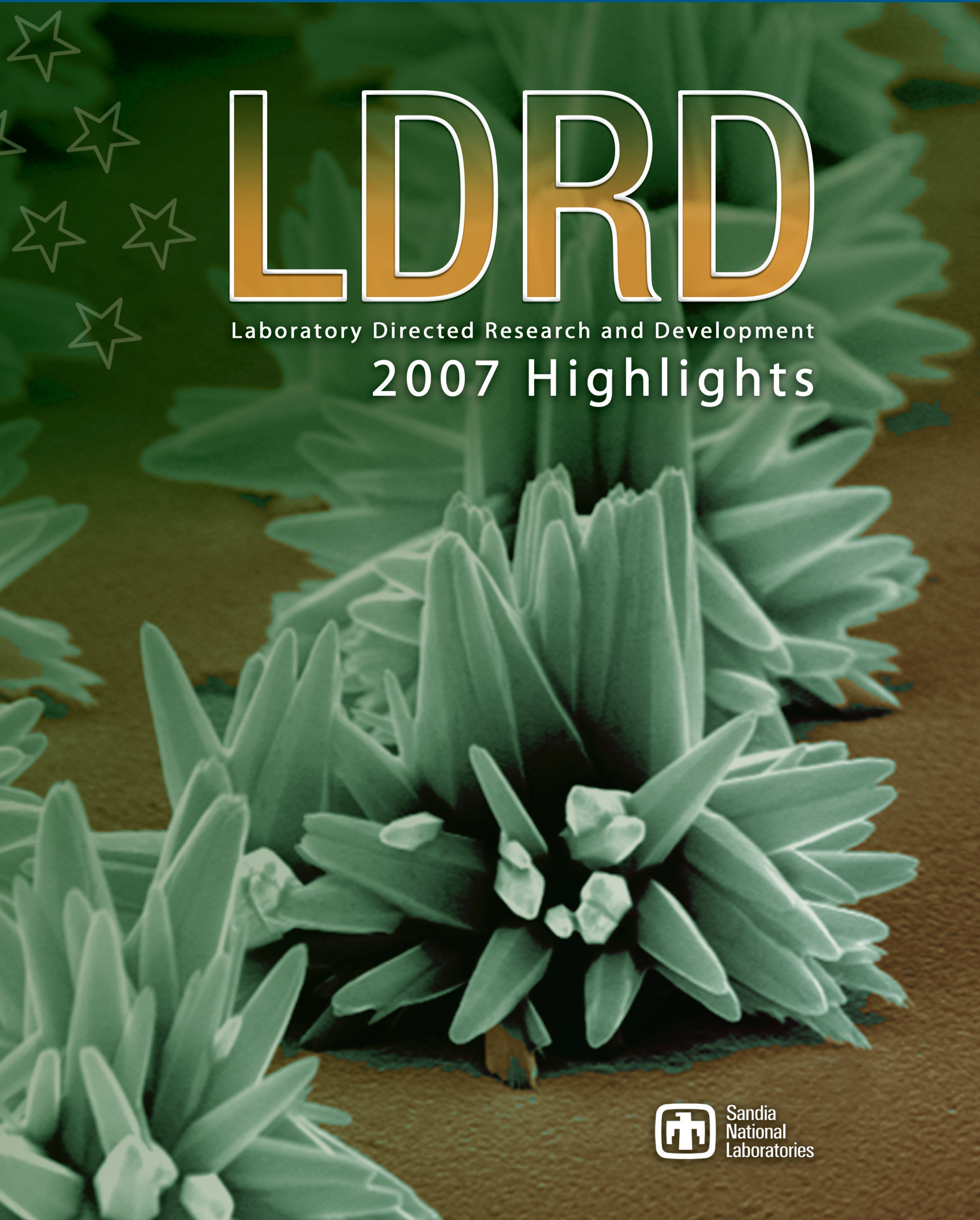

LDRD

Laboratory Directed Research and Development

2007 Highlights

Sandia National Laboratories

From the Chief Technology Officer

Throughout history, imagination and the capacity to dream have always driven great scientific and technological leaps forward. This results partly from stepping outside the boundaries imposed by mainstream scientific thinking, and partly from an ability to anticipate the future and what it may demand of us. A great national laboratory ensures that imaginative new research and development (R&D) ideas are cultivated from dedicated scientists and engineers who seek innovative solutions to our national security mission needs. The LDRD Program at Sandia National Laboratories supports such leading-edge ideas by funding high-risk, potentially high-return R&D in support of those missions.

The LDRD program is unique in that it has the flexibility to respond to present mission needs and anticipate future ones. As such, LDRD funds projects that pursue technological solutions to the most-urgent challenges facing our nation or that validate concepts or approaches offering firmer science and engineering foundations from which to propel new R&D ideas. Stretching the boundaries of the present, they generate landmark accomplishments for peers to emulate and a nation to utilize.

This brochure offers an overview of 39 current or recently concluded Sandia LDRD projects, highlighting six that were deemed worthy of Sandia's LDRD Awards for Excellence. These project summaries are but a small sampling of the LDRD program, but they demonstrate the breadth of the leading-edge R&D and their potential impact.

Richard H. Stulen
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About LDRD

Maintaining Sandia's world-class science, technology, and engineering capabilities and anticipating their evolution in response to future challenges are absolutely essential to the Laboratories' ability to address national security needs. Authorized by Congress in 1991, the Laboratory Directed Research and Development (LDRD) Program reflects precisely that congressional intent — to encourage and sustain preeminent science and technology by investing in high-risk, potentially high-payoff research and development. The program is designed to proactively anticipate the breadth and depth of research and technological development that oncoming challenges will require.

LDRD projects seek innovative technical solutions to our nation's most-significant challenges, often in collaboration with corporate and academic partners. LDRD allows Sandia to recruit and retain outstanding scientific and engineering talent in service to the Laboratories' five primary strategic business areas: nuclear weapons; energy resources and nonproliferation; defense systems and assessments; homeland security and defense; and science, technology, and engineering foundations.

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CONTENTS

Note on The Organization of this Brochure

Many projects overlap two or sometimes even more topical areas. Hence any attempt to categorize them — including the five-fold categorization employed, herein — is, by definition, somewhat artificial. For example, a project categorized as "nanoscience" might employ computer simulation in its execution, involve some microsystem engineering, and have obvious proximal applications in homeland security via bioagent detection, with potential longer-range applications in energy security or nonproliferation. Such a project therefore transcends categorization by the topical areas used to organize this publication or by other organizational schemes.

Cover Image:

Award-winning science-as-art, zinc oxide "yucca cactus" nanostructures, courtesy of Julia Hsu, Sandia National Laboratories (see page 5).

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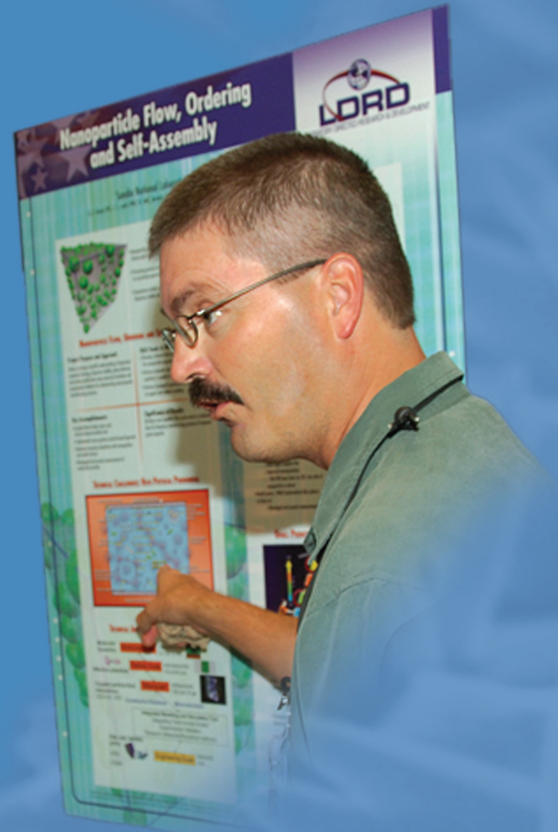
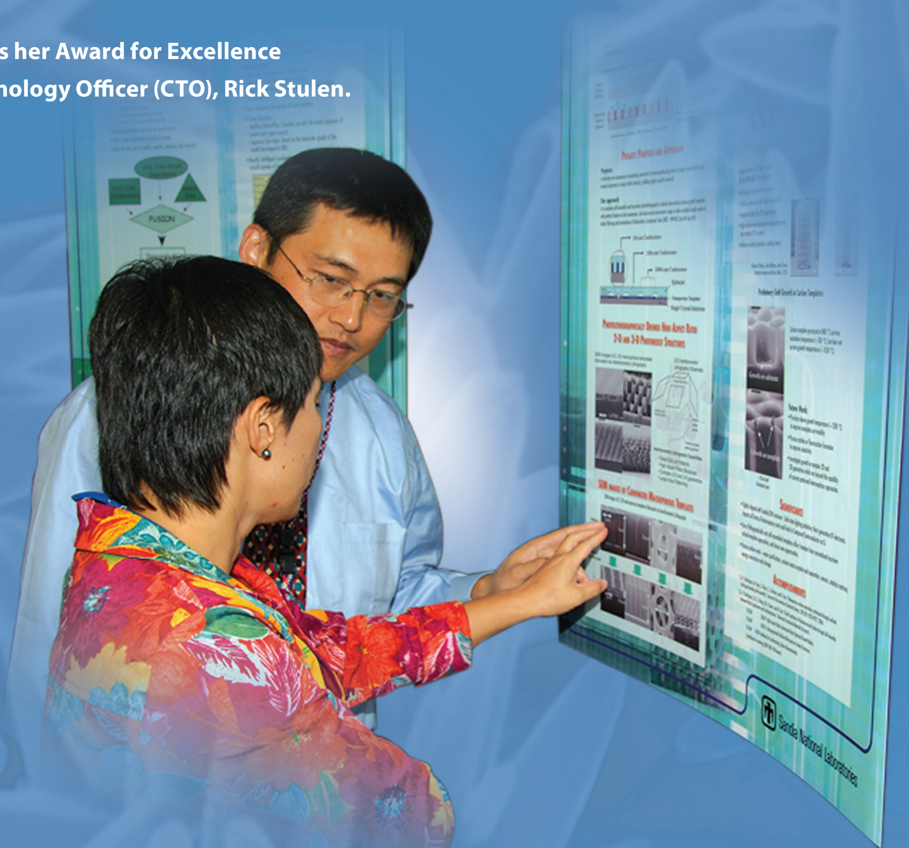
Julia Hsu accepts her Award for Excellence from Chief Technology Officer (CTO), Rick Stulen.



Randy Schunk explains the great variety of physico-chemical forces governing nanoparticulate interactions.

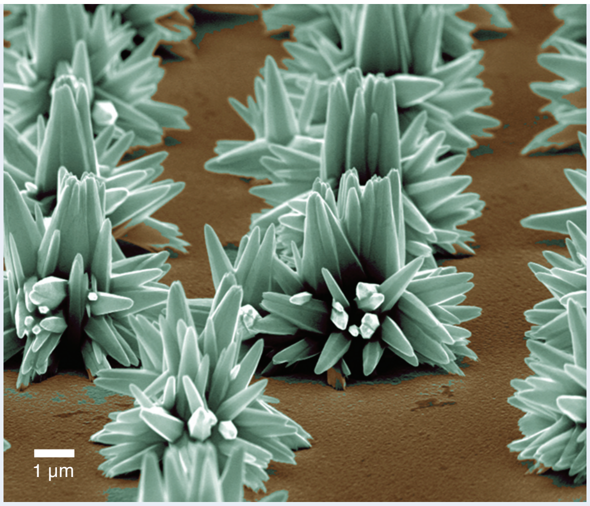


Hongyou Fan and Julia Hsu discuss potential future directions for his research.

Nanolithography Directed Materials Growth and Self-Assembly

Julia Hsu

The white cliffs of Dover, England, are spectacular carbonate structures facing continental Europe, across the English channel. Remarkably, they are built from the shells and skeletons of biological creatures. These shells have fascinated nanomolecular chemists because their intricate three-dimensional patterns grow from the mineralization of pattern-forming bio-organic molecules (typically proteins). Modern-day chemists would like to mimic such biological processes to control the formation of three-dimensional nanostructures for semiconductor applications. Typically semiconductor chips are patterned two-dimensionally by photolithography, but this process is not conducive to three-dimensional patterning of nanostructures. In this project, the general strategy of biological pattern formation was, in a sense, adapted to growing zinc oxide nanostructures, which have desirable electronic and optical properties.



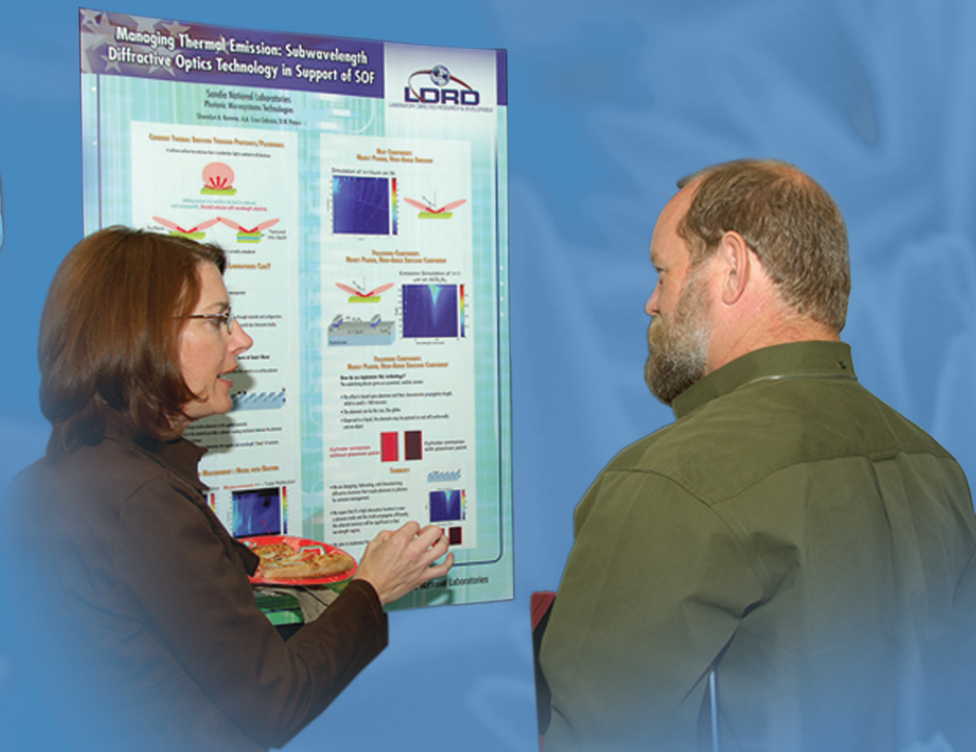
Science-as-art: award-winning zinc oxide nanostructures.

The project pursued a complex process of oriented crystal growth. Taking place in several steps, different added substances and different concentrations produced different structures through control, at each stage, of the surface chemistry of the substrate upon which crystal growth occurred. For example, seeding a glass surface with zinc oxide crystals and subsequently adding the organic substance citrate (found in orange juice), led to the growth of fatter and shorter structures than would otherwise have resulted. Several other organic molecules, used as growth modifiers over the course of multiple stages, assisted in producing a fantastic variety of nanostructural architectures. Electrical currents were sometimes applied to encourage growth in particular directions.

By systematically controlling the surface chemistry of multiple crystal growth steps, this team has been able to generate a wide variety of crystal micro- and nanostructures, even to the extent of an award-winning image for "Art as Science," the so-called "Zinc oxide yuccas," which were grown on silver foils. A key aspect of this chemistry is its environmentally benign nature.

More important than the artistic aspects are the scientific possibilities. In addition to zinc-based nanostructures, titanium-based nanotubes and calcium carbonate nanowires have been generated. Moreover, research on silicon- and cadmium-based nanostructures is ongoing. Oriented nanocrystalline shapes are demonstrating powerful optical and electronic attributes, and their properties are key for next-generation solar cells, in which efficient light (photon) and electron (current) transport will be crucial to improving the present generation's relatively low efficiency, which limits many practical applications. If the efficiency of transforming absorbed sunlight to electrical current could be significantly improved, the dream of a nonpolluting, non-fossil-fuel-based solar economy might well become a reality. Therefore, in addition to its many other applications in nanoscience, this research is at the forefront of transforming our energy future. ■

Mark Lee (above) and Hongyou Fan (below) accept their Awards for Excellence from CTO, Rick Stulen.

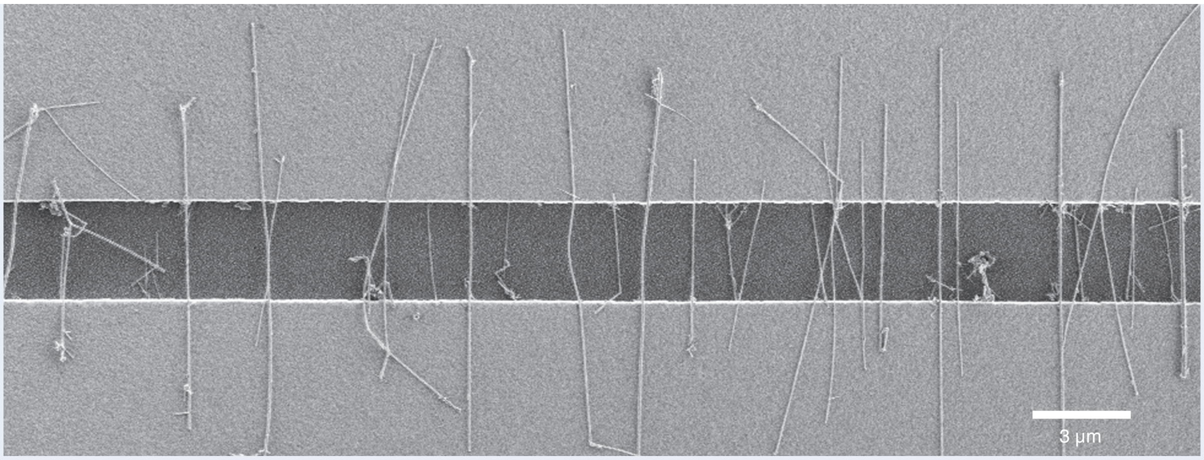


Shanalyn Kemme discusses the possibility of a paint that might mask infrared emission from a surface.

Jeff Cederberg answers a question about the properties of his self-assembled quantum dots.

Microwave to Millimeter Wave Electrodynamic Response and RF Applications of Semiconductor Quantum Nanostructures

Mark Lee



Silicon nanowires assembled along a waveguide.

Currently, electronic devices operate at frequencies ranging from those of radio waves (typically thousands [kilohertz] or millions [megahertz] of oscillations per second) to microwaves (in the gigahertz [or billions of oscillations per second]) region. These waves are typically the result of the coherent ("choreographed") oscillation of particles of matter, often electrons. Much higher frequencies of oscillation are characteristic of light waves, in photonics, oscillations of red light in the 400 terahertz (trillion oscillations per second) region. Between the electronic and the photonic lies a region around 1 terahertz that has been difficult to tame. Essentially, classical physics presents a barrier to coherent vibrational motion of particles at this extremely high rate. There are other barriers as well.

This project has overcome several of these barriers by fabricating solid state electronic nanostructures that exhibit quantum coherence. Rather than the conventional "flow" of electrons that we rely on in solid-state electrical circuitry that might produce radio waves or microwaves, the unit of oscillation becomes a plasmon, a coherent charge wave that can oscillate far faster than the actual particles, the electrons from which that charge wave arises. Oscillations in the terahertz region have been achieved.

The project used both self-assembling silicon nanowires and single-walled carbon nanotubes, assembled in a parallel arrays to demonstrate progress toward the goal of a solid-state 1-terahertz transceiver capable of outputting significantly greater than a milliwatt of average power. Traditionally, the domain of large and unreliable gas-tube and free-electron lasers, this goal of solid-state terahertz microelectronics would represent a significant breakthrough.

There are numerous national security applications of a terahertz device in secure communications and other areas. For example, many materials are opaque or reflective to other frequencies, but relatively transparent to terahertz radiation, bringing forward the possibility of "see-through" imaging or radar applications. And the spectral resonance vibrations of many molecules in the terahertz region can be used to detect and identify substances with high specificity (currently infrared and ultraviolet light are commonly used for such spectral analysis). This offers the eventual possibility of precise identification of potentially toxic substances crossing borders in sealed transport containers — without ever opening those containers. ■

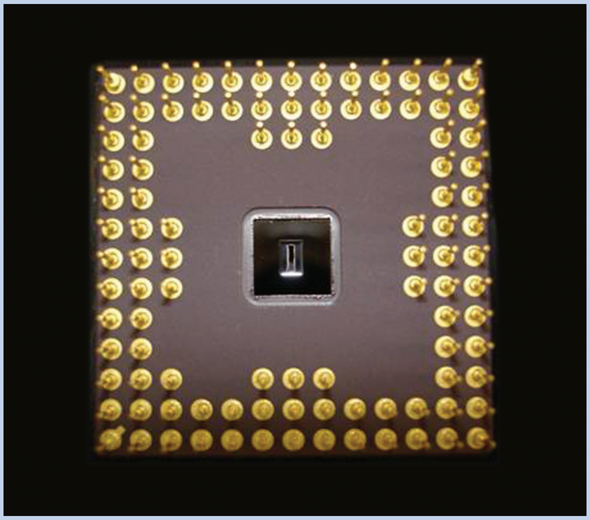
MEMS-based Array of Micro Ion Traps for Quantum Simulation Scaling

Matthew G. Blain

Working with colleagues at Los Alamos National Laboratory to simulate puzzling but groundbreaking quantum systems (such as the recently discovered plutonium-based superconductor), this team has fabricated ion-trap chips using microelectromechanical systems (MEMS) processes. It has also developed novel bonding epoxies to flexibly bind components together to form the viable ion-trap chip.

The complexity of quantum systems requires that such traps, scaled at the micrometer (millionth of a meter) level, allow experimenters to manipulate ions (charged particles) by varying the electrical potential and through the use of laser light. They also require an optical apparatus for detection of the changes in behavior (state) induced by such manipulation. Such trapped ions offer a system for simulating the multiple spin states of multi-body quantum systems.

In addition to studying quantum-level physical chemistry puzzles like superconductivity, these activities have implications for the understanding of devices for quantum information processing (so-called "quantum computing") and the scalability of devices for that purpose. Sandia's expertise in micro-level fabrication partnered with Los Alamos' strengths in theory and modeling have moved us a step closer to realizing quantum computing.



Rear view of ion trap chip (approximately 2 millimeters on a side).

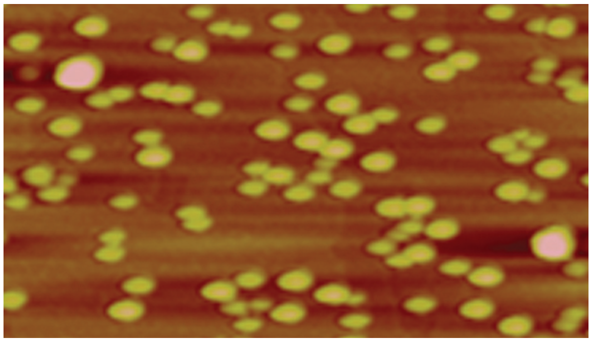
Nanoscience

Long-wavelength Infrared Detection Using Self-assembled Quantum Dots

Jeff Cederberg

Detecting infrared (IR) radiation is a key issue for both civilian and military applications, since IR can be a signature for detection of intrusion or infiltration by both personnel and electronic devices. All objects in our environment emit radiation in the infrared region, a signature of molecular motion that we sense as heat and measure as temperature. Currently, long-wave IR detectors implement a mercury-based alloy that can operate only cryogenically (at extremely low temperatures). Although these detectors are efficient, engineering an alternative operating at higher temperatures and using less-toxic materials that are easier to integrate with other electronic devices would be a significant advance. This project has made several strides in that direction, for specific IR photodetection applications.

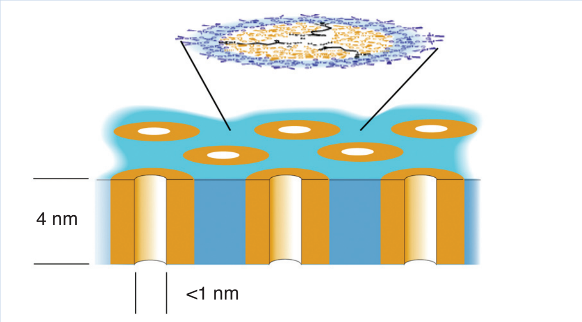
The project has pursued IR detection through the use of self-assembling quantum dots based on the metals indium and gallium rather than mercury. Although the detector shows responsiveness in the desired frequency range, improvements are being pursued in several project areas that may allow further advances. From uniformity of the quantum dots through fabrication processes through pixel design, such improvements may engender better performance and move closer to a viable replacement for mercury-based detectors.



Micrograph of self-assembled quantum dots; yellow dots about 25 nm (billionths of a meter) in diameter.

Exploiting Interfacial Water Properties for Desalination and Purification Applications

Randall T. Cygan



Artist's rendition of water pores in a silica membrane, showing the detailed molecular structure of the wall of the pore (top).

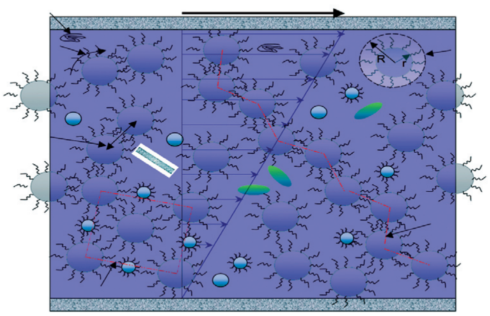
Water shortages affect half the world's population, and where water is scarce, 80% to 90% of diseases and 30% of deaths are connected to poor water quality. The production of fresh water from seawater, brackish water, or water otherwise contaminated by toxins such as arsenic is expensive and energy consumptive. If purification costs could be reduced, states like New Mexico, with extensive brackish groundwater resources, could gain access to precious fresh water resources. This project has addressed this critical issue through nanochemistry, as part of Sandia's mandate to focus on improving fresh water resources.

The project is devising and employing novel materials to fabricate better separation membranes. In addition, this team is using computational modeling and a study of naturally occurring biological pores (known formally as "ion channels") to assist them. The project is essentially creating active nano-sieves to serve as interfaces where water pores can allow water to be separated from dissolved substances. Through a study of both man-made materials like nylon, and naturally occurring minerals, such as zeolites, this clever chemistry tries substituting one substance for another in order to devise membranes — molecular sieves — that are selective for the passage or exclusion of a variety of substances.

The team has generated a greatly enhanced understanding and ability to model the interaction of water molecules and dissolved substances with a variety of molecular sieves, so that taking the next steps forward toward fabrication of efficient and cost-effective structures for water purification is becoming a more realistic outcome.

Nanoparticle Flow, Ordering, and Self-Assembly

Gary S. Grest



Drawing of the numerous interparticle and particle-solvent forces.

The juice of a peach and honey: both are sweet, both mainly aqueous (watery) solutions of the sugar, fructose. Yet one is more viscous (thicker) and slowly flowing, the other is thinner. This illustrates how flow properties (rheology) of fluids can change markedly even when the same components are present in different proportions. The physics of fluid flow can become far more complicated when many different particle types are present.

Fluids containing nanoparticles are quite complex in terms of the many and varied chemical interactions that occur among the suspended and/or dissolved particles. This project is attempting to computationally simulate these chemical forces in order to better predict how nanoparticulate fluids will behave during manufacturing processes. Multi-million atom simulations are possible, and the methods can integrate particle interactions across several different scales from molecular dynamical interactions occurring at the nanosecond (billionth of a second) timescale through engineering dynamics at the multisecond scale.

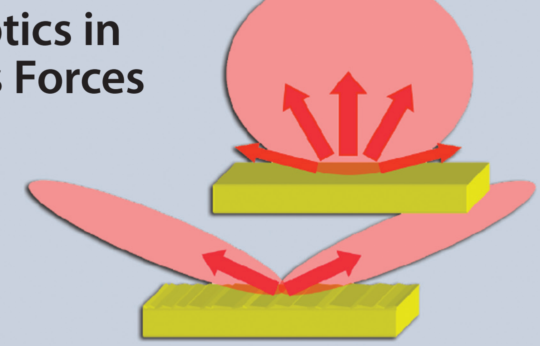
This capability should provide important guidance for designing manufacturing processes involving nanocomposite materials. The importance of this predictive capability is illustrated by a May 2007 Cooperative Research and Development Agreement (CRADA) reached among Sandia and corporate partners, including Procter and Gamble , Corning, 3M, BASF, and Imperial Chemical Industries. Its purpose is to develop production-level computational capabilities for nanoparticle flow-processing strategies.

Managing Thermal Emission: Subwavelength Diffractive Optics in Support of Special Operations Forces

Shanalyn Kemme

Any object having a temperature above absolute zero emits infrared (IR) radiation. For the most part, that IR is radiated in all directions from an opaque object's surface, most of it perpendicularly. This project is investigating methodologies for altering an object's pattern of IR radiation and has its roots in the field of plasmon-photon (light) coupling. If an electricity-conducting metal like copper is thought of as a regular organization (lattice) of atoms within a sea of mobile electrons that carry electrical current, then at the surface of the metal, a plasmon is a measurement of coherent electron waves, parallel to that surface.

These computational studies have indicated that imposing a regularly repeating pattern or grid of appropriate dimensions into an object's surface can control those plasmons, which in turn, acts to alter that surface's IR emission. Choosing the appropriate details for the repeating pattern at an object's surface can dictate that a majority of emitted IR radiation occurs at extreme angles (for example, at a 10-degree angle) to the surface, rather than perpendicularly (at 90 degrees).



Comparison of infrared emission from a smooth (top) versus a patterned (bottom) surface.

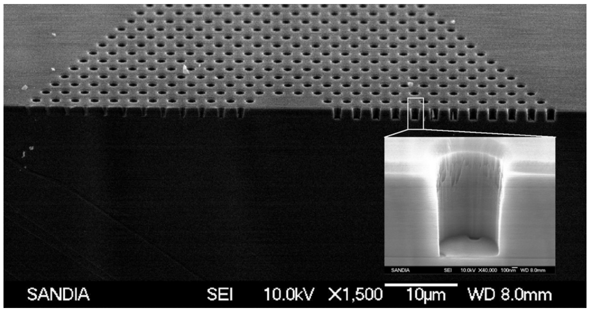
There are several potential applications: Since IR radiation dissipates heat (thermal energy) from an object, controlling emission direction implies a greater control over radiative cooling of objects, an important parameter, for example, in semiconductor chip operation. Higher-efficiency incandescent lamps and thermophotovoltaics are possible. Another application involves the ability to "hide" objects from thermal detection. The plan is to fabricate a "glitter"-like paint, where instead of glitter, the suspended objects will be tiny versions of the grid pattern that when painted onto a surface will alter IR emission, potentially masking the object from thermal detection.

Nanoscience

Mid-infrared Quantum Dot Emitters Utilizing Planar Photonic Crystal Technology

Eric A. Shaner

As a consequence of their energy-state properties, quantum dots also have unique optical properties that may lead to new or higher-efficiency devices. By growing "islands" of indium arsenide quantum dots in a specially configured electronic fashion, this project successfully demonstrated an "all-electron" mid-infrared emitter. Essentially, this device is similar to a single stage in a quantum cascade laser with quantum dots replacing quantum wells in the active region. In part, a consequence of the development of a good theoretical understanding of electron transport in these systems, the team was able to obtain room-temperature light emission. As shown in the image, this material will be integrated with photonic crystal cavities in the near future, in order to increase efficiency and create wavelength-tunable devices (devices in which the output wavelength [perceived "color" for visible light] can be controlled).



Micrograph of a photonic crystal and one of its cavities.

In another effort to potentially control the output wavelength and enhance photon extraction, surface plasmon output couplers were developed. At this project stage, these elements are primarily used as bandpass filters, but they may ultimately be directly implemented to enhance coupling out of quantum dot material and may also play a role in electrical tuning of certain quantum cascade lasers.

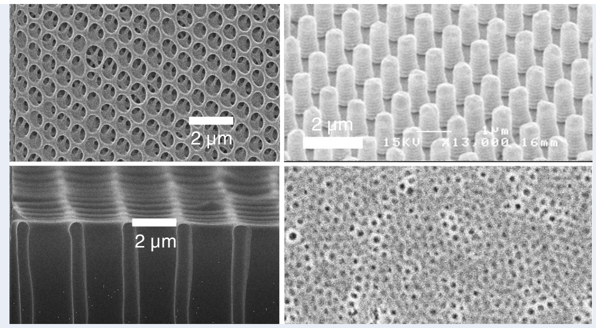
Nanoporous Films for Epitaxial Growth of Reduced Defect Nanomaterials

Hongyou Fan

Minuscule electronic devices that store and play gigabytes of music and video — twenty years ago, only leading-edge scientists could have envisioned this scenario; yet, today, they are a fact of life. The high-tech world is obsessed with data density and nanotechnologies as the means to build smaller devices with more memory storage. However, as a corollary to ongoing chip miniaturization, one must also consider the quality of the materials used to fabricate such microprocessors. This project is pursuing unique approaches toward fabricating better-quality nanomaterials.

Defect-free semiconductor nanomaterials (for example, gallium nitride), the underpinning structures of chip miniaturization and likewise critical to the ubiquitous LED (light-emitting diode) are difficult to fabricate. Normally, these are made by a combined crystal growth / photoetching process that ultimately forms the industry-standard printed-circuit semiconductor chip. At the molecular level — the nanometer (billionth of a meter) scale — there are several sources of chemical-interaction issues during the growth of crystals that can provoke defects. According to the National Institute for Standards and Certification Information, the defects of semiconductor materials grown on hard inorganic (such as sapphire) substrates can be effectively rectified, but only through processes that are costly, adding "significantly to the cost of the end product."

By contrast, this project team predicted that it could reduce nanostructural defects by growing nitrides on patterned organic (carbon-based) substrates (underlayers). True to that prediction, the team has developed new nanoporous templating materials for growth of semiconductor materials on organic patterned substrates to reduce defect density, yielding higher-quality material. The team



Micrographs of various patterned nanoscale templates.

used a technique known as interferometric lithography (etching), light rays interfering with one another to produce periodic patterns of light (high-intensity) and dark (low-intensity) regions; this phenomenon was employed to etch nanoscale patterns. These were then carbonized at high temperatures, producing a substrate underlayer with a controlled pattern of pores or holes that can range from the nanometer to micrometer (millionth of a meter) dimension.

A second technique relies on the self-assembly molecular properties of carbon-based nanostructures (illustrated by the well-known carbon nanotubes and infamous "Buckyballs"). Beginning with sugars and other organic molecules, which self-assemble into periodic nanostructures, this method likewise yields intricate two- and three-dimensional patterns upon which semiconductor materials can grow in a reduced-defect fashion.

With immediate impacts in LED and laser fabrication, the more-reliable, more-cost-effective process should ultimately be poised to support advances in semiconductor fabrication for a more-global electronics and communications market, as well as for national security arenas such as surveillance. There are other potential applications in both nanoscale electrochemistry, cellular and molecular biology, and in generation of terahertz-frequency signals. ■

Bioagent Detection Using Miniaturized NMR

Todd Alam

NMR (nuclear magnetic resonance) spectroscopy (and its medical-imaging relative, MRI) has found enormous utility in medical, industrial, and research areas. As a non-optical technique, NMR is not hampered by partly opaque fluids such as milk or blood, and hence can serve as a detector of chemo- and biotoxins in such fluids. But the technology is hampered by its size and cost.

Suppose the technology could be miniaturized and its price tag reduced, using much smaller magnets and analyzing much smaller samples, thus making the technology field-operations relevant. This project's goal was to create or locate the various elements of such a miniaturization initiative. Beginning with a coffee-mug-sized, Sandia-created 1-Tesla magnet, the team devised and optimized a coin-sized magnetic-detection platform. It then seized on iron oxide nanoparticles, dubbed "SPIONS," as the magnetic vehicle within a microfluidics system. Finally, it employed biological detection-specificity offered by antibodies, proteins that can specifically cling to a broad range of toxic chemicals and microorganisms. Coupling antibodies to the magnetic SPIONS rendered the system agent specific.

A powerful Sandia-created magnet suitable for use with this miniaturized technology.

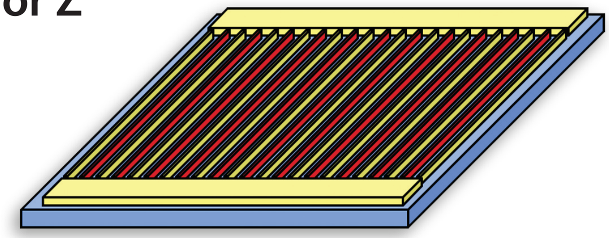
So, for example, in identifying the possible presence and concentration of the bacterial toxin causing botulism, a blood sample exposed to SPIONS coupled to an appropriate antibody would cause a positive response. Since the SPIONS are magnetic, they are readily detected by NMR.

Beyond the technology's specificity is its sensitivity, another prerequisite for miniaturization. And indeed, the designers have demonstrated that their micro-NMR is usable with fluid volumes in the range of 10 one-millionths of a liter. This technology is now poised for a myriad of possible applications in both threat detection and military and civilian medicine.

Microfabricated Wire Arrays for Z

Mike Cich

Stockpile stewardship without the resumption of underground testing requires analysis and understanding of the behavior of materials at extreme conditions. Critical to this understanding, the Sandia Z-machine serves as a pulsed-power x-ray source to deliver such extremes. Employed by all three weapons laboratories, Z performs this function by the sudden creation of plasmas (ionized gases) that implode onto target materials of various types. To create these plasmas, extreme electrical currents are pulsed through arrays of microscopic wires that explosively vaporize. The wires are consumed during the experimental process as their constituent atoms form the plasma. The exact configuration and composition of the wires determine different characteristics of the plasma, which, in turn, defines the extreme conditions imposed upon the target material.



Drawing of the type of wire array fabricated by this method.

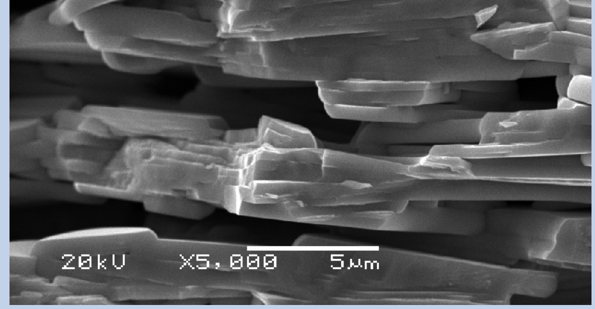
Such wire arrays for Z must currently be fabricated by hand, through precision machining. A repeatable, mechanized process for microwire array fabrication would facilitate more-rapid experimental setup on Z, thus improving complex-wide capability for performing such stockpile-stewardship-crucial experiments.

This project team has engineered such a reproducible mechanized microfabrication process that relies on selective etching of materials placed under controlled strains. In addition to the production of currently utilized microwire arrays, novel arrays from this effort should also expand the spectrum of experimental designs that can be attempted on Z.

Microsystem Engineering

Advanced Manufacturing of a Novel Functional Material

Christopher DiAntonio



Micrograph showing the stacked-grain microstructure of a bismuth- and titanium-based ceramic.

In part, a consequence of the Federal ban on lead paint enacted in 1978, it is fairly common knowledge that lead is a harmful substance, one capable of adverse effects on the central nervous system, particularly of children. This project has progressed toward the fabrication of novel materials that can substitute for lead-containing electrical components, and has also developed a novel microstructural engineering process for their fabrication.

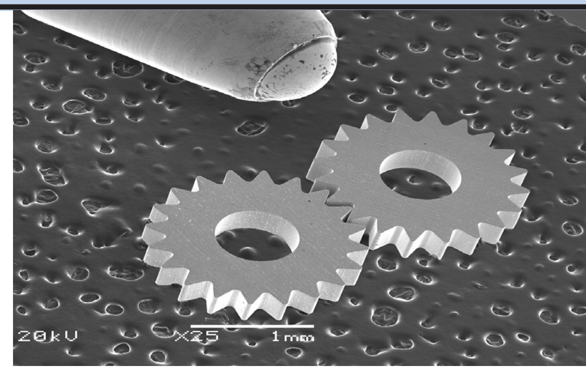
A handful of dominoes thrown into the corner of a room would end up in all sorts of orientations: some lying flat, parallel to one another, some perpendicular to those, still others standing on edge against the wall. Contrast this with a carefully created stack of dominoes forming a pyramid, all oriented in the same direction. Analogously, at the microstructural level, bulk materials are often formed of polycrystalline grains that may be arranged either randomly or in specific orientations.

Terming it "texture engineering," this team has developed methods to template the formation of such crystalline materials and to employ physical shear stresses to control material growth from individual grains, the grains conforming to particular orientations. The project has produced ceramic materials for electronics with lead replaced by bismuth and in which certain electrical properties can be controlled depending on grain orientation. Such grain-templated materials can provide improved capabilities for weaponry, advanced sensing technology for homeland security, superior sonar materials for Navy systems, and higher-resolution ultrasound components for medical diagnostics.

Microsystem Engineering

Low-Cost, Mesoscale Parts Fabricated from Nanocrystalline Metals

David Gill



The first-ever mesoscale parts from nanocrystalline metal, shown near the tip of a ball point pen.

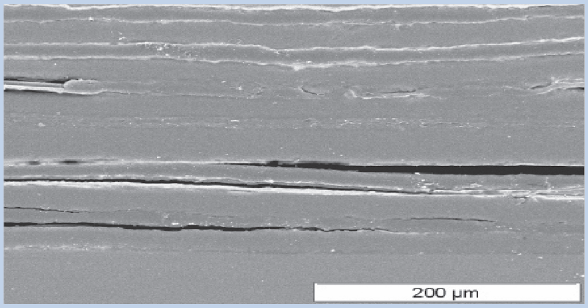
How can millimeter-size parts with ultrahigh strength and hardness be made from a pile of metal powder? This is the problem currently being addressed by the Nanocrystalline Metal team. Nanocrystalline metals exhibit extremely high strength, superior hardness, and are expected to have very low wear rates, as well. However, the methods for creating nanocrystalline metals from high-strength alloys produce powder instead of bulk material (what we would commonly think of as a "block" of metal). Adding to the challenge is the fact that this powder cannot be formed into bulk material using available techniques: the pressure, heat, and time required to form the material into bulk shapes cause the metal's microstructure to change, leading to the loss of the unique properties deriving from its nanocrystalline structure.

This project has been studying high-strain-rate processes for joining the metal powder, including cold spray and shock compaction. Cold spray impacts the particles onto a surface at extremely high velocities creating bulk material with functional properties. Shock compaction uses a gas gun to fire a projectile into a mold full of nanocrystalline powder, forming the powder into a bulk material so fast that the microstructure doesn't have time to change. Through these methods, the team has created bulk nanocrystalline material that is large enough for mesoscale (millimeter size) parts to be machined from that bulk material — the first-ever mesoscale parts from nanocrystalline material.

The team is testing these parts for strength, ductility, corrosion resistance, wear, and other mechanical properties. The technology being produced by this project will provide designers with a whole new suite of super materials to satisfy the demanding requirements of mechanical microsystems including those required by key national security customers.

Multilayer Coextrusion Processing for Micro-Nano-Layered Devices

Joseph L. Lenhart



Micrograph of a multilayered extrusion showing a separation defect that the project seeks to rectify.

A relatively lightweight shipping container that maintains the temperature of its contents without coolants; clothing that responds to changes in body temperature by adapting its heat dissipation properties: Such seemingly futuristic advances are rapidly emerging, as engineers learn to assemble the appropriate multilayered structural materials. Properties such as strength, permeability, and adhesiveness can be controlled by selecting and fabricating the appropriate layered structures.

This project is devising methods to extrude multiple layers of polymer materials of micro- (one-millionth) and nano- (one-billionth) meter thicknesses, in order to efficiently manufacture such structures.

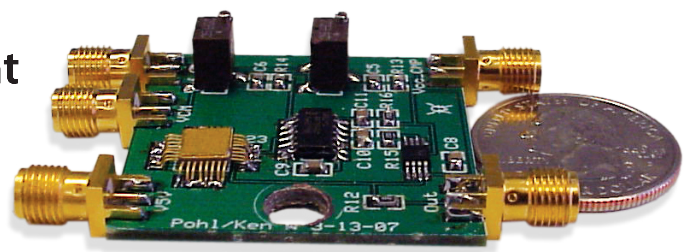
This is, of course, more difficult than it might sound, because in addition to controlling flow rate of extrusion to obtain uniformity of laminar (layered) flow, the chemistry of the extruded materials becomes a challenge, particularly as layers become thinner. Atomic and molecular interactions among the particles and suspending medium in the extruded material become an issue, especially if the particles show a tendency to clump together. Viscosity ("thickness") of the extruded materials is important, particularly when multiple layers of material are being simultaneously pushed out by the extruder mechanism. A viscosity mismatch in adjacent layers can easily produce instabilities.

The team has succeeded, to date, in extruding 8, 16, and 32-layered structures of total thickness less than a half-millimeter; it has employed a number of ingenious physical chemistry and engineering strategies to control viscosity, surface chemistry, and particle shape. It has demonstrated that individual layer thicknesses of less that 10 one-millionths of a meter are possible. Everyday encounters with futuristic materials may be just around the corner.

Microsystem Engineering

Post-CMOS Compatible Aluminum Nitride Resonant Accelerometer

Roy H. Olsson



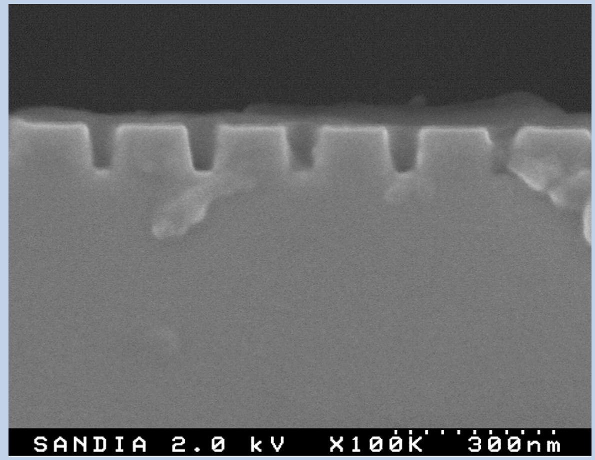
Miniaturized circuitry for the device compared with a US quarter-dollar coin.

As the name suggests, an accelerometer is an instrument for detecting and measuring acceleration. Perhaps surprisingly, such devices are a significant part of everyday life. For example: the deployment of airbags in your automobile is triggered upon sudden decelerations; and prior to hitting the ground, your laptop switches off, if it falls from the surface of your desk. There are many other industrial applications such as in measurements of the severity of vibration in machinery. This project has developed a resonant accelerometer, based on a circuit that compares the change in the frequency of vibration of two delicate tuning forks, positive acceleration (as in your laptop falling) increasing vibration frequency of one fork and decreasing vibration frequency in the other. This piezoelectric arrangement (altered motion transformed to altered electrical parameters) changes the flow of current in a circuit designed to convert the changes into a measurement of acceleration.

The entire package, including the circuitry, is merely a few centimeters in size. Moreover, compatible materials-processing conditions and compatible chemistry ensure that the device can be placed directly atop semiconductor circuitry. It has been tested and validated in sensitivity, showing extremely accurate performance. Its design renders it more reliable, less sensitive to fluctuations in temperature, and relatively simple to fabricate.

Nano/Micro–Engineered Interfaces for Improved Performance & Reliability

E. David Reedy



Micrograph of the exemplary patterned, nanoscale roughness imposed on a surface film.

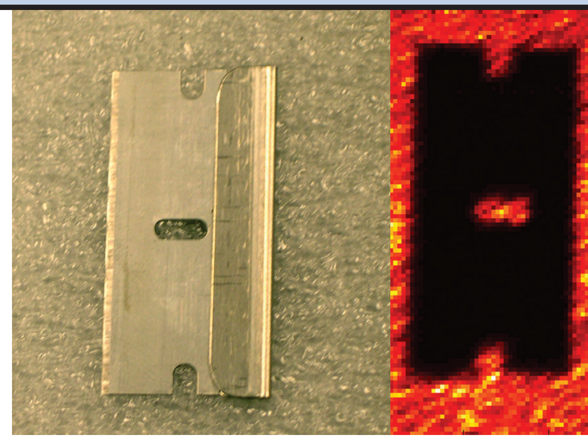
Today's microelectronic devices are composed of multiple thin-film layers. Many of these layers are brittle, and consequently, the devices contain numerous brittle interfaces. This situation defines a strength issue, where the interfaces between thin films can be a failure point that diminishes reliability of an electronic component. This project investigated methods for increasing the reliability of the interface between brittle films.

Employing both atom-level and continuum simulations as well as an experimental approach, the project team used existing nanolithography techniques to introduce regularly patterned, nanoscale roughness between thin-films. Tests indicated that the toughness (resistance to fracture) at the interface between two thin films increased as a result of this patterned roughness. Simulations also suggested that the current models used in nanoscale analyses of such fracture events might require modification.

In addition to microelectronics, thin films are also found in protective coating applications in a variety of products, as well as in nuclear weapons components. Clearly, the consequences of improving interfacial toughness can be quite significant.

Terahertz Microelectronic Transceiver

Michael C. Wanke

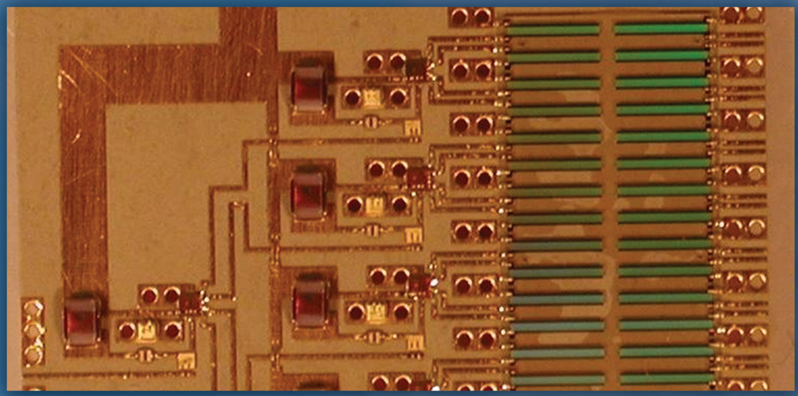


A razorblade and its image, recorded through a layer of Styrofoam with terahertz radiation.

Based on the seminal theoretical and nanoscience research of other Sandia staff, this project seeks to lay a foundation in microelectronic technology for a terahertz transceiver (transmitter-receiver of signals encoded into electromagnetic waves).

With the terahertz regime of electromagnetic radiation just recently brought into more-realistic control with the advent of terahertz quantum cascade lasers, this project focused on integrating the laser with a Schottky diode, a device with very rapid switching. By micromachining prototypes of waveguide components, the project team fabricated a prototype integrated transceiver.

National security applications of a terahertz device in secure communications and other areas are numerous. For example, many materials are relatively transparent to terahertz radiation, but opaque or reflective to other frequencies, bringing forward the possibility of "see-through" imaging with a compact device, such as in unobtrusive weapons detection or sealed package examination. And the spectral resonance vibrations of many molecules in the terahertz region can be used to detect and identify substances with high specificity. A key corollary is that there are no known health hazards associated with milliwatt exposure to terahertz radiation.

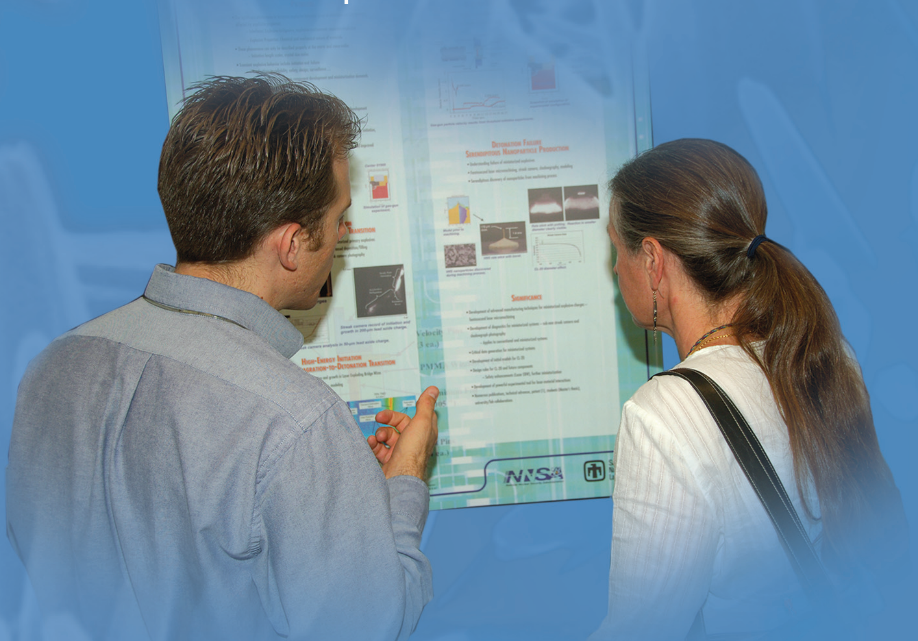


The circuitry in Larry Bacon's Just-in time technology that splits an incoming signal into parallel frequency-analysis channels.

Larry Bacon accepts his Award for Excellence from CTO, Rick Stulen.

Sal Rodriguez points out the essential aspects of his model coupling hydrogen production to nuclear power.

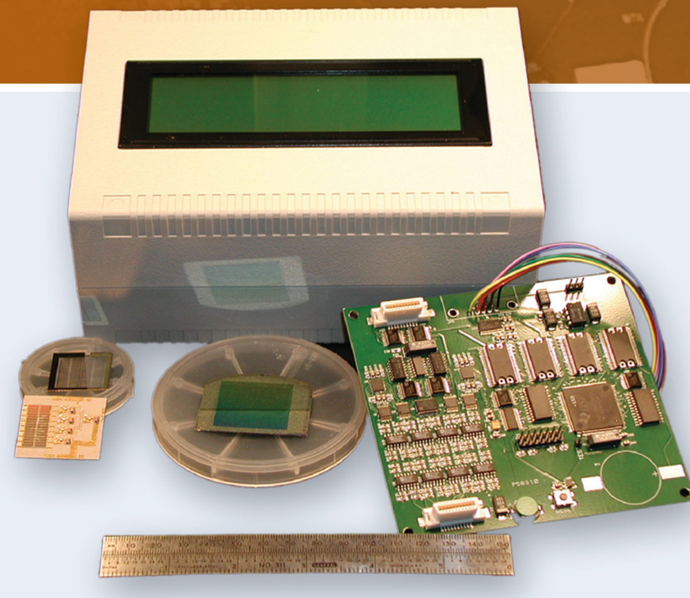
Dan Dolan illustrates how synthetic diamonds might be used in ZR Machine dynamic compression experiments.



Alex Tappan explains a streak camera image of explosive initiation.

Just-in-time Jamming

Larry Bacon



Components of the jammer adjacent to a six-inch ruler.

Every day, American personnel encounter the threat of improvised explosive devices (IEDs) triggered, most often, by radiofrequency (RF) signals, crude, but perversely effective remote detonation apparatus. Such devices can be best contravened at the source by jamming the triggering signal. Currently, the cost is high: broadband multi-frequency jamming signals that can reliably disable such triggers also interrupt all other communication signals during the jamming interval, thereby creating communication-downtime vulnerabilities of their own. Similar drawbacks ensue from broadband jamming of other communication signals: when jamming is not frequency selective, undesired interruptions can occur.

But suppose that the specific radiofrequency of the triggering signal could be rapidly discerned, such that a precise narrow-frequency band could be broadcast as a jamming signal — over the time necessary to prevent IED detonation? Based upon Sandia-invented acoustic, silicon-germanium and other components, this team has devised just such a detector-jammer that functions as an analog (full-frequency spectrum) device. Silent until activated, and consuming very little power from its battery, it awakens upon detection of a detonation-trigger signal.

The detected trigger signal is routed into multiple parallel channels at adjacent precise signal frequencies within the band being analyzed. A given channel thereby detects the exact frequency of the detonation signal. Then, the device transmits an appropriate, frequency-precise jamming signal before the detonation signal is completely transmitted to its IED. Since the jammer is silent until this moment, it is itself difficult to detect and counteract.

Threat foiled — and personnel protected — without the broadband jamming transmission that would interrupt other critical communications. Moreover, by integrating this analog functionality with a digital signal processor, the jammer is kept well within the hand-held size range.

The prototype 16-band device operates in a known crucial frequency range. From this adaptive and ingenious foundation, devices operating in both alternate and broader-frequency bands can be crafted — the technology is scalable, covering as much bandwith as is desirable. Several smaller units can be stacked to cover a number of different frequency ranges, while still keeping the unit at the single-personnel portability level. A larger unit can also be upscaled to vehicle size and crafted to monitor a much broader range of signal-transmission frequencies.

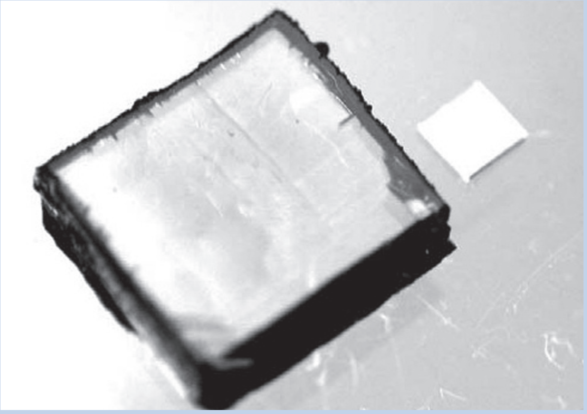
Other applications include wireless sensors for aircraft and detection of covert transmissions at or near secure facilities. ■

Dynamic Compression of Synthetic Diamond Windows

Daniel H. Dolan

Extreme conditions of rapid material compression are quite essential to many types of experimental work, for example, to understand weapons components and to study the stresses that can cause material failure. But such dynamic compression experiments require extremely strong viewing windows that are resistant to both physical and electrical current invasion. Based on their transparency to light, mechanical strength, and electrical resistance, diamonds are one of the premier materials for this application. But diamonds are not only expensive but artificially inflated in price. Hence, cost makes the use of natural diamonds as viewing windows for material compression experiments prohibitive.

Consequently, this team has thoroughly investigated the use of synthetic diamonds. By sandwiching a mirror between two synthetic diamond windows from which light waves were collected for interferometry — a standard measurement technique — the team found that even at extreme pressures,



Two square synthetic diamonds, two millimeters (left) and one millimeter (right) in thickness.

the synthetic diamonds retained their elasticity and transparency far better than other options. Synthetic diamonds appear to be ideal for a range of shock and other dynamic compression experiments essential to Sandia (ZR Machine) and other national laboratory programs, for example, assessing elastic-plastic deformation and phase transformations in various materials. Ongoing investigations may indicate broader applications in other areas of experimental work, as well as in detection of fissionable materials.

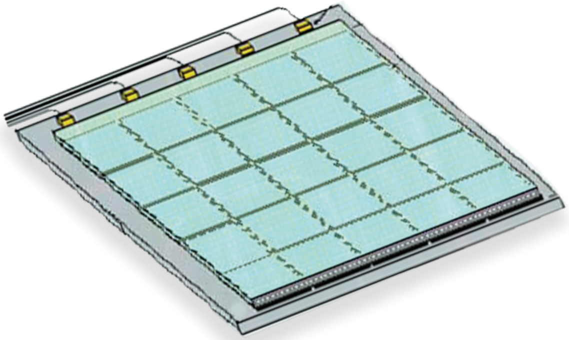
National Security Applications

Highly Pixelated Hypertemporal Sensors for Global Awareness

Randolph Kay

We live in an age in which our enemies are no longer overt. Ascertaining the presence and nature of covert enemies is now a primary focus of ensuring national security, and Sandia has a long history in developing and refining technologies to monitor global events that provide clues to the location and nature of threats. In this project, large arrays of fast-sampling integrated-circuit chips have been devised and assembled as pixels to sample the environment for detection of transient optical or infrared events (explosive detonations, for example).

Each array is a thin wafer of detector tiles, with arrays stacked upon one another to increase detection sensitivity. Interconnections are all-optical. Designing and assembling the arrays required integration of several teams responsible for modeling, fabricating silicon circuits, devising a viable means of packaging the sensor, and designing a high-speed interface to digitize the optical data and quickly move it to a digital processor.



Drawing of a five-by-five pixel array of chips on a wafer-scale motherboard.

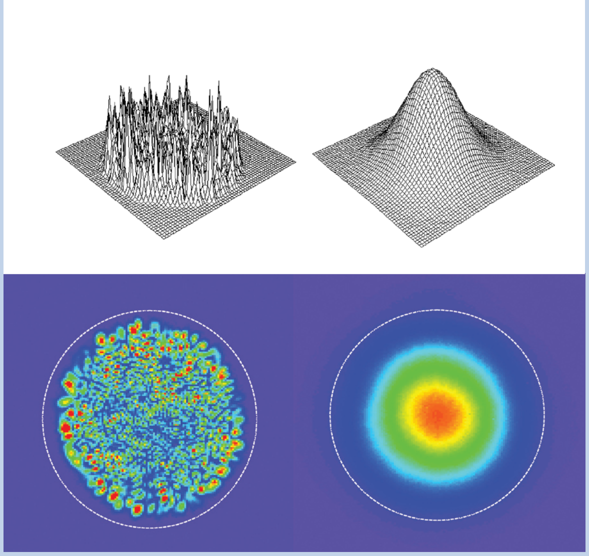
All these activities had to incorporate the consequences of the fact that the sensor and associated hardware would be speeding through space on a satellite platform, where it would contribute to truly global monitoring and detection of transient optical and infrared events. This and other Sandia teams continue to strive for global coverage with detection that is increasingly more sensitive, higher in resolution, and more rapidly transmitted and analyzed.

Fiber Laser Grand Challenge

Dahv Kliner

Optical-fiber lasers have many desirable properties, but the inability to boost their power output has limited their use in industrial and military applications. This project has overcome those limitations. A fiber laser is similar to the optical fibers commonly used to transmit information, the difference being that those optical fibers are passive carriers of light-encoded information. By contrast, by doping the optical fiber's core with particular metal ions, that core can be induced to "lase," that is to coherently emit light following electronic excitation of the ions.

In conventional crystal lasers, the more atoms that can be excited and induced to emit light, the greater the power of the laser. But conventional lasers are inefficient, bulky, unreliable, and typically require elaborate cooling systems, because they convert only a small fraction (generally less than 5%) of their electrical input energy to light energy. Nonetheless, they are capable of peak power outputs in the megawatt (millions of watts) range. By contrast, fiber lasers can exhibit efficiencies of 40%, dissipating much less heat, and so, can be air cooled. In addition, they can be far more compact, and portable. But their power has typically been limited by the fact that to maintain beam quality, their metal-doped core must be kept relatively small, with not enough ions to generate high power.



Measured images of the output beam profile of a high-power fiber amplifier before (left) and after (right) coiling.

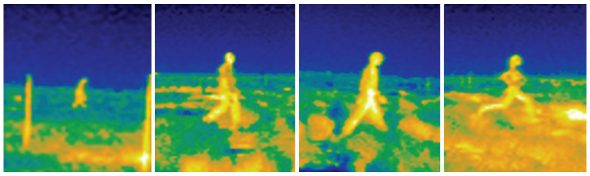
The conventional approach has been to increase the fiber's core diameter, thus diminishing beam quality. But this project, an R & D 100 Award winner, has discovered that bending the fiber — strategically coiling it around a spool — eliminates this degradation in quality, essentially filtering out unwanted output light ("modes" of the fiber). Power is increased by a hundred fold, into the megawatt peak-power range, without loss of beam quality. The result is a higher-power fiber laser that retains all other advantageous properties. With immediate applications in chemical and biological sensing, future applications will be found in materials processing, medical instrumentation markets, and in secure communications and target tracking to name just a few.

Using Infrared Video to Detect Humans and Improve Nuisance Alarm Rejection

Mark W. Koch

Border security is an issue that mandates development and deployment of appropriate and best-possible technologies for detection of human intrusion. This project aims to develop an unattended intelligent infrared detector that can distinguish humans from wildlife and other nonhuman moving objects such as vehicles, by combining results from multiple image frames.

Considering the vast range of human motion behavior and its similarity with that of other animals, as well as the range of scales at which objects would be registered by this system, the system employs algorithms to assist in determining "human-ness." In addition to obvious and objective measures such as velocity, the system attempts to, for example, classify movement behavior as human or nonhuman.



Infrared images of humans in motion.

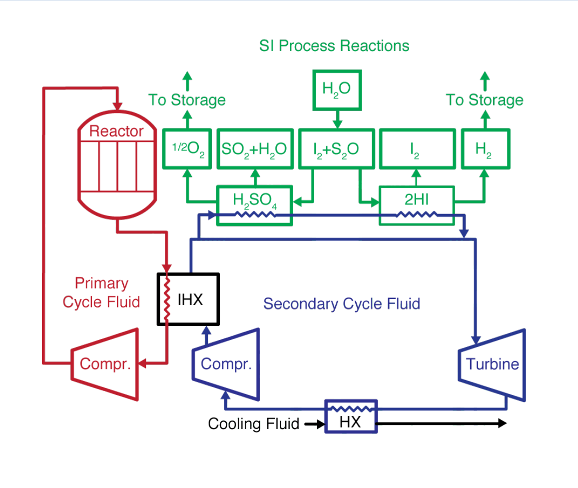
Future improvements will entail categorizing response to a stimulus in terms of its probable intent and therefore its human-ness, and integrating the results of this sensor's analysis with that of other sensors. In any case, the goal of reducing nuisance alarms should become increasingly attainable as these refinements are incorporated.

Development of Design and Simulation Models for Large-scale Hydrogen Production Plants Using Nuclear Power

Sal B. Rodriguez

Nuclear power, an important aspect of the US energy-independence equation, offers a partial solution to stationary electricity generation, but not, directly, to transportation energy requirements. Can nuclear power be adapted to drive the production of a transportation-relevant fuel such as hydrogen in an economically feasible fashion? This is the question critically evaluated by this project.

Two complex thermodynamic systems — one chemical-energy and one nuclear-energy driven — must be assessed both individually and in terms of their interaction, in order to guide experimenters into the most time- and materials-economical paths. The sulfur-iodine process for hydrogen production is thermodynamically "uphill," requiring an external energy source to drive it. Clearly the specter of global climate change and diminishing fossil fuel resources, imported from volatile global regions, dictate that combustion of fossil fuels to drive the sulfur-iodine process is untenable. But if energy liberated in nuclear power plants can be efficiently coupled to the process, hydrogen production may well become economically feasible. This team and its collaborators have thus far successfully modeled the process and are poised to optimize reactor designs and processes



Schematic of the linked processes for nuclear-energy-driven hydrogen production.

that couple reactor neutronics to hydrogen production. MELCOR-H2, the derivative software tool, estimates that each gas-cooled-reactor-based nuclear power plant can produce about 420,000,000 kilograms of hydrogen (H_2) per year at a cost of $1.38 per kilogram, while simultaneously generating close to 600 Megawatts of electricity. This could place hydrogen into viable economic status as a transportation fuel.

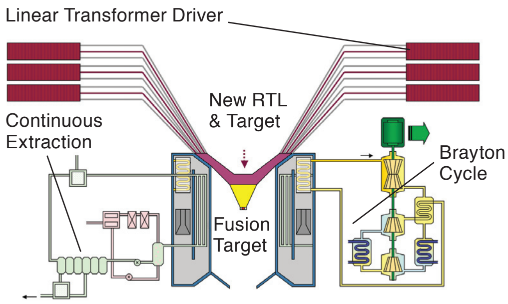
National Security Applications

Advanced Fusion Concepts: Neutrons for Testing and Energy

Daniel B. Sinars

Energy analysts generally agree that, at least in the short term, nuclear energy must be one aspect of the solution to energy independence that phases out fossil-fuel combustion. But the biggest issue with nuclear-fueled electricity generation in light-water reactors is the long-half-life of the so-called "spent fuel" byproducts, which must be stored in a repository such as Yucca Mountain. In addition to plutonium, much of this residue is comprised of the minor actinides, neptunium, americium, and curium. "Burning" these to produce energy and shorter half-life byproducts — sometimes referred to as "closing the nuclear fuel cycle" — could increase the functional capacity of Yucca Mountain by 50% to 100%.

This project is developing a spent-fuel burner, the In-Zinerator, which provides an alternative to the fast reactor, the currently favored option. The In-Zinerator can burn both TRU (plutonium



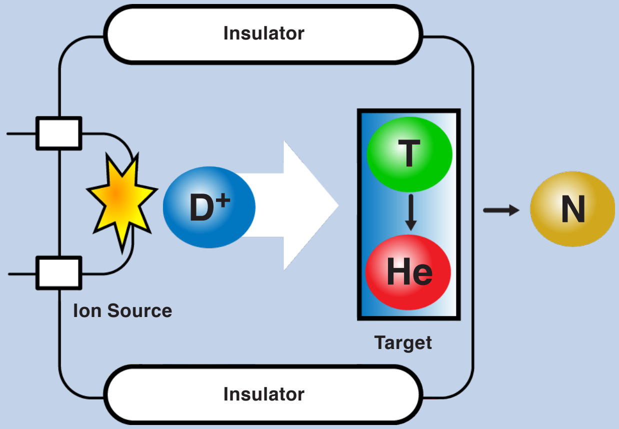
Components of the In-Zinerator power plant.

and enriched uranium) or minor actinide byproducts of light-water reactor operation. It uses a liquid fuel and a molten salt mixture to remove fission products; tritium is also extracted. The economics of this option are comparable to the use of fast reactors. Many experts believe that realization of this capability is essential to the ongoing viability and increased use of nuclear energy–driven electricity production in forthcoming decades.

In Situ Optical Diagnostics of Neutron Generator Target Films

Clark S. Snow

Neutron generators are important in many civilian, military, and homeland security applications. In addition to protection against proliferation through detection of nuclear materials and explosives, petroleum exploration and cement process control also exemplify the range of non-research applications. While other neutron sources are either prohibitively large, expensive, or problematic in other ways, Sandia-developed sealed neutron tubes offer a compact, inexpensive neutron source. This project's focus is the clarification of the thermodynamic and kinetic assumptions used in production of the tritium-containing targets within the tubes, with an eye toward improving the metal hydride films upon which the tritium is loaded.



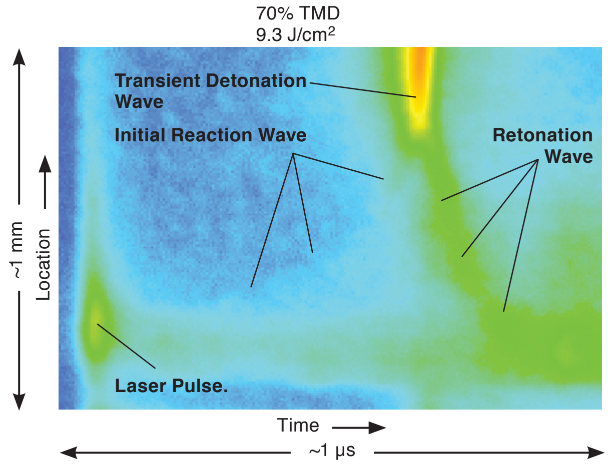
Schematic representation of neutron generator components.

Using both the Sandia-developed Multi-beam Optical Stress Sensor (MOSS) technique and computational modeling for these metal films, the project team examined the relationship between optical properties of the films and their stoichiometry (the ratio of the various elements in a chemical compound, in this case, metal and hydrogen). It was able to use optical methods to monitor the hydriding process to determine the crystallographic and stoichiometric properties of the films, as they formed. With ongoing research, this project hopes to answer critical questions that can improve the production and operation of these important diagnostic and research instruments.

Micro- and Meso-Scale Detonics of Explosives

Alex Tappan

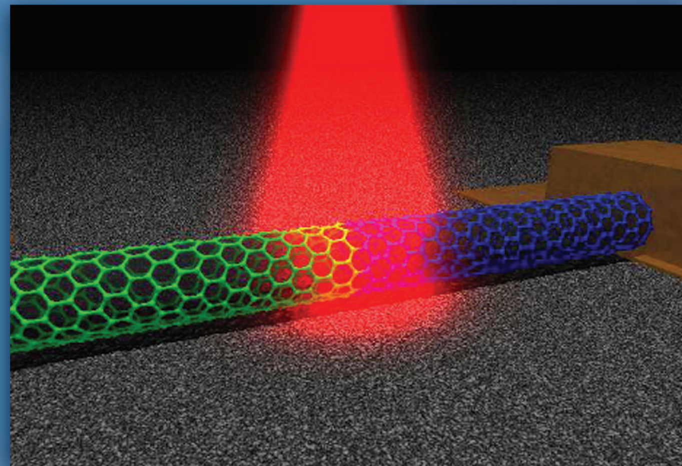
Detonator safety is of critical importance in civilian (mining, demolition), military, and research applications. There are still several incompletely described processes in explosive behavior both during initiation or triggering and during spread of energy through an explosive, particularly within an irregularly confined space. This project is studying these issues within the context of detonator miniaturization, working from the assumption that understanding the unknowns in explosive behavior requires description at both the micro- and meso-scales.



Caption: Streak camera image of initiation phenomena in laser exploding bridge wire detonation

Using both traditional experimental methods (such as gas gun shock initiation) and computational modeling, the project has unearthed several factors potentially relevant to failure, with a possible role for serendipitously discovered nanoparticles. The team has begun developing and implementing processes, including laser micromachining, and diagnostics, such as streak-camera and shadow graph imaging, for miniaturization.

Advantages of miniaturizing detonators include safety, with quantitatively less explosive, and better functionality / more reliability through the higher precision that is necessary in miniaturized systems.



Artist's rendition of current flow being switched on by light in a single carbon nanotube.

Tammy Kolda elaborates on the concept of mathematical tensors.

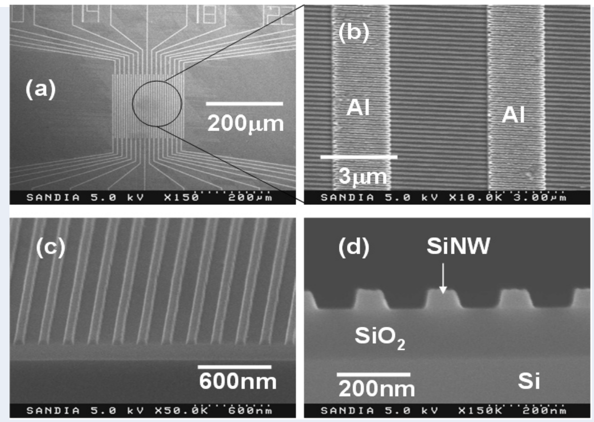
Francois Léonard, above, accepts his Award for Excellence from CTO, Rick Stulen. Below, Mark Derzon accepts Paul Galambos' award.

Mark Boslough fascinates a listener with his models of low-altitude airbursts.

Controlled Fabrication of Nanowire Sensors

Francois Léonard

Devising a novel fabrication technique for silicon nanowires — microscopic components of semiconductors and miniaturized sensors — this project not only went on to demonstrate their usefulness, but additionally, was able to develop a new method for using light to control the electrical properties of nanowires. Computational approaches — simulations of nanowire performance — underpinned and paralleled the experiments.



Micrographs of silicon nanowire arrays.

Accurate component miniaturization, device performance, and lower production costs are key parameters for both commercial communication industry ventures and national defense concerns. Traditional fabrication of semiconducting nanowires is ridden with defects, so this Sandia project team took the novel approach of starting with a precise silicon template — analogous to an ink-pad stamp — with which it impressed a pattern of minute parallel lines onto a wafer, then chemically etched the pattern into its surface. Electron microscopy showed a resulting precise pattern of quite uniform, evenly spaced nanowires. The advantages include a high density of wire fabrication over a large area, with a high degree of individual wire uniformity. Characterizing the electrical responses of these elements indicated quite acceptable voltage-current relationships, suitably similar to other types of semiconductor devices.

Moreover, in a highly touted set of experiments featured in *Nature Nanotechnology*, this team was able to march an important step forward in the development of so-called "field-effect transistors," miniaturized devices whose wide-scale use in transmitting wireless signals makes them a cornerstone of modern civilian and military communication.

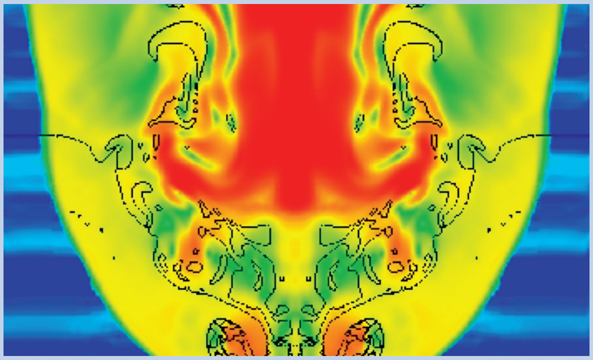
To demonstrate functionality as transistors, the nanowire arrays were employed as sensors asked to discriminate between different concentrations of two similar chemicals, nitrobenzene and phenol dissolved in the same liquid, cyclohexane. The sensitive performance indicated that the fabrication technique might hopefully offer a simpler, more-precise methodology for the fabrication of chemical and biological sensors.

In another set of studies with nanowires, this team utilized familiar carbon nanotubes, and reversed the sequence: current flows, light switches on; to the converse: light switches on, current flows. They were able to coat the nanotubes with the common dye (or "chromophore"), Disperse Red 1. This dye has the chemical property of changing molecular shape when exposed to blue light. The shift in molecular shape of the dye acts as a switch and greatly increases the electrical conductance or current-carrying capacity of the nanotubes, simplistically switching current flow on. The switching is reversible: when the dye has one molecular shape, current flow switches off, and in the alternative shape, it switches back on. Traditionally it has required laser light to control current flow in carbon nanotubes; this breakthrough has now demonstrated that light of much lower intensity can be used for this purpose. ■

Low-Altitude Airbursts and The Impact Threat

Mark Boslough

Siberia, 1908: the impact of an asteroid or comet razes a thousand square miles of Siberian forest. Libya,1932: British explorers discover a mysterious yellow-green glass scattered across the surface of the desert strangely resembling those generated by asteroid impacts.



Simulation of the vortices present in an airburst event.

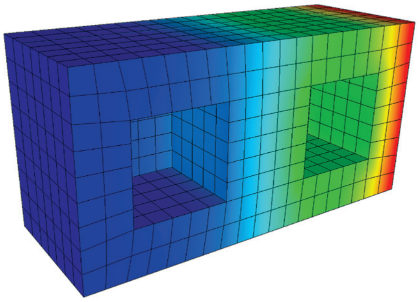
Intriguing, certainly, but more pertinent, what is the physics of and the potential future threat from these interactions between near-earth objects (NEOs) and our planet? In 2005, Congress mandated that NASA discover and catalogue 90% of NEOs larger than 140 meters in diameter by 2020. The remaining threat to earth will be dominated by objects that explode in the atmosphere as so-called "low-altitude airbursts." For several years, using nuclear weapons codes, this project has been modeling the physics on Sandia's Red Storm supercomputer in order to thoroughly characterize this hazard.

Simulations indicate that, in general, such atmospheric explosions can result in fireballs hot enough to melt quartz on the ground, creating the types of glasses found in the Libyan desert. The models suggest that surface damage from these events is much greater than for nuclear explosions of the same yield because the NEO-impact fireball is ballistic, moving downward in complex vortices toward the earth's surface. Hence, for example, an earlier consensus was that the 1908 forest ablation would have required an atmospheric event on the order of 10 to 20 megatons, whereas this model predicts that only a 3- to 5-megaton explosion would have been adequate to produce the observed damage. These conclusions have already been incorporated into the NASA white paper. Naturally, one goal would ultimately be to extend this research to discover potential mitigations for such events. An ancillary outcome has been a better understanding of the weapons codes.

Computation and Simulation

Multi-Physics Coupling for Robust Simulation

Russell Hooper



Three-dimensional representation of a thermal gradient.

The software package developed by this project is especially well-suited to simulations that use two separate simulation codes, able to couple these codes in a variety of ways that will provide a best solution. The underlying rationale for this work is the observation that many current and future modeling scenarios will depend on the simultaneous solution of very different physical phenomena, and that in trying to couple the codes that model these phenomena, there are fundamental issues that have not been addressed. For example, in modeling next-generation nuclear reactors as part of the Global Nuclear Energy Partnership (GNEP), modelers must deal with several physics issues. Nuclear fuel consumption at reactor cores couples to thermodynamic processes describing the efficiency of how energy released in nuclear processes is transferred to non-nuclear physical phenomena such as the heating of water and other fluids that will then transfer this energy to turbines for electricity generation. These are vastly different but coupled physics problems involving very disparate time and length scales that often must be accurately resolved together.

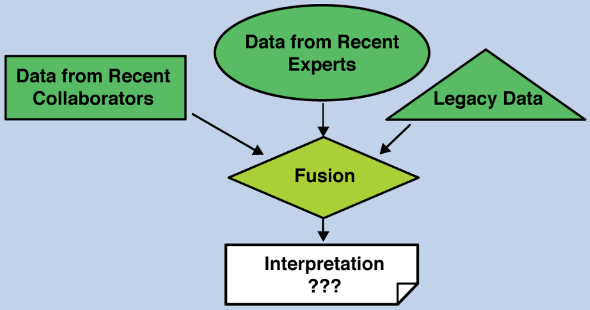
The project has thus far provided coupling algorithms in several key impact areas of Sandia research, for example, weapons engineering and stockpile stewardship. It has demonstrated improvements both in robustness of solutions and in reduced simulation times, important considerations as computing demands continue to grow.

Computation and Simulation

Data Pipelining for Heterogeneous Data Fusion

Genetha Gray

Like different camera angles of the same scene, essentially the same or similar information sets can appear to be totally disparate without some indication of the relationship among them. In an age of information overload, this is a growing problem in science. Similar to the brain's ability, given cues, to reconstruct a three-dimensional image from different-angle photos, this project has developed algorithms for fusing different data sets, both current and legacy, into a more unified representation.



Schematic representation of some elements in data fusion.

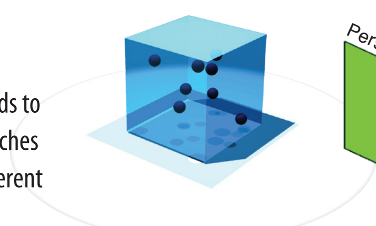
Exemplifying the approach is data on the phosphorylation of proteins, an elegant biological control mechanism of primary significance. Proteins are complex structures and determining the exact site of this chemical alteration is often difficult and fraught with ambiguity. Several software routines that predict likely phosphorylation sites exist, and they yield sometimes conflicting results. This project team was able to intelligently combine results from these packages such that an overall reduction of errors occurred when compared against actual experimental data.

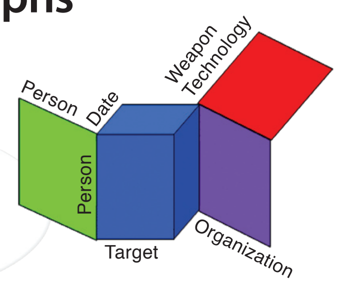
In addition to experimental science, this technique has obvious applications in clinical medicine, where data from different tests can sometimes obfuscate rather than clarify a physician's diagnosis of a patient's state of health. And in nuclear weapons stockpile stewardship, in light of the moratorium on testing, data from smaller-scale materials experiments and simulations must be intelligently combined with legacy test data collected before 1992.

Computation and Simulation

Data Mining on Attributed Relationship Graphs

Tamara G. Kolda





Left: Illustration of a (sparse) third-order tensor. Right: Schematic representation of multi-way links among heterogeneous data.

Most of us are familiar with search engines that use key words to extract links to sometimes thousands of websites. Such searches underline a key problem in informatics, that is, how can different sources and types of information be combined so that their relationship to one another is sensible and useful. This project explores that information space by refining and expanding a technique previously used in psychometrics and other fields. Attributed relationship graphs provide a methodology for combining disparate pieces and sources of information — telephone, email, newspapers, etc. Intelligence analysts use such graphs as a way to integrate data from somewhat incongruent sources.

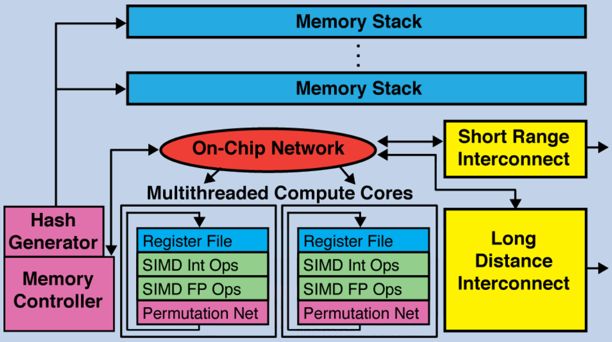
Representing these information sources as a matrix provides a convenient and efficient way of grouping and showing the interrelationships that characterize them. For example, such matrices of interrelationship characterize the way web search engines evaluate the links among web pages. But matrices are most commonly two-dimensional. This project makes use of mathematical tensors, which provide a multidimensional (three or more) representation of such interrelationships among groups of information such that they can be analyzed, for example in terms of their importance or rank. The technique is globally applicable. With obvious applications for enriching the relationships on the internet and increasing its value to both search engines and users, tensor analysis of information is poised to become a valuable tool in the area of threat detection. This application derives from its ability to decompose and characterize relationships among different types of message traffic over networks, even to the point of making predictions about the meaning of these communication patterns.

Building More-Powerful, Less-Expensive Supercomputers Using Processing-in-Memory

Richard Murphy

Universally sought, faster computing is more important to scientists addressing complex problems on supercomputers than to the average PC user. In assessing the possible limiting factors to increasing supercomputing processing speed, this team considered issues such as number of processing units and branch prediction. Clearly, improving running software's ability to correctly predict which of its processing branches would apply to a particular operation would speed up its execution. However, the team found that even perfect branch prediction would not improve performance as much as increased speed of memory access, a machine's fetching stored data essential to an operation.

Given this understanding, that memory latency is the most limiting aspect of performance, this project aims to develop



Schematic of X-Caliber Architecture.

a novel hardware architecture that decreases this latency. In X-Caliber Architecture, memory units are physically located on a processing chip, connected directly, silicon-to-silicon, to decrease memory latency. In light of the growing number of pressing national issues — for example, climate modeling and stockpile stewardship — that will require supercomputing, success of such an improved architecture would be of great value in a next generation of supercomputers. In the interim, the architecture has shown significant promise in solving large graph-based informatics problems in the intelligence arena.

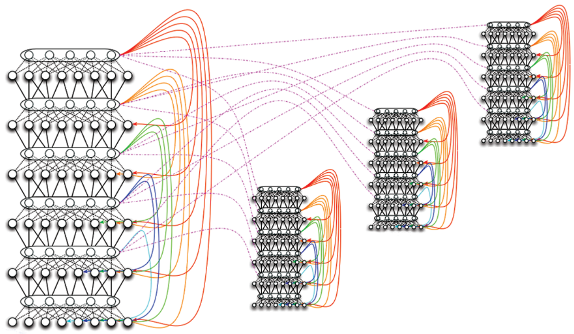
Computation and Simulation

Adaptive Peircian-Based Decision Aid

Michael Senglaub

Information overabundance is a common aspect of Twenty-first Century life. Such "cognitive overload" is especially problematic for critical decision makers in our civilian and military leadership. Computational models of decision making have, thus far, suffered from a variety of flaws that must be rectified before intelligent machine reasoning can become of more value. This project has designed a computational decision-making algorithm that both attempts to reduce cognitive load and incorporates several aspects of human reasoning into decision making.

Human decision making encompasses the convolution of current information with stored knowledge in order to generate understanding against the backdrop of what we commonly think of as a belief system. Encompassed in these belief systems are aspects of risk aversion that clearly impact the ultimate decision about action. In addition to this aspect of human cognition, machine decision making must also duplicate or mimic the



Schematic model of the types of interconnectivity among nerve cells and modules of the human neocortex.

different routes which human reasoning can sample to solve a problem.

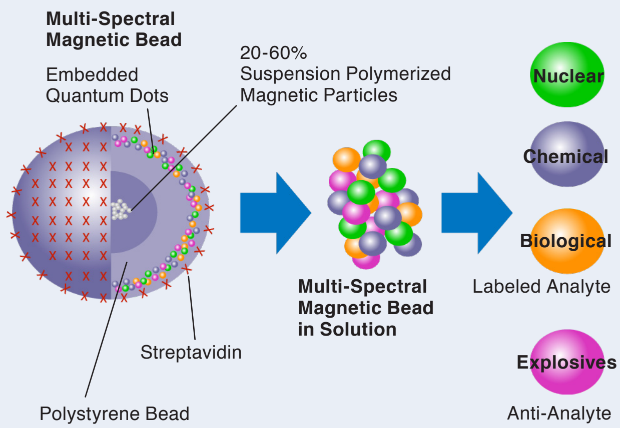
Using Peirce's model for reasoning, this project also makes use of the neuronal (nerve-cell) connectivity model of the neocortex (highest, most-evolved human brain structures). Ultimately, the operational model becomes a decision aid that includes the key human components of belief and reasoning. It is scalable, that is, can be run on a mainframe for predictive analysis and even scaled down to a personal digital assistant (PDA) for simpler applications. In addition to its implications for decision-makers and analysts, the conceptual design has implications for the design of sensors and information architectures.

Bead-based Multiplexed, Orthogonal Biowarfare/Infectious Disease Detection Microsystem and Technologies

Paul Galambos

Threat detection, in this age of covert enemies, has become a primary necessity in ensuring homeland security. Yet possible threats to the health of civilian and military populations are seemingly too numerous to count: radiation; viruses, bacteria, and their toxins, and numerous toxic chemicals.

Conventional wisdom suggests a different approach to detecting each of these noxious categories: radiological, biological and chemical. Undaunted by that limiting opinion, this project seeks to field a detector that can register and sort-out instances of all three threat types, while retaining exacting specificity and small size.



Drawing of the components of a polystyrene bead; in this case, the surface binding molecule, streptavidin, is specific for binding chemically modified DNA

A key component is a bar-coding system that maintains order amid a chaotic inventory of potential toxin sources. The bar-coding system consists of quantum dots embedded in polystyrene beads. Each type of dot can be stimulated to emit a unique signature of light. By using dots to create bar-coded beads, one can also make each bead barcode specific to the detection of a single agent.

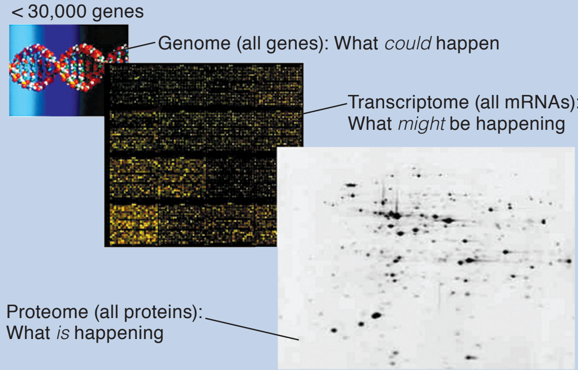
For example, biological antibodies can be used as detection agents. Antibodies have exquisite specificity for identifying chemicals and microorganisms. If, for example, all beads bar-coded to emit light from quantum dot "A" (emitting, for example, orange) were also tagged with an antibody specific for binding botulinum toxin, then any botulinum toxin present in the environment would stick to the beads bar-coded to emit orange. In turn, beads labeled with quantum dot "B" (emitting purple light) could contain an antibody or other molecule that binds and detects the chemical toxin, serin. Since A beads emit light of a different color than B beads, they can be optically separated. Since the polystyrene beads are also rendered magnetic, magnets can be used to concentrate them and guide them into particular flow patterns within an also-developed microfluidics system. The beads thus serve as carriers to chaperone their bound substances to analytical assay stations.

At these assay stations, there would also be methods to more-sensitively quantify the amount of material (for example, botulinum toxin) adhering to each set of beads. For example, standard immunological "sandwich" methods can be used, by which a target substance like botulinum toxin is sandwiched between two antibodies, one of them optically labeled with a fluorescent dye. Each threat or toxic agent would be precisely quantified by a particular, already existing (in most cases) chemical or optical method affixed to the surface of a bar-coded bead.

Detection has been demonstrated for the radiological emitter, europium, using a straightforward chemical assay. In principle, there is no limit to the number of agents that can be detected and quantified, simultaneously. ■

Shotgun Protein Sequencing

Jean-Loup Faulon



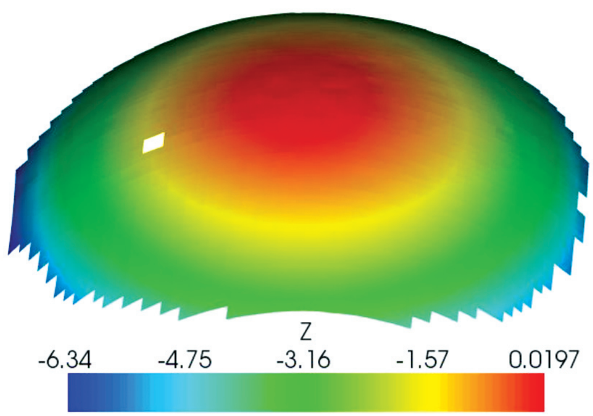
Combined drawing and data illustrating the disparity between number of genes and number of proteins.

For decades, the "prime directive" of molecular biology was "one gene (segment of DNA) equals one protein." Then came modern technology and more-detailed looks at the plethora of proteins produced by cells from far too few genes. Biologists realized that there were multiple ways that a gene could encode the information for several proteins. The problem of determining the structure of those proteins became of paramount importance, since knowing DNA sequences (genetic information) no longer ensured a knowledge of protein structure. And knowledge of protein structure is the key to understanding metabolism from the perspective of its key molecular players, protein molecules.

This project, a combination of biochemistry and computational algorithms arrived at a method to quickly and efficiently establish the primary structure (or amino acid sequence) of proteins. Using seven different enzymes to digest (cut up) proteins, the team then employs standard methods to separate and analyze the fragments. Using a sampling algorithm, it ultimately finds overlaps among the different generated fragments, enabling unambiguous identification of the different forms ("splice variants") of a protein that may derive from the same DNA information (gene). Such accurate protein-structure information is critical for several national security initiatives, including biofuels production and biodefense initiatives that depend on accurate understanding of the immune system and population susceptibility to biothreats at the molecular level.

Multiphase Dynamics of Soft Biological Tissue

Reese E. Jones



A displacement map of the cornea under fluid pressure.

Keratoplasty — reshaping of the eye's cornea to improve vision — has become a common aspect of everyday life. But despite a high success rate, the procedure is not always applicable and is sometimes unsuccessful. Understanding the structural dynamics of the cornea could favorably change those statistics. And for individuals who develop corneal injury, corneal transplantation is sometimes their only option.

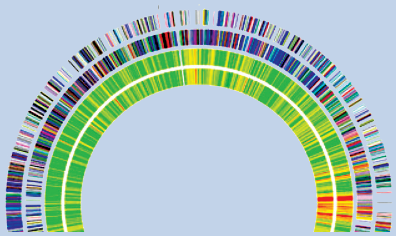
In this project, a Sandia team is modeling soft, visco-elastic biological tissues such as the cornea to provide a detailed understanding of the mechanics of such tissues under deformation. A closely integrated experimental and computational program unique to Sandia forms the foundation of this work. Using animal, experimenters subjected the tissue to both tension and inflation to measure characteristic parameters. In conjunction, the project team created a predictive model of the tissue's mechanical response. Together, experiments and model provided detailed understanding of how the tissue's structure affects its behavior.

Artificial materials resembling skin that might form a completely supple, conforming, and impact-resistant body armor; artificial biomimetic prosthetics for damaged corneas (or similarly constructed biological tissues): these are a few of the possible applications of this project. Similar to the case of hard tissues, such as bone, soft tissues offer insights into material composition-property relations that can, in turn, inspire new man-made materials with desired properties.

Synthetic Biology of Novel Thermophilic Bacteria for Enhanced Production of Ethanol from 5-Carbon Sugars

Rajat Sapra

Imagine the liquid biofuel, ethanol, derived from the leftover inedible chaff of crop harvesting rather than a from a specific food crop, like corn. Vehicular fuel from what is normally considered waste: this possible scenario springs from the work of a Sandia team's genetically engineering a thermophilic bacterium to become a biochemical factory for ethanol production.



Map of the sequenced DNA of *Geobacillus thermoglucosidasius*.

The current problem: The preferred agent of bioethanol production, yeast, is limited in the sugars it can use as feedstock for ethanol production and operates only at ambient temperatures around 30 °C. But the optimal temperature for the breakdown of plant fiber to its component sugars is significantly higher, around 60 °C. As a thermophilic ("heat-loving") bacterium, *Geobacillus thermoglucosidasius* is ideally suited to ferment most sugars to ethanol at this higher temperature, and in addition, can be genetically engineered to overproduce ethanol. Engineering bacteria is relatively simple and Geobacillus is innately tolerant to high ethanol concentrations that might intoxicate and disable other organisms. Considering that the project team has already achieved sequencing of Geobacillus DNA, it has progressed to a point where this organism is now much better understood metabolically. Therefore, paths to optimizing its functioning as an ethanol producer will be that much more transparent.

While liquid biofuel production is, in principle, a quite necessary part of the solution to US energy independence, the often-touted use of corn as a feedstock and yeast as the biological fermenter is actually not that highly favorable, economically. By contrast, this solution shifts the economic landscape in a quite favorable direction.

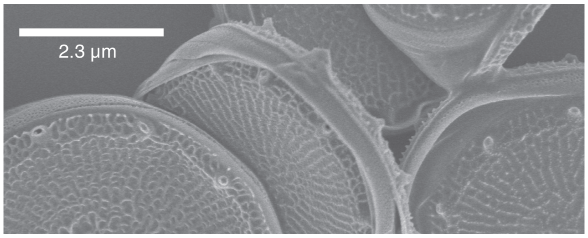
Understanding Biosilicification: Diatoms as Bioarchitects

Blake Simmons

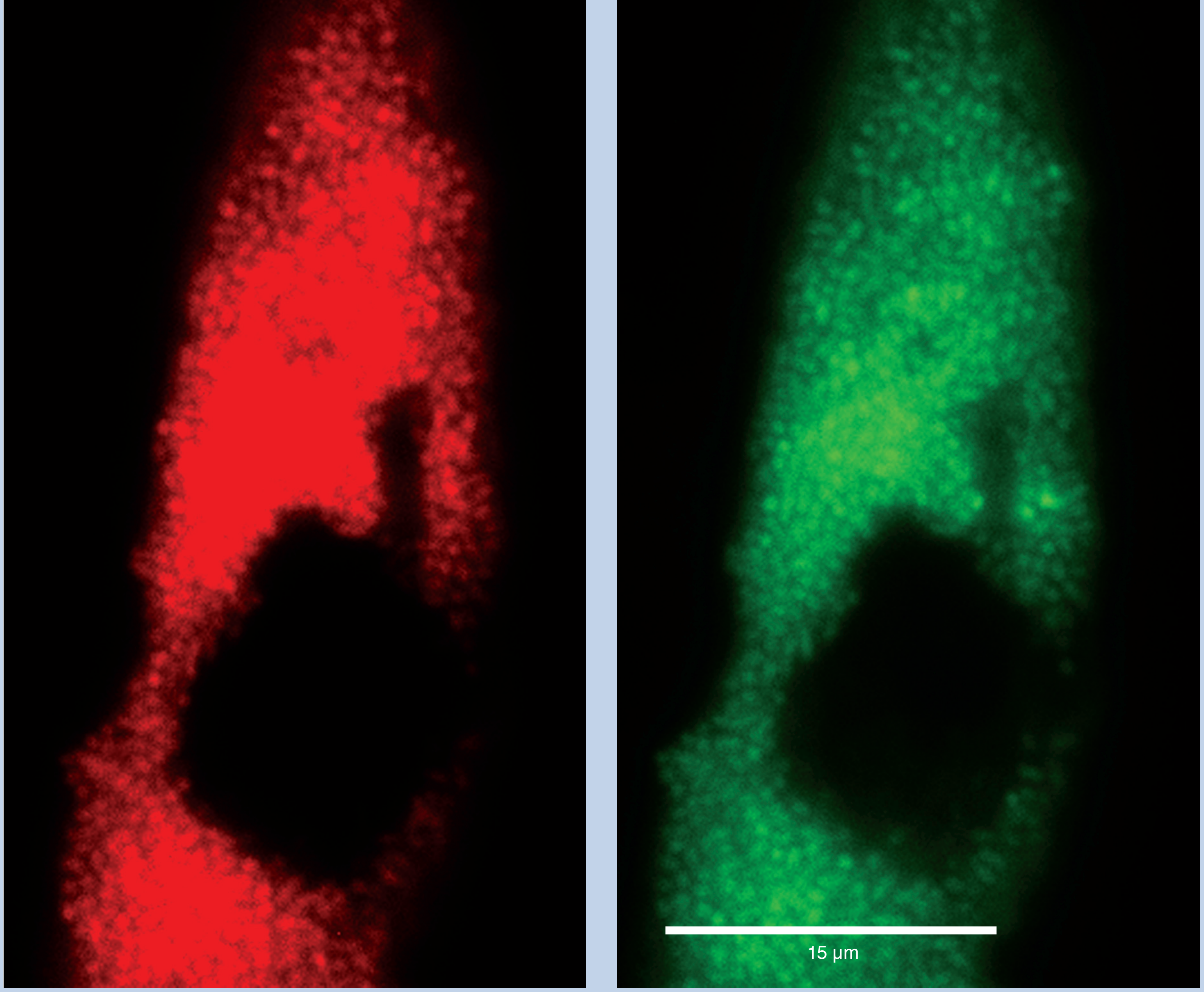
Diatoms are an important component of the microscopic photosynthetic organisms (phytoplankton) that serve as the base of aquatic food webs, and they possess unique properties. They build intricate, elaborately patterned outer shells of either silica or calcium carbonate (limestone). This project's attempt to understand the process of pattern formation in these organisms' shells has potential implications for the templated growth of nanostructures.

Recent work at Sandia has utilized organic substrates upon which to grow inorganic nanostructures, and that approach has, in fact, been the one of choice for diatom shells for millennia. For diatoms employ proteins and other organic molecules to template the deposition of silica during the genesis of their intricate shell patterns.

In addition to computational simulation, the project also made use of the knock-out mutation technique — by which selected genes are inactivated, thereby more-readily allowing assessment of their function within a metabolic process. As a result, the project has increased the detailed molecular understanding of these biochemical and nanostructural processes. Given that silicon-based nanowires are an important area of semiconductor research, this understanding has potential significance beyond its advance of knowledge in molecular biology.



Micrograph illustrating some of the intricate patterns found in the silica shells of diatoms.



Optical microscopy of macrophages (a type of "white blood cell") with differently colored fluorescent reporters potentially indicating internalization of different microorganisms.

Microscale Immune Studies Laboratory

Anup Singh

Understanding the immune system at the systems level is an enormous challenge: It is a "liquid brain" that processes information about invasion of the human body by organisms or toxins. And it employs a myriad of cells and informational-protein messengers ("cytokines"), in a network of interactions with a very large number of permutations. Clearly, given the numerous biothreats that we face, a detailed understanding of the intricacies of the immune response is key to the development of countermeasures, be they vaccines or other strategies.

A comprehensive systems approach that informs this project, which assembles a number of microchip-based microfluidics assays for both cells and the cytokines by which those cells communicate. One example is a microchip that assays phosphorylation (the addition of a phosphate group) to the protein cytokines; phosphorylation is one of the foremost molecular control mechanisms employed in biological systems. The project employs long-lived mouse immune cells, which are well-characterized and robust. Mouse and human immune systems are fundamentally similar, but the project will, ultimately, progress to research with the white blood cells of humans.

By integrating chips performing different assays onto a single microfluidics platform, the numerous interrelated cellular and molecular aspects of a given immune response can be tracked and assessed in tandem, with resolution at the single-cell level. And this capability, together with the development of novel analytical processes accelerates pathological assays, so that what might have previously required several days for conclusive results can now be accomplished in a matter of minutes. The addition of hyperspectral imaging with fluorescence-based assays and computational modeling to integrate results ensures that the project team offers a truly comprehensive systems-based picture of immune responses. The project therefore has the potential to revolutionize public health approaches through infectious disease analysis; to enhance biothreat awareness, detection and explicit characterization; and to improve civilian and military biosecurity.

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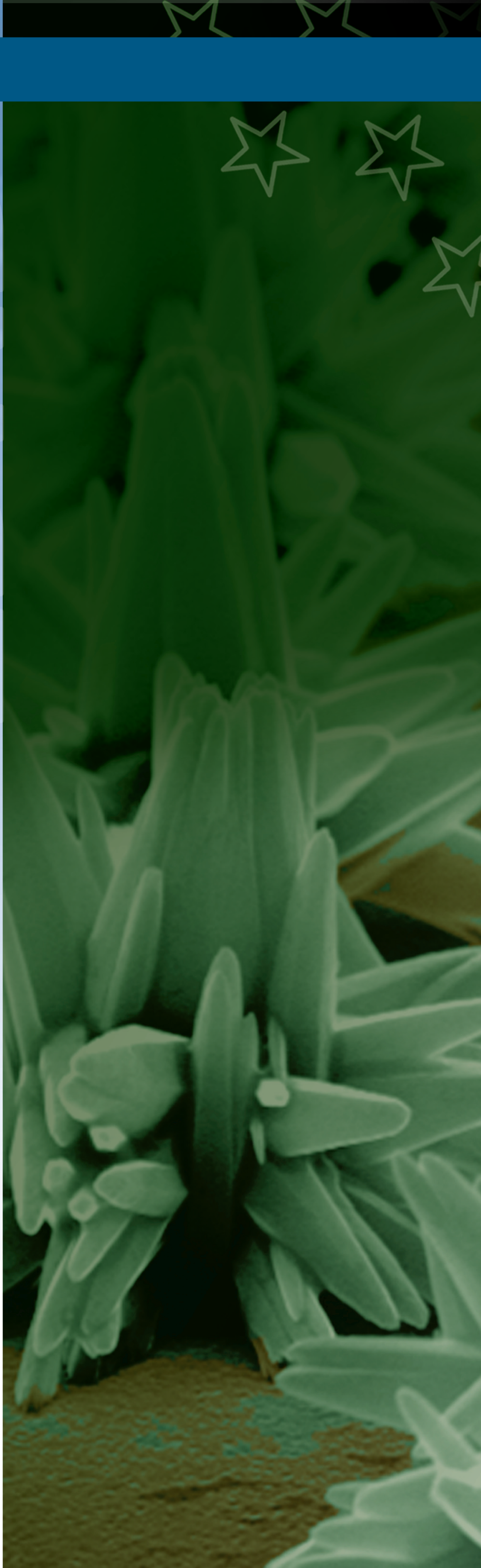
2007

Conference presenter
David Gill

Award for Excellence recipients with CTO Richard Stulen (center)

Poster session discussants



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.

SAND No. SAND2007-6769P