

Story by Neal Singer

A recently completed pilot study conducted with the University of Michigan shows that a Sandia handheld device determined in minutes — from a tiny sample of saliva alone — if a patient has gum disease and quantitatively how advanced the disease is.

— Reported in the *Proceedings of the National Academy of Sciences*

Sandia researcher Amy Herr prepares a microfluidic cartridge containing saliva and reagents for later use in Sandia's clinical diagnostic instrument.
Photo by Randy Wong

"The gold-standard validation of any new medical diagnostic is using the instrument to assess human patients," says Sandia researcher Amy Herr. A recent study, published in the March 27 issue of the *Proceedings of the National Academy of Sciences*, reports on analysis of a pilot patient population using a clinical diagnostic instrument recently developed at Sandia.

The results of the Sandia measurements were then compared to accepted clinical measurements for that same group of human patients.

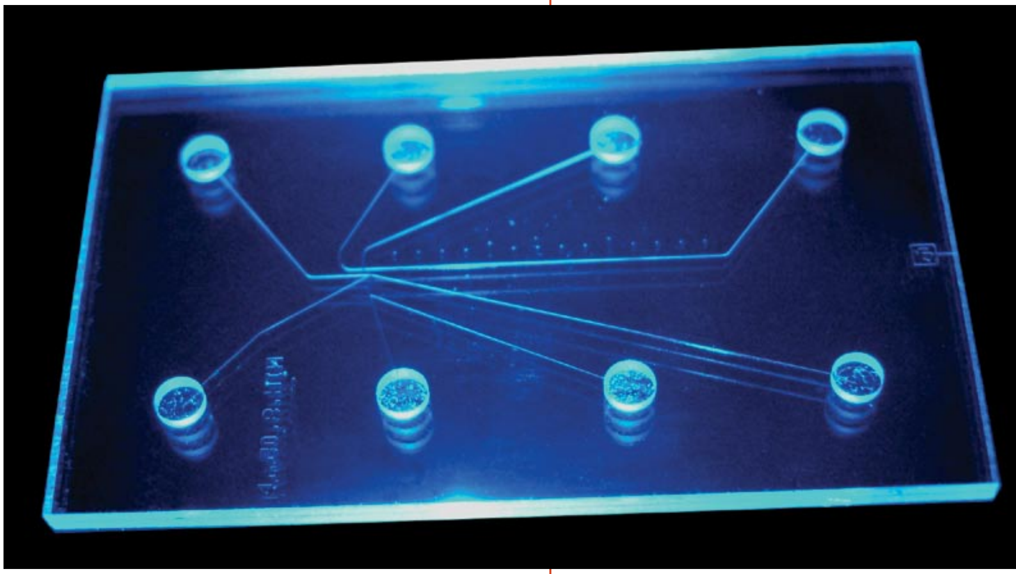
"We achieved faster and more reproducible results because we combined steps that ordinarily require time-consuming manual handling by many people, into a single automated device," she says.

Because the amount of sample fluid needed for testing is so small, Herr sees further applications in other disease areas — including potentially improved diagnosis of prostate and breast cancer — as well as rapid measurements of serum in animal models employed in vaccine development research.

"This technology also has great promise for Sandia's efforts in homeland defense," says Sandia researcher Anup Singh. "We have efforts to use the diagnostic platform to detect biotoxins and other markers in bodily fluids to be able to diagnose exposure to a biological agent."

Sandia has filed patents and technical advances to protect the work, Herr says. "The study has sparked commercial and university interest in our inventions. Our team — an interdisciplinary group of internal and external collaborators — believes Sandia's contributions in this area could advance personalized medicine. So we're motivated to extend the limits of Sandia's lab-on-a-chip tools."

"Lab-on-a-chip" refers to an entire laboratory on an area the size of a computer chip, requiring only tiny amounts of material to perform automated chemical analyses.



This microfluidic chip, about an inch long and a half-inch wide, is the core of Sandia's diagnostic instrument. The glass channels (lines connecting circular fluid reservoirs) are the diameter of a human hair. The channels make analysis of the saliva possible.

How it works

While components of the saliva-detection technique were reported earlier by Sandia, this is the first comprehensive study of Sandia's integrated clinical method.

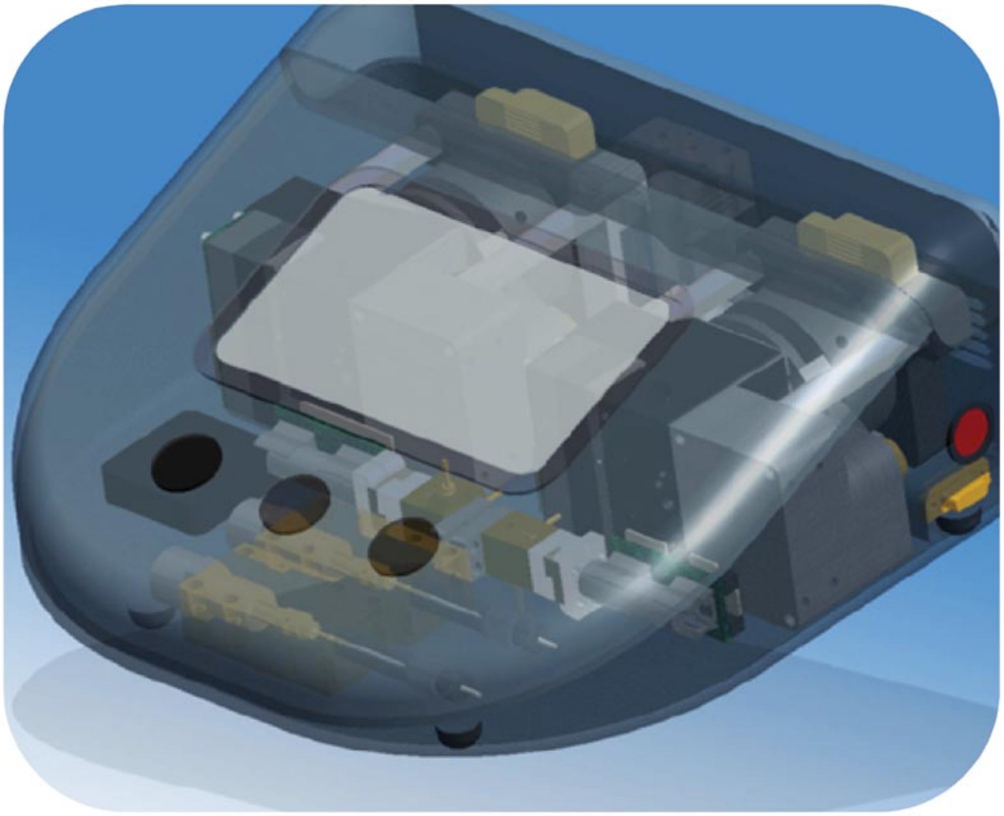
"Biomedical researchers have suspected that changes in the amount or type of proteins present may be useful as biological markers in disease diagnosis," says Herr. "Our current work with a particular enzyme in saliva supports that hypothesis regarding periodontal disease."

Aiding dental practitioners, the pocket-sized device measures the state of biomarkers to determine how much the disease has been set back. Its progress may be cloaked, silently advancing or retreating without showing any signs.

"Periodontitis can be episodic in nature," says Herr. "You need to know the stage of disease progression to diagnose and treat the illness most effectively. The enzyme [biomarker] that we monitored decreased or stabilized if the treatment was working well."

Often, owing to the time and expense involved, practitioners formerly had not been able to perform extensive biochemical investigations.

The work, funded by the National Institute of Dental and Craniofacial Research — one of 20



Engineer's rendering of proposed Sandia clinical diagnostic. (Diagnostic test and internal hardware are complete.)

institutes in the National Institutes of Health — is the first application using microliters of saliva, a painlessly and easily secured fluid. The real-life alternative to diagnose periodontitis has been quasi-subjective physiological measurements, such as gum recession and gum bleeding upon probing.

Unlike Sandia's MicroChemLab — its patented version of a lab on a chip — which reports multiple protein signatures in fluids of interest, the clinical diagnostic instrument described in *PNAS* is designed to quantify the amount of a specific protein (or panel of proteins) present in particular biological fluids. Monitoring quantities of *specific* proteins makes the tool useful as a clinical diagnostic.

Disposable cartridge

Using a disposable lab-on-a-chip cartridge, the device makes use of a molecular sieve made out of a polyacrylamide gel. The location of the sieve in the microfluidic chips is determined using photo-lithographical methods adapted from the semiconductor industry. The gel is porous, with very small openings. A low electrical current (measured in micro-amps) is passed through the gel and a process called electrophoresis moves charged proteins through it. The gel has a gelatin-like consistency and, by permitting the easy passage of smaller molecules and slowing the passage of larger ones, quickly separates proteins contained in the saliva. Prior to this separation, the proteins are brought into contact with specific antibodies chosen for their ability to bind to the biomarkers. The antibodies are pre-labeled with fluorescent molecules attached to them. Interrogation by laser of these combined molecules — fluorescent antibody and fluorescent antibody bound to the biomarker — determines the amount of biomarker present, indicating the degree of disease.

Sandia authors of the study, in addition to Herr and Singh, the NIDCR project primary investigator, include Anson Hatch, Daniel Throckmorton, James Brennan, and Huu Tran, as well as Will Giannobile of the School of Dentistry at the University of Michigan, Ann Arbor.

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Computer simulation tracks nuclear contraband traffic

A Sandia researcher has developed a simulation program designed to track the illicit trade in fissile and nonfissile radiological material to predict who is building the next nuclear weapon and where they are doing it.

“By using a cluster analysis algorithm coded into a program,” says Sandia researcher David York, “I evaluated traffic patterns and routes in which thefts, seizures, and destinations of materials were reported.” Data from these examinations allowed York to depict the A. Q. Kahn network before it was uncovered. Kahn is a Pakistani scientist linked to the illicit proliferation of nuclear technical knowledge.

Cluster analyses link data of common place, time, or material. Testing a computer simulation on a known past event is one accepted means of establishing the program’s validity. In the Kahn analysis, York looked at networked routes indicative of a nuclear trafficking scheme between countries. In several verified incidents, inspectors seized uranium enriched to 80 percent, as well as other items indicative of small-scale development of crude nuclear devices.

York developed the program as part of his master’s thesis while a student intern at Sandia. He collected and collated data from 800 open-source incidents, from 1992 to the present. He plotted the incidents on a geographic information system software platform. He came up with a network of countries and routes between countries indicative of an illicit nuclear and radiological trafficking scheme.

“The number of incidents and the quantity and quality of material seized is disturbing,” York says, “particularly because this may represent a small percentage of the actual amount of material being trafficked.” The situation may be worse than it appears because much information about nuclear material traffic is classified, he says.

York presented his results in October at the International Safeguards Conference sponsored by the United Nation’s International Atomic Energy Agency (IAEA) in Vienna, Austria. He has also been invited to present his methods and conclusions to the European Union’s Illicit Trafficking Working Group at a summer meeting of the IAEA.

For the tool to be effective, “Enough information must be collected under a cooperative international framework,” York says. “Then info must be analyzed to separate patterns from noise, essentially creating intelligence.” “We’re trying to develop a market niche for this kind of tracking program,” says Sandia manager Gary Rochau, “and I think we’re ahead of everyone’s headlights.”

The method can be used to track other materials, such as drugs. “We have a lot of interest from a lot of agencies,” says Rochau.

A trafficking analysis computed with factors deduced from available intelligence results in a probabilistic route. Actual seizure site for this in Chechnya is depicted by the star.

David York (left) shows John Reynolds a simulation program designed to track illicit trade in radiological materials.
Photo by Randy Montoya

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INSIGHTS

Scaling down to the micro-dimension

Story by Nigel Hey

One of the great revelations of engineering at the micro- and nano-scales is that the micro-world is quite, quite different from the world we can see and touch.

Dr. Arthur (Art) C. Ratzel III is the Director, of Sandia's Engineering Sciences Center. He has thirty years experience in both theoretical and experimental work in the areas of fluid/thermal sciences and energetic materials working at the Lab as a staff member and manager.

Sandia's determination to do great things with tiny technology has spawned an exciting cross-disciplinary surge of interest, attracting new talent in a number of disciplines, from mechanical engineering to microbiology.

- At the micro-scale, Sandia has pioneered a number of microelectromechanical systems, or MEMS, innovations.
- Understanding the science at the nano-scale and using unique MEMS properties can increase energy efficiency, improve healthcare, and strengthen national security.
- The technical community is fairly well agreed that, with time, micro- and nano-scale devices will revolutionize engineering, and that the manufacture of these devices will be transformed by nano-scale assembly.

However, progress in developing complex MEMS devices has been slow. The more successful MEMS innovations to date are relatively simple devices like accelerometers for airbag sensors, ink-jet printer heads, and digital mirrors for video projection. In the case of more complex systems with multiple components, problems of reliability begin to appear.

Sandia is speeding up MEMS development by learning more about the unusual nature of micro-engineered mechanisms and devising ways of turning their peculiarities into assets. Advances in modeling and simulation — where nano-scale physical effects can be formulated to describe more general aspects of MEMS systems — are currently generating a high level of enthusiasm.

One of the great revelations of engineering at the micro- and nano-scales is that the micro-world is quite, quite different from the world we can see and touch. If we don't learn to operate in that realm — if engineers don't learn to think like physicists — then the full potential of MEMS technology will most likely remain beyond our grasp.

Complex assumptions

Because many of the old assumptions don't work and the new ones are much more complex, micro-scale engineering is likely to reap great dividends from the growing interest in modeling and simulation, while relying less on conventional problem solving.

"We are moving from the early, relatively unenlightened days of 'making macro solutions smaller' to doing things a new way, through micro-scale enabled solutions," says Art Ratzel, director, Sandia's Engineering Sciences center. Ratzel authored an article on the state of the art in the March 2007 issue of *Mechanical Engineering*, flagship magazine of the American Society of Mechanical Engineers. One conclusion: "Engineering at the microscale introduces an appreciation of the complex physics at the feature scales of the devices. It demands the appreciation of a ground-up approach to design and problem-solving."

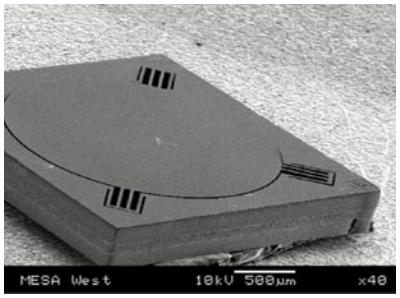
As a result, emphasis on computerized design support is increasing dramatically, and modern mechanical engineers are becoming software experts. Some are arguing that, since MEMS production is an automated two-month process, model-based design verification should be completed before fabrication begins.

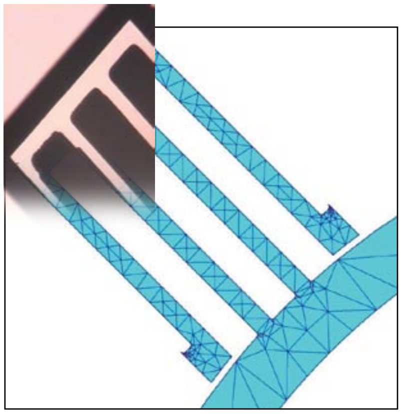
Cleanroom worker at keyboard in Sandia's Microelectronics Development Laboratory.
Photo by Randy Montoya

"It's exciting that you can review the design and check out the 3-D solid model, before it's actually made," says Channy Wong, manager of the Labs' Applied Mechanics Development department. "You predict the performance, evaluate the response from different design variations, and analyze the results. Applying modeling and simulation allows us to conduct concurrent engineering and optimize the design thus reducing costs significantly. There are lots of new things to do. I think that's the most exciting thing about working in the micro and nano worlds. Science and engineering can be very different at those lengths."

Lessons learned

Interest in computational simulation blossomed as the result of lessons learned with the Sandia micro-engine — an early MEMS product initially developed in 1995. The basic design was simple, and the first micro-engines were built under stringent clean room conditions, but they proved to be only somewhat reliable. After 477,000 cycles, an electron microscope image clearly showed the reason — accumulation of debris detached from rubbing surfaces. The Sandia team conceded they had insufficient understanding of the wear mechanisms and accelerated the labs'





Sandia engineers learned that microsizing a macroscale spring mass device (top) would have benefited from early modeling and simulation to optimize the design. Blue design for support spring (below) shows mismatches with black and white, as-built spring.

Nigel Hey is a retired Sandian, a science and technology writer, and the author of two recent books: *Solar System* and *The Star Wars Enigma: Behind the Scenes of the Cold War Race for Missile Defense.*
Photo by Randy Montoya

Sandia's Microlab and Microfab facility completed 2006. Replacing a lab built in the 1980s, the building has space for more than 250 workers.
Photo by Bill Doty

research into micro- and nano-scale science and engineering.

The built-and-test approach, which was relatively expensive, was supplemented with discovery experiments, model development, and computational simulation. This shed new light on the mechanisms that were causing imprecise precision control and lateral instability, as well as wear.

Deposition and etching

MEMS structures are built by depositing and etching polysilicon at selected areas using a multi-layer, multi-stage photolithographic process. Each deposition and etching process exposes a new surface which, when examined with an electron microscope, can be seen to include a large number of points, known as asperities, which project at various heights above the "real" part of that surface.

In the macro world, the effect of these asperities gives rise to an averaging-out notion of "slick" or "rough" surfaces and thence to the idea of sliding friction, the force that resists relative motion between two bodies in contact. On the micro scale, friction behavior depends on discrete contacts, because each asperity is relatively large and a small number of them will interact and produce effects of their own — for example breaking off and generating debris. However at nanoscale the physics of friction is an active area of research.

Many surface interaction models depend on statistical description of the asperity heights for high contact forces, since the real contact area increases with load as asperities are flattened and more come into contact. With light contact only the outlier asperities are engaged. Thus, at the macro scale, where a surface will have many contacting asperities, the real contact area varies directly with load — the heavier the package, the harder it is to slide along a counter top. But at the micro scale, unfamiliar effects can increase static friction. Forces such as stiction, the force required to get an object moving, result from the interaction between single asperities.

New questions

Since the micro-engine experiments, Sandia's micro-scale modeling and simulation community has been occupied with questions like "What went wrong?," "Can computational simulation ensure that a component will perform up to expectations?," and "Can computational simulation suggest better operation and improved design?" The next step is to bring about microscale-enabled engineering solutions — ultimately a transformation in component design — through shared innovation by individuals specializing in components, engineering, and microelectronics.

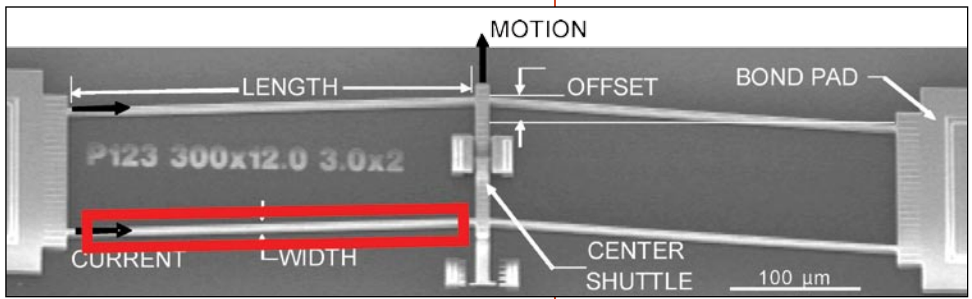
Physical models must be modified, sometimes drastically, as length scales shrink because the dominant physical phenomenon is different as length scale changes. For example, gravity is more easily overcome by adhesion; friction models break down; ballistic phonon transport in solid can be as dominated as the diffusive phonon transport.

Such effects are especially important in polycrystalline silicon (including structures made with Sandia's SUMMiT® V process), which have several levels and have geometry features up to 10 micrometers and grains in the 10s to 100s of nanometer range.

How things work

Computational simulation of a Sandia-designed microscale thermal actuator provides examples of how size affects how things work. In this device, electrical current passes through four mechanical legs, causing them to expand and displace a shuttle with a reciprocating motion. Remarkably, conventional methods predict the beam temperature at 750 Kelvin, whereas Sandia's "non-continuum" calculation, using nano-scale data, puts it at a more accurate 900 K. (See graphs at right.) With some materials, this could make the difference between melting and not melting.

The fledgling MEMS industry has a limited knowledge of materials physics at micrometer size, and currently commercialized devices are designed for specialized purposes. Partly for this reason, they do not have a broad user base, and therefore have not generated industry standards or the design and process software that would be built based upon those industry standards. However, this may change as Sandia's materials science, engineering, and computer sciences organizations develop engineering systems which, while designed for their own use, could migrate into the private sector and revitalize the pace of invention.



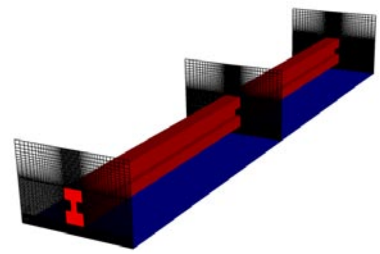
While Sandia is seeing a major effort to harness nanoscience for the improvement of applications such as micro-machines, big benefits are visualized for everyday products by Jim Redmond, manager of Sandia's Strategic Initiatives department.

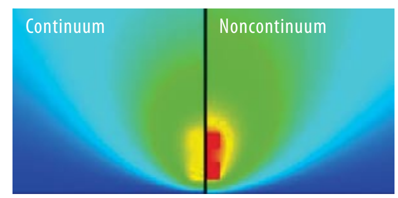
"For example, carbon black can be considered a 'nano material' that has been used for years to enhance the performance of tires, a product that we are all familiar with," he says. "This benefit was determined largely by trial and error. With modern computing and production tools, we ought to be able to engineer similar improvements for many products."

Blurring the lines

"As these new perspectives evolve into reality, a new breed of engineer is coming into existence," says Ratzel in *Mechanical Engineering*. "In fact, the line separating the computer scientist, the materials scientist, and the engineer is becoming blurred and indistinct. Mechanical engineering cannot help but benefit from this exciting new horizon. MEMS is here to stay, and it will transform the future."

"One cannot scale down confidently from macro-dimensional assumptions when the final product is measured in micrometers . . . When engineers attempt to apply traditional methods at such small scales, they often find themselves face-to-face with the unexpected —situations for which the macro-world design experience can no longer provide all the answers."





Micrograph of a thermal actuator (top) and a 3-D model of the actuator leg (middle.) The temperature contour plot (bottom) illustrates that microscale heat transport is noncontinuum in nature as molecules and phonons travel between material interfaces without collisions. Neglecting noncontinuum heat levels could result in structural integrity and other problems.

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Read more: To see the full story in *Mechanical Engineering*, click on the March, 2007 issue:
www.memagazine.org/backissues/back.html

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In *Mechanical Engineering Magazine*

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