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 **ON THE COVER**

Sandia Labs nanosystems engineer Mike Lilly keeps an eye on two individually powered nanowires, embedded one above the other, in a few atomic layers of Sandia-grown crystal. The unique test device has yielded new information about electron flow in the nanoworld.

(Photo by Randy Montoya)



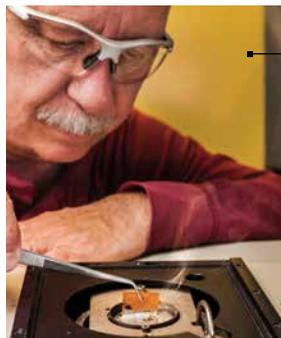
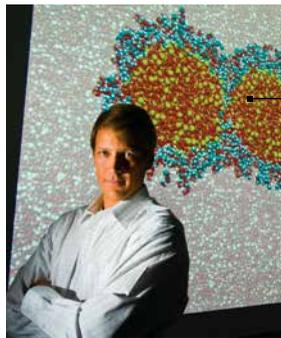
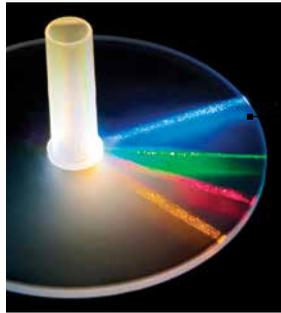


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MATERIALS

DEFINE THE TIMES

Materials – they are everywhere and make up everything. “That’s obvious!” you say? Well, yes, of course. But when you consider the breadth and depth of materials science knowledge that’s necessary for the performance of photovoltaic solar energy cells, the circuits in your electronic devices, a bridge, a pressure vessel or a weather satellite, it can be daunting. Some of today’s common engineering materials have been in use for thousands of years, some for decades — however, it’s amazing what we still can learn about them!

Sandia’s national security missions require fundamental materials understanding so that we may have confidence our products will perform safely, reliability and as intended in a variety of environments. A long, reliable lifetime in harsh environments (e.g., extreme temperatures, high radiation doses, severe shock or fire accidents, etc.), like those relevant to a nuclear weapon, a satellite or a nuclear power plant, places stringent requirements on our materials. Since the very beginning of the creation of a “fundamental physical sciences” program at Sandia in the late 1950s, materials (e.g., semiconductors, ferroelectrics) have been part of the Sandia research landscape. The breadth of materials that are critical to our missions spans semiconductors to stainless steels, carbon composites to ceramics, polymers to nanocrystals. When you add the variety of processes that impact material structure, properties and performance – the broad scope of materials science at Sandia becomes apparent.

In this fourth issue of *Sandia Research*, we’ve assembled a number of articles to give you a window into materials science research at Sandia, and a peek at some of the high-tech tools we develop and use. You’ll also meet several of our leading materials researchers. From predicting materials performance at the nano and mesoscale to understanding hydrogen embrittlement to developing next generation semiconductor materials, our materials scientists participate in and have impact across the research-to-development-to-application spectrum.

By integrating core scientific understanding into the design of high-consequence hardware, and looking to future capability made possible by new materials, materials science enables confidence that Sandia’s products will perform as required, when required. The Materials Science Research Foundation provides a key component of the technical basis for Sandia’s engineering decisions and mission success today and in the future.

Carol Adkins
Director
Materials Science Research Foundation



THE BREAKING POINT

By Sue Major Holmes

Metals have been used for thousands of years, but there's still a lot about them we don't understand. And an engineer can't just consult a chart that shows how much stretching, bending or compression a metal will take. That's determined by its mechanical properties, and those can vary widely, even within and between parts made of the same material.

Sandia Labs three years ago began an ambitious long-term, multidisciplinary project called Predicting Performance Margins, or PPM, to fill gaps in the fundamental understanding of materials science. From the atomic level to full scale, the research links variability in materials' atomic configurations and microstructures with how actual parts perform.

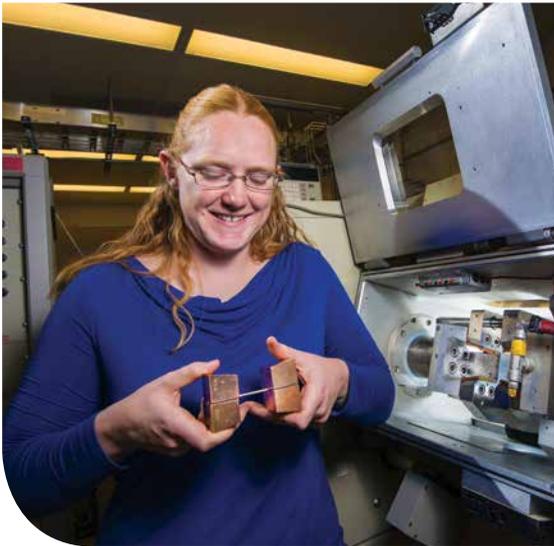
A material can take only so much stress.

Scientists want to predict how a machined part will behave, and ultimately perform, before it hits the assembly line.

“Too often, we are unable to predict precisely how a material will behave, and instead we must rely on expensive performance tests,” says program manager Amy Sun. “Capturing variability by tests alone is too expensive and not predictive.”

PPM is used to change that by identifying how material variability affects performance margins for an engineering component or machine part. The goal is a science-based foundation for materials design and analysis that enables us to predict how a material will behave in a specific application, particularly with regard to its requirements. Researchers use the information to design better high-reliability components and systems.

“Achieving this goal will require coordinated efforts of several Sandia communities,” says Terry Aselage, a senior manager in materials science research and development. “It’s a natural marriage between materials science and engineering science.”



crystal intersect and where the crystal level and the component level intersect — to predict collective behavior,” says lead investigator Brad Boyce, who works in metallurgy and materials joining.

Researchers examine how and why metals deform so they can predict that behavior and ultimately make them stronger. Better understanding could lead to improvements in how materials are processed as well as better materials. “It’s one thing to predict failure; it’s another to make metals better so they don’t fail,” Boyce says.

The impetus for PPM came from former Chief Technology Officer Steve Rottler, now vice president of Sandia’s California lab, and others who proposed a far-reaching investigation into a critical materials science question relevant to the laboratories.

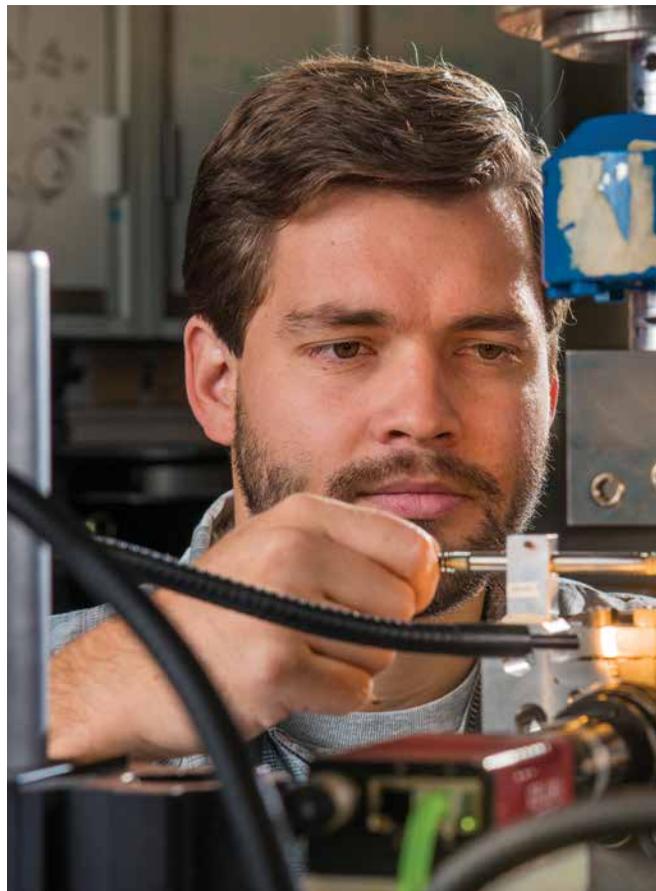
“The goal is to have enduring funding and focused expertise, and then ensure that it has impact on real

Lisa Deibler, left, gets ready to test a tubing specimen in a thermal-mechanical experiment system. She helped develop a simulation for an annealing process to soften tubing that was too hard to do a particular job. Below, Brad Salzbrener tests laser-welded objects in pure tension, shear and mixed tension-shear loading. The tests offer insight into weld performance.

Going to extremes

It may sound simple to imagine progressing from atoms to engineering-scale performance, but attacking such a multistate problem is a research challenge in itself. PPM approaches it by working from the outside in, tackling fundamental materials science issues at the atomistic and microstructural scale and challenging engineering problems at the macroscopic scale.

In the end, success requires connecting the two extremes. “The research focuses on where the scales connect — where the atomistic level and a single



problems in the nuclear weapons community and in other mission areas,” says Rick McCormick, a senior manager in radiation, nano and optical sciences.

Sandia’s core mission of nuclear weapons stewardship and national security requires it to meet the highest standards. “Few entities in the world are asked to guarantee lifetime performance of complex engineering systems,” Sun says. “We have to put a label on ‘best used by’ and determine the scientific data that back our claims. We have to support our results with sound, quantitative evidence.”

Materials science fundamentals aren’t important just to Sandia. Performance is crucial to safety and reliability in the wider world, in space, bridges, power grids, automobiles, nuclear power plants and other engineered systems.

The problem of laser welds

PPM brings together experimental and computational experts and tools to study the behavior of materials at different length scales. From the bottom up, it studies how atoms rearrange to cause defects in response to mechanical stresses and strains (nanoscale); how these crystalline defects evolve, multiply and interact (mesoscale); and how an ensemble of polycrystals works in concert to govern deformation and failure of

a component (macroscale). PPM looks at how manufacturing processes determine the microstructure of a material and examines macroscopic testing data and failure statistics to better understand the relationship between the microstructures and performance of engineering materials.

As an example, one pilot study at the top-down engineering scale involves laser welds used in a wide variety of Sandia components. Understanding the performance of laser welds is a long-standing problem, with issues in materials science, engineering and processes, Sun says.

Weld performance can be unpredictable because a weld’s microstructure isn’t homogenous, and geometric imperfections such as cracks and pores can be introduced by processing. The aim is to understand how the microscopic variability of a weld impacts the mechanical reliability of the welded component.

“We could say that if you weld it with this margin of overdesign, you’re probably OK, you’re probably safe,” Sun says. “But as a materials scientist, you’re not going to be happy with that answer.”

Instead, material scientists and systems designers want to predict the effects of porosity on weld properties such as strength, ductility and toughness. “How do these little microscopic pores or any kind of imperfections in your microstructure affect the actual material properties?” she asks. “How do we measure that? What is that fundamental mechanism for the pore to start to initiate a failure?”

Inter-atomic forces

The bottoms-up approach starts with a study of pure metals such as tantalum or iron. Knowing how atoms in crystals interact allows researchers to calculate inter-atomic forces. These forces are used to predict the ways that single crystals of the metal will respond to external stresses and the way engineering materials, aggregates of small single crystal grains, will perform. While it’s not possible to model every atom in engineering-scale codes, “if you understand the atomistic effects well, you can approximate it very accurately in the high-level codes,” McCormick says.

Boyce illustrates this approach with images of microstructure-scale strain fields in a tantalum tensile bar. The images compare experimental measurements





MEET

Jonathan Madison

of strain within individual grains as shown by scanning electron microscopy (SEM) to a digital image correlation model, to a two-dimensional slice of a three-dimensional simulation of strain inhomogeneity. The SEM imagery and the computer model look nearly identical.

"It's very encouraging," Boyce says. "These predictions, and their detailed validation by experiments, are truly at the forefront of the field."

Researchers also use such tools as transmission electron microscopy to view individual atoms as they bend and break tiny components or parts. "They can see what's happening to these grains and these boundaries, how the stresses build up. They can see it at a microscale, where they're looking at collections or aggregates of grains," McCormick says.

Then they scale up, running experiments on bigger components at Sandia's large engineering science test facilities.

PPM's approach draws on other successful Sandia collaborations, particularly QASPR, the Qualification Alternative to Sandia Pulsed Reactor, which began in 2005 as a multidisciplinary, science-based alternative to the decommissioned Sandia Pulsed Reactor. QASPR, which has expanded into new research areas over the years, uses technology development, experimental research and computational simulation to study and predict radiation effects in electronics.

The next generation

The PPM effort launched in 2010 has seen success. On the engineering side, nuclear weapons programs are using PPM to help component engineers understand



Madison spends much of his free time volunteering in professional and civic organizations. A favorite is his role as New Mexico area director for Alpha Phi Alpha Fraternity Inc., the first intercollegiate fraternity established for and by African-American men. It boasts such members such as W.E.B. DuBois, Paul Robeson, Thurgood Marshall and Martin Luther King Jr. Madison says he enjoys overseeing the Albuquerque chapters and helping members live out their fraternity's creed of "manly deeds, scholarship and love for all mankind."

STATS

- Bachelor of science in engineering science with a concentration in mechanical engineering, Clark Atlanta University, Atlanta, magna cum laude.
- Master of science in materials science and engineering, University of Michigan, Ann Arbor.
- Ph.D. in materials science and engineering, University of Michigan, Ann Arbor.
- Madison's graduate school thesis produced the first large-scale 3-D reconstructions of experimentally derived mid-solidification dendrites in a directionally cast nickel-based super-alloy. These datasets were used as direct inputs for 3-D models of fluid flow in dendritic structures, producing a better numeric predictor for casting defects. Madison says the work combined experiment and simulation in a unique way to better inform metals processing. It was memorable because it started as a failed solidification experiment from a broken mold.
- Madison's current research includes 3-D reconstructions and 3-D quantitative descriptions of microstructure as well as microstructural evolution models.
- He received a Sandia National Labs Early Career Laboratory Directed Research and Development award, 2010-2011.

ROBOTIC TOOL BUILDS SLICES OF DATA INTO 3D IMAGES

A robotic arm slices through a piece of metal, taking image after image, like a mechanical MRI.

It's called RoboMET.3D, and Sandia uses it to study materials. It does autonomous serial sectioning — removing small amounts of material by mechanical polishing, cleaning the samples ultrasonically, air-drying them and

ture instead of just the surface," Madison says.

Researchers can analyze how internal features are arranged, how they're positioned in comparison to one another and their shape. "Since the emergence of 3-D reconstructions, previous approximations in models have been improved by increasing the accuracy of what we think we know about microstructure," Madison says.



Jon Madison works Sandia's RoboMET.3D to better understand the behavior of materials.

imaging each slice by optical microscope. The system repeats the process over and over at a fixed rate, and researchers then assemble the images into a 3-D volume. The result provides information on structure, defects and imperfections not otherwise seen.

The system is one of Sandia's many specialized characterization tools being used for a project called Predicting Performance Margins (PPM), a far-reaching program to address gaps in the fundamental understanding of the impact of materials variability on performance. Researcher Jon Madison, who works on PPM, says it's important to study the quantity, size and variability of internal features to better understand a material's behavior. Variations in how materials perform are related not only to large-scale geometric factors but also to differences in their microstructure.

Many models represent pores induced by laser welding as circles or spheres. But Madison says this may not be a good approximation under certain conditions. "We've found in many cases, the curvature and morphology are not spherical at all," he says, pointing to pores in a 3-D reconstruction. The pores look lumpy, like eroded hills of different sizes. Three-dimensional reconstruction reveals not only surface features, but also those in the interior. "It brings to bear a 3-D understanding of the microstruc-

Without an automated system, serial sectioning must be done by hand. Madison says the painstaking and time-consuming process could, at best, result in up to 10 slices per day, with varying uniformity. The RoboMET.3D system, on the other hand, has demonstrated serial-sectioning rates anywhere from 1 to 50 microns per slice with high uniformity, while providing as many as 50 sections in a day.

It can take from a few minutes to more than half an hour per slice, depending on the material and the desired image resolution. Typically, the more pristine the surface finish, the more steps are required. The machine has a robotic arm that works in conjunction with pads containing diamond suspension to polish samples using abrasive action to remove small amounts of material at a time. The polish determines the quality of the image used to reconstruct the 3-D volume.

Sandia acquired its system at the end of 2011 and spent the next year installing and customizing it. Researchers began using it for material investigations in September 2012. "It's a research tool," Madison says. "It's not meant to replace human metallographers or be a rapid diagnostic tool. We don't use it for everything, but it's a great tool for specific tasks." ■

— Sue Major Holmes

how to better design and qualify structural components and modify material processes such as recrystallization to boost performance. In fundamental science, PPM can point to more than a dozen articles in scientific journals, symposia at international conferences and 100-plus presentations, including more than 20 keynote or invited addresses.

PPM has helped develop the next generation of materials scientists by creating an environment where young staff can grow and mid-career researchers can lead. Much of PPM's technical work is done by early-career staff members, guided by mentors and mid-career staff members responsible for various aspects of the project, Aselage says. "We are concerned about how early-career staff members develop expertise, skills and reputation as experts in their field," he says.

One early-career researcher, Jon Madison, says transferring knowledge to newer hires maintains Sandia's expertise. "Younger staff on high-impact projects can interact with some of Sandia's best minds. It's an opportunity for new staff to make their mark and bring capabilities Sandia might not have had before. For me it's been a really good opportunity not only by bringing capabilities and tools to bear but to have them recognized in a larger team effort that impacts how we address national concerns."

"This sort of enduring funding on a high-impact problem and the chance to work on state-of-the-art equipment brings the best and the brightest to Sandia," McCormick says.

It didn't take long to assemble a core PPM multidisciplinary team of about 20 staff and postdocs augmented by a large network of people doing interrelated projects, the "friends of PPM."

"Everyone wanted to work on this problem," Sun says. "It was so interesting and relevant to pretty much everything we do."

The project's funding comes from three sources in Sandia's nuclear weapons program: the Technology Readiness Program, part of Readiness in Technical Base and Facilities; Advanced Simulation and Computing through its Physics and Engineering Models program; and the Enhanced Surveillance Program.

Supporters expect funding will grow with the project's impact.

PPM draws on expertise across Sandia centers for materials science, engineering science and physical, chemical and nanoscience at campuses in New Mexico and California. It uses the laboratories' outstanding experimental and computational science abilities, including advanced characterization and testing such as 3-D microscopy, focused ion beam and digital image correlation, as well as quantum and atomistic simulations and models of mesoscale material mechanics.

The early success suggests PPM could become a prototype for tackling other difficult material issues at multiple length scales, such as the aging of polymers and foams, friction between electrical contacts and failures in glass-to-metal seals, and in solders and interconnects.

PPM itself will evolve. "As we solve some problems, we discover gaps and we move on to work on those gaps," Boyce says. ■



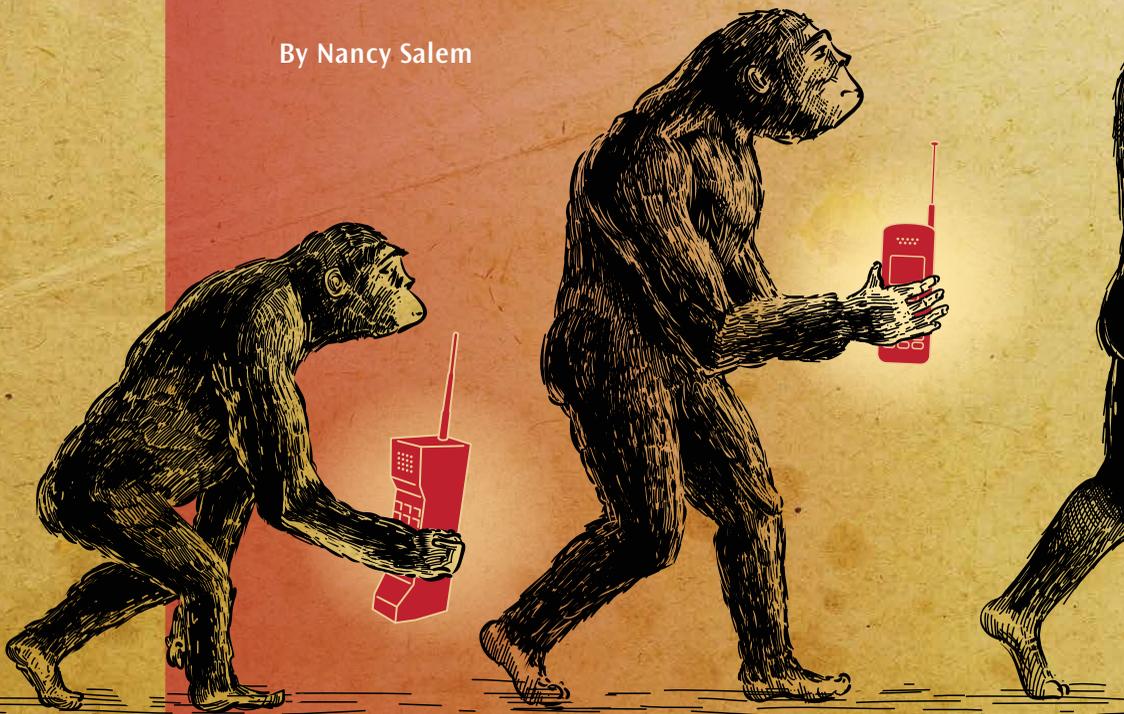
Cy Fujimoto demonstrates a flexible polymer membrane that could help make possible a hydrogen car.



POWER **to the PEOPLE**

Semiconductors have had a mindboggling impact on society. But your sleek cell phone and trusty GPS are only the beginning. Smaller, faster electronics are still to come.

By Nancy Salem



Semiconductors are sneaky. Little by little they permeate your life, unnoticed until you stop and think. Remember mammoth cell phones and boxy computers? Remember being lost? “Our lives become more convenient, flexible, dynamic and agile every day,” says Sandia Labs Fellow and materials scientist Jerry Simmons. “Semiconductors are the reason why.”

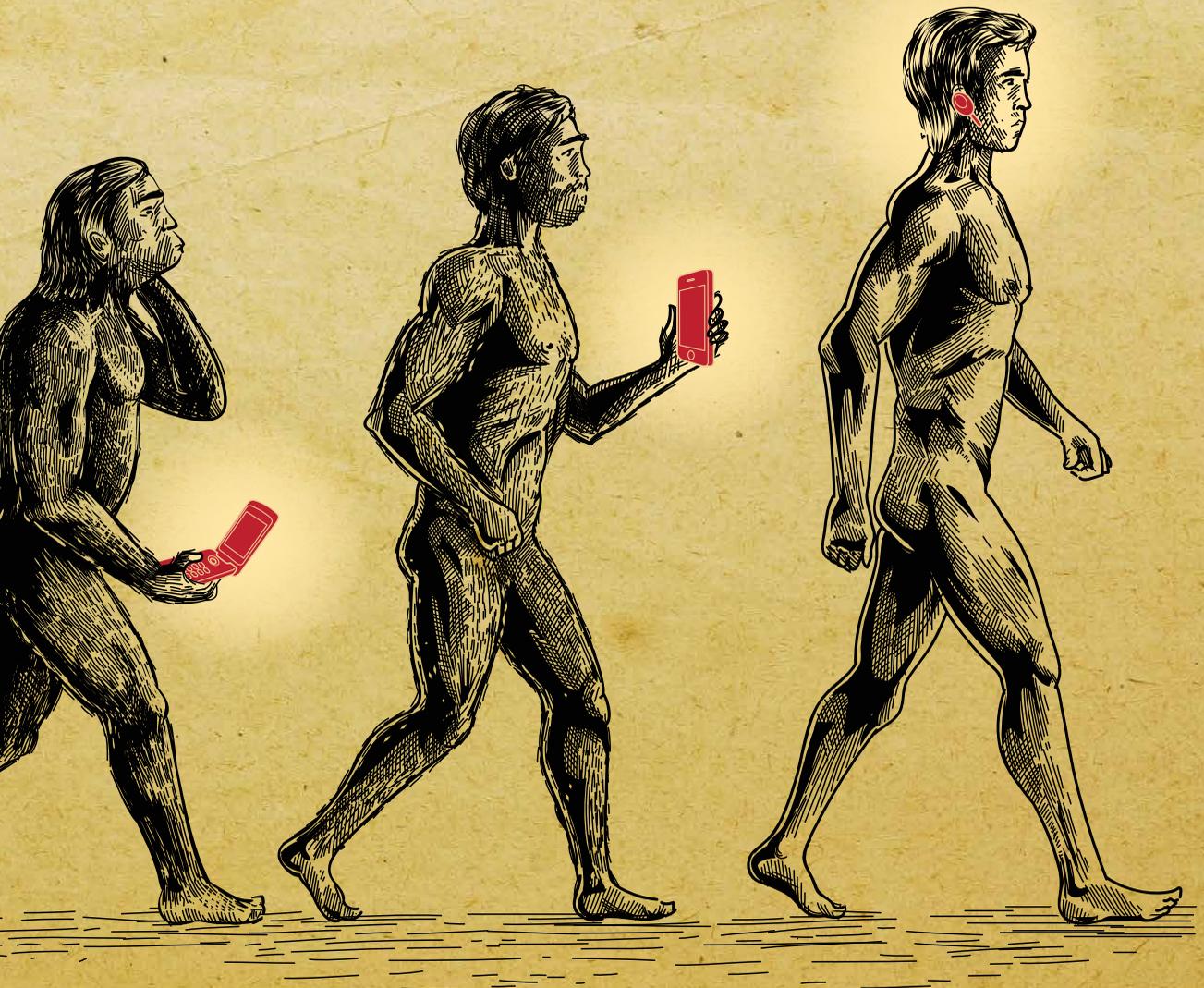
All modern electronics need semiconductors, which at the most elemental level simply switch electricity on and off. At opposite ends of the electrical spectrum are conducting materials, such as copper and aluminum, used in wires through which electricity is sent, and insulators that keep electricity from flowing out of the wires, causing shocks. “In between are semiconductors that can switch back and forth from conducting to insulating,” Simmons says. “When hooked together in complex ways, you get high-performance computing. But semiconduc-

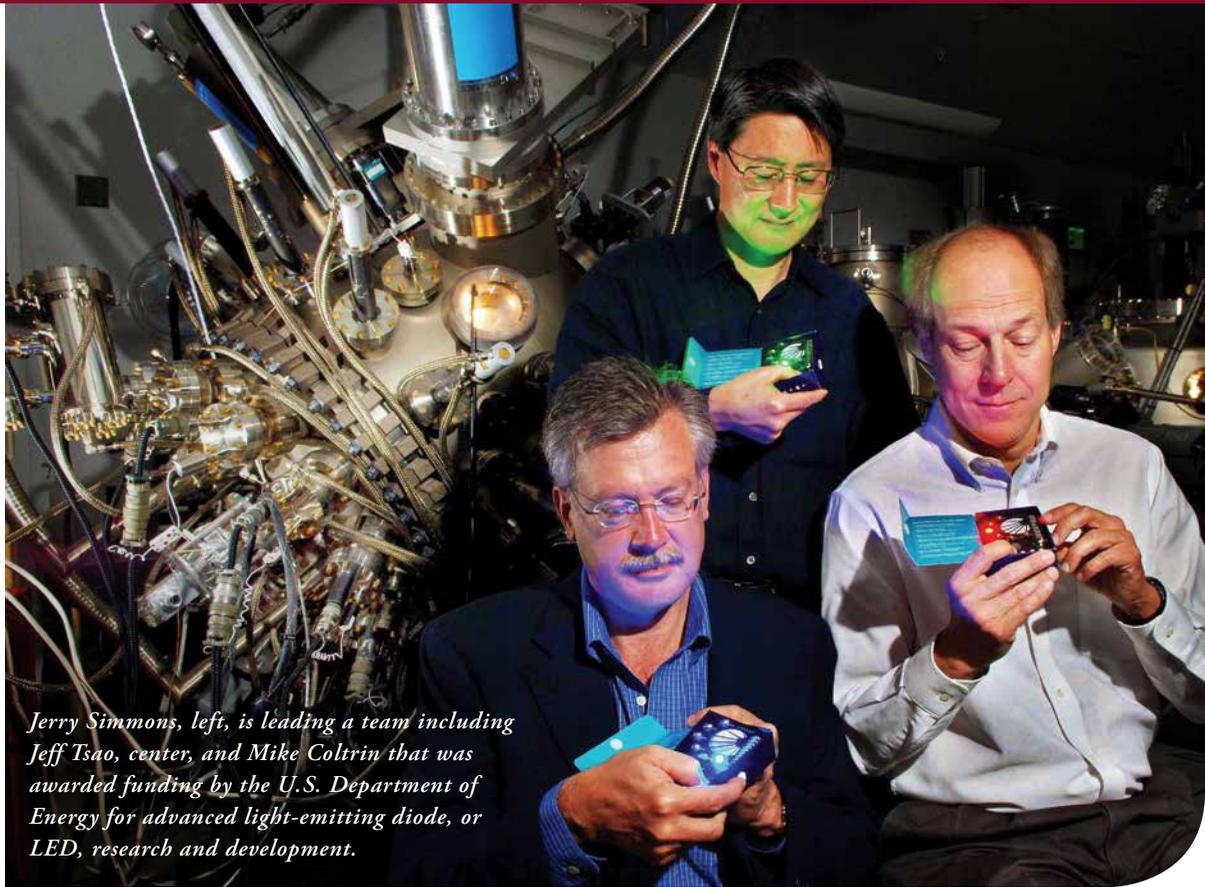
tors serve other functions like optical communications, imaging and switching electrical power — also known as power electronics. As the semiconductors get more efficient, so do entire systems.”

Silicon, as in Silicon Valley, has long been the go-to semiconductor material for computing and power electronics. But a new generation of materials is taking hold that could lead to smaller, lighter, more powerful and versatile devices. The rising stars are III-Vs, graphene, wide bandgaps and metamaterials, each of which will push electronics, and modern life, to new places.

III-V: See the light

Simmons says one area in which silicon falls short is the handling of optical processes. “There are a lot of applications where you want something to absorb a particle of light or emit a particle of light,” he says. “People have used various non-silicon semiconductors to do that.”





Jerry Simmons, left, is leading a team including Jeff Tsao, center, and Mike Coltrin that was awarded funding by the U.S. Department of Energy for advanced light-emitting diode, or LED, research and development.

That research helped revolutionize telecommunications because optical fibers use light to carry computer signals. “The Internet is based on semiconductor devices that absorb a photon on the receiving end or emit a photon on the transmitting end,” Simmons says. “It was a generation of semiconductors that began to be studied in the 1970s and ’80s that allowed optical internet communication to take place.”

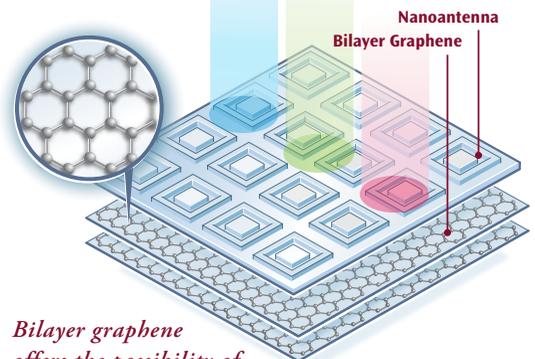
Sandia is developing optical materials that will do even more. One innovation is solid-state lighting powered by a new class of III-V semiconductors, so called because they combine elements from groups III and V of the periodic table. Using indium gallium nitride and aluminum gallium nitride, Sandia engineers made some of the first high-intensity blue and ultraviolet light-emitting diodes, or LEDs. “We had to learn how to grow the material thick enough to make an LED inside a growth chamber,” Simmons says. “You have different layers in the LED structure. The thickness of the quantum wells has to be well-defined and controlled to within a single atomic layer.”

Sandia was a pioneer in that material system and helped make possible the white LEDs that are penetrating the market, replacing incandescent and fluorescent bulbs. Also developed were LEDs that emit at ultraviolet wavelengths used in military applications and to purify water.

Researchers are extending the same gallium nitride-based materials into power electronics. “Instead of an information signal in your computer — tiny little currents of micro- or nano-amps — we’re looking at switching hundreds of amps to supply electricity from the grid to entire neighborhoods,” Simmons says. “The materials will make everything smaller, lighter, more efficient and more reliable.”

Graphene: Strength in layers

Graphene is a one-atom-thick layer of the mineral graphite in which carbon atoms are arranged in a hexagonal pattern. It’s strong, light and nearly



Bilayer graphene offers the possibility of real-time tunable infrared photodetectors. Adding nanoantennas increases absorption, making atomically thin graphene a plausible detector material.

transparent, an excellent conductor of heat and electricity with the potential to create ultra small and fast components in electronics. Wafer-scale graphene can be engineered and integrated with other semiconductors, producing tailor-made components for applications such as spintronics, biosensing and bioanalytics.

“Graphene is just in its infancy, but the potential number of applications is mind-blowing. Because it is only one atom thick, it is easy to modify the surface or the edges of a strip of graphene to control its properties. So this can make very tiny, low power switches,” Simmons says. “Or you can put two layers of graphene on top of each other and make a photon detector.”

Metamaterials: Second nature

Metamaterials are engineered to have properties not found in nature. Atoms and their arrangement in a material determine its properties. “It turns out you can make artificial atoms by shaping the material on a nanoscale, and as long as the shaping is significantly smaller than the wavelength of the energy it’s interacting with, it looks homogenous,” says Rick McCormick,

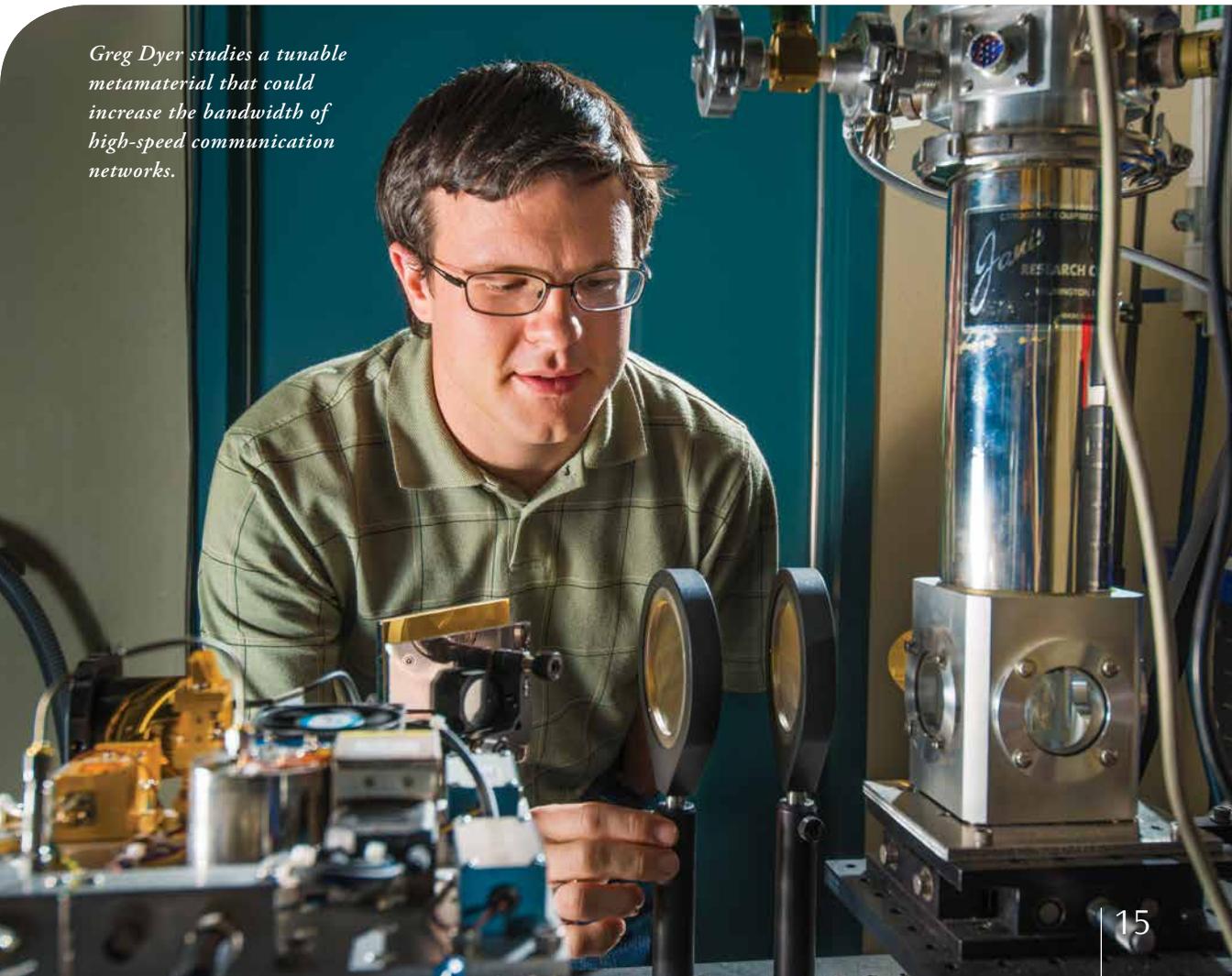
senior manager in radiation, nano- and optical sciences. “You can’t tell the difference between the atomic response and the response of the shaping.”

By changing geometry at the nanoscale, materials can be artificially engineered to create a response that doesn’t exist in nature. “It opens the door to making artificial atoms at artificial frequencies,” McCormick says. “Theoretically, that gives you a big knob to turn on material properties. We’re not stuck with what nature gave us.”

An example is the way a material responds to light. “Normally, when light passes through glass, like a prism, the light gets bent in a certain direction,” McCormick says. “By using metamaterials, we can make the light bend in an *opposite* direction to what occurs in nature. This allows us to do new things with light including non-visible light, like infrared and radio waves, that were never imagined before.”

Examples include ultra-thin lenses, ultra-efficient cell phone antennas and ways to keep satellites cool and

Greg Dyer studies a tunable metamaterial that could increase the bandwidth of high-speed communication networks.



photovoltaics more efficient. A recent Sandia Grand Challenge research project headed by McCormick and funded through Sandia's Laboratory Directed Research and Development program (LDRD) advanced the state of the art in metamaterials from two-dimensional metafilms to three-dimensional materials, research that won an R&D 100 award.

The work led researchers to look at optics in new ways, including using metamaterials in an invisibility cloak to shield something from view by controlling electromagnetic radiation.

"Metamaterials have given us a bunch of new theoretical, computational and experimental tools to explore the way light interacts with matter at a very small scale," McCormick says. "Now we can play with that in a new way."

Wide bandgap: Hot topic

Electronic bandgap is a fundamental materials property. Wide bandgap (WBG) materials such as silicon carbide and gallium nitride are semiconductors with bandgaps significantly greater than that of silicon. Wide bandgap materials already have revolutionized lighting. But as transistors, or switches, in modern power electronics they also have the potential to vastly improve the performance of electrical power grids, electric vehicles, motors in buildings for elevators and HVAC systems, and even computer power supplies.

WBG materials can handle high temperatures and voltages, properties that could lead to simpler, less costly power conversion systems. WBG has the potential to substantially reduce the estimated 10 percent energy loss between generating electricity and transmitting it into a home or business. A wide bandgap allows faster switching.

"In a decade or two the giant transformers in your neighborhood distributing power from the electric grid to homes that now weigh 10,000 pounds will be replaced by things the size of a suitcase that weigh 100 pounds," Simmons says.

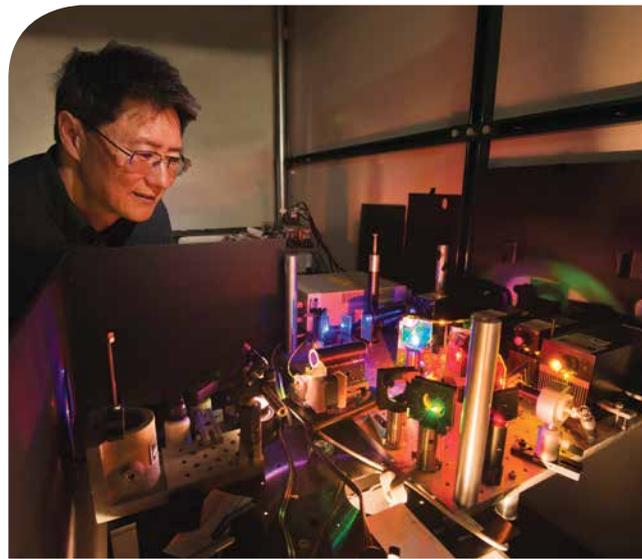
And if electric vehicles could tap the potential for WBG power electronics to withstand higher temperatures, they might not need a liquid cooling system, reducing the system's complexity and improving vehicle range because the car would weigh less.

Modern family

Simmons says Sandia is looking ahead to new classes of semiconductor materials that could help meet the labs' national security mission. Photon detectors are an example. "New photon detectors can image battlefields or landscapes in frequencies that we haven't looked at before," he says. "It's a new generation of materials that gives us that capability."

Where is the next generation of semiconductors leading? Simmons says to dramatic changes in the way people live. Some revolutions transform life in a striking way, such as buying an LED light bulb that uses less energy, saves money and lasts longer. Others sneak up, such as the realization over time that cell phones do much more in a much smaller package.

"Semiconductors have progressed over time to the point that the density of transistors and computing chips is mindboggling," Simmons says. "They are



Jeff Tsao looks over the set-up used to test diode lasers as an alternative to LED lighting.

embedded in systems like cars and cell phones and home appliances. They allow us to have our modern-day lifestyle.

"But we always have to be out on the frontier looking for the newest discoveries and picking things to develop further. So if we talk about semiconductors again in two or three years, the topics will likely be dramatically different but equally exciting." ■

what's next

Crystalline cells give solar power more oomph

By Neal Singer

Jeff Nelson's group at Sandia wants to get more power, more cheaply, out of photovoltaic materials, and they're succeeding.

They need materials that can absorb the widest range of wavelength spectrum the sun sends to Earth because solar radiation is lost when wavelength regions are ignored. Sandia is integrating five materials to capture spectral regions ranging from the infrared through the visible.

"Integrating dissimilar materials is difficult because of differences in atomic lattice size and chemistry," Nelson says.

To solve the problem, Nelson's team has developed a wafer bonding and integration approach for materials that are optically clear and have thermal expansion properties that minimize complications during the stress created by thermal cycling.

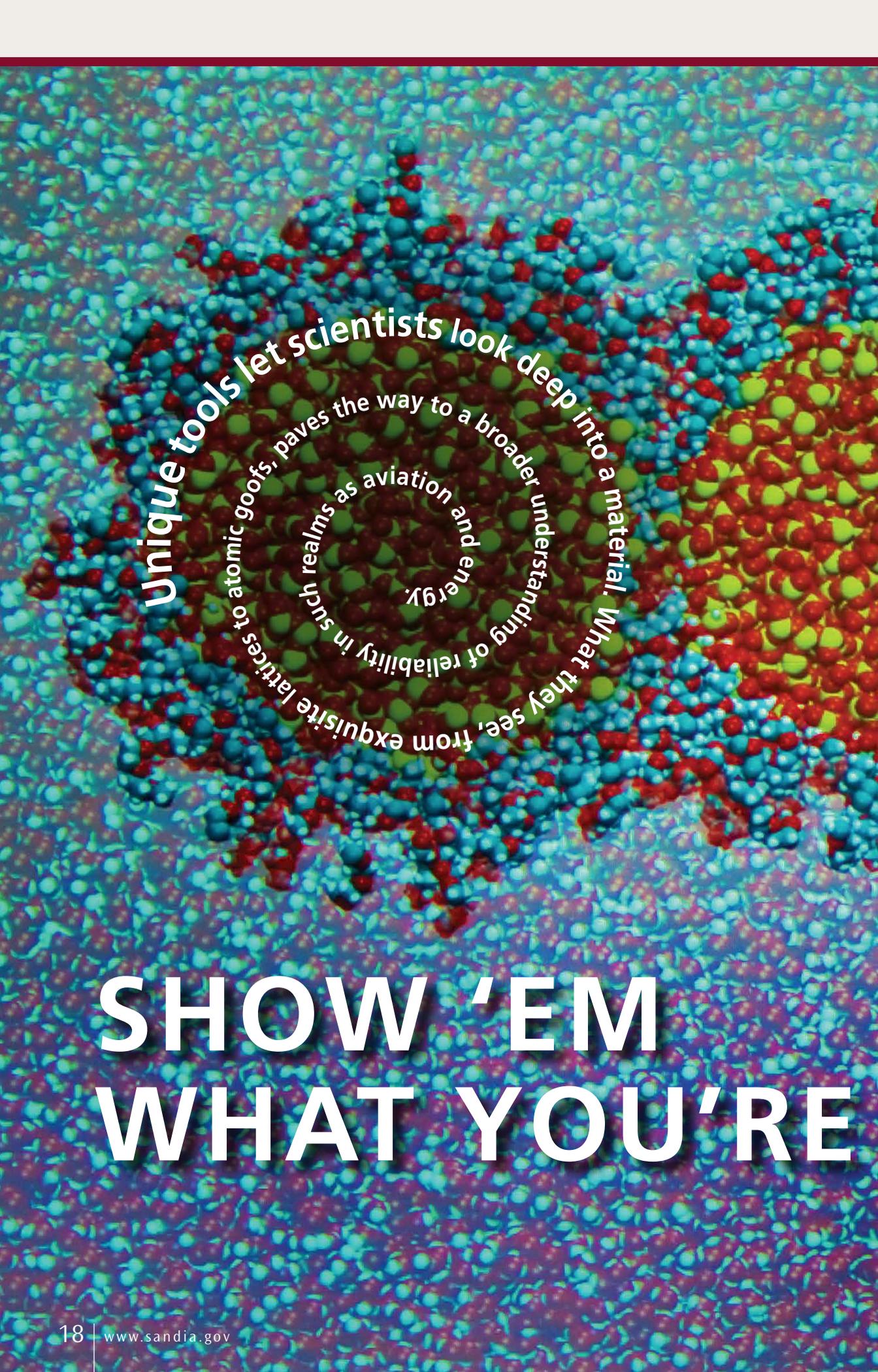
The Sandia strategy uses a technique unique in the solar industry to keep cost and device weight low while improving the electric current harvest. Microsystems-enabled photovoltaics (MEPV) is a way to make tiny crystalline solar cells that are measured in millionths of an inch instead of the inches of conventional cells.

A key element of MEPV technology is its ability to manufacture the 10-micron thick, 250-micron wide multimaterial cells within the existing manufacturing infrastructure using standard microdesign and microfabrication techniques. The miniaturized cells can then be transferred to a lightweight, flexible polymer or glass substrate that harbors embedded electrical contacts.

Materials of choice for these unique cells include silicon (efficiency around 20 percent) and compounds involving gallium-indium-arsenide-phosphide, with efficiencies demonstrated by industry to be greater than 40 percent. The compound method, however, is about 100 times more expensive than silicon, and must be combined with inexpensive optical lenses that, by concentrating sunlight onto the glitter-sized solar collectors, minimize the amount of material needed.

"It's a nice solution," Nelson says, "because we can make crystalline, micron-dimension cells, dose them with sunlight, and integrate them with flexible plastics or concentrator systems, depending on the application."

The work has national security and commercial applications in recharging batteries in fixed or mobile operating bases, powering vehicles, tents and UAVs in the field, and collecting energy in solar farms and rooftops. ■



Unique tools let scientists look deep into a material. What they see, from exquisite lattices to atomic goofs, paves the way to a broader understanding of reliability in such realms as aviation and energy.

**SHOW 'EM
WHAT YOU'RE**

In earlier centuries, it was enough for experimenters to know whether a material was cold or slippery, hard or light, flammable or explosive.

Today researchers working to understand the crystalline structure of a solid use powerful imaging tools to visualize a dizzying regularity of atoms stretching in every direction — above, below, behind and before their probes. They can see defects when atoms have dislocated from their expected positions in a lattice — atomic “goofs” — or where others have shifted *en masse* to different locations, like the moving fold that occurs when one shakes out a carpet, because the material has been placed under a severe enough strain to generate bands of dislocated atoms looking for a home.

Understanding these reactions is a major interest at Sandia Labs, where machines with unusually fine capabilities are used to figure out where and how materials may fail before they actually do. Such information saves money, time and expense, and reduces risks.

“We’re designing experiments to understand the role of microstructure on resultant properties like ductility, strength and fracture tolerance,” says Sandia researcher Blythe Gore Clark.

“For example, we want to understand where strain is concentrated during the deformation of polycrystalline materials. Polycrystalline means that the material has grain

Matt Lane shows a computer model depicting polymer-coated silica nanoparticles.

MADE OF

By Neal Singer



boundaries, sections of atoms aligning with different rotations, like countries with three-dimensional borders. Regions of high strain are believed to lead to void formation, where atoms are absent. As the voids grow and coalesce, they form cracks that propagate through the material. Among our charges is to understand the initiation and propagation of damage to develop higher fidelity predictive simulations.”

To do this well takes the best tools. The scanning transmission electron microscope (STEM) is widely used to investigate material structure and defects, but had drawbacks in its previous incarnation. The machine transmits an electron stream and creates an image of the atomic lattice under investigation. If the electron beam probe was truly a point source, like the tip of a sharpened pencil, the investigation would be invaluable. But unremediated, it is not precise.

“The highest resolution would be achieved if the electrons were focused to a point,” Clark says. “But the lenses aren’t glass, they’re electromagnetic fields produced by electricity flowing through copper coils. The further off-axis an electron is, the more strongly bent it is by the field.”

Thus, she says, the beam focuses to a disk rather than a point.

Enter the aberration-corrected STEM, or AC-STEM. Materials scientists Paul Kotula and Ping Lu say the

microscope uses computer software and double hexapole lenses, each of which alternates a north-south magnetization in its six poles. The software helps measure spherical aberration and then uses the poles to push electrons back into the right place to create an actual point-source beam.

The new, very fast machine has been compared to a telescope powerful enough to show two peas side by side on the moon. It can identify what element it’s examining by measuring characteristic X-rays emitted from single columns in the material. It’s located in New Mexico but can be controlled remotely from Sandia’s California location and by other research partners across the labs.

Another unique machine is the In-situ Ion Irradiation Transmission Electron Microscope (I3TEM), which shows better than any other what happens to certain materials in ion irradiation, gas-solid interactions, liquid cell work and quantitative nanomechanical testing.

“There are roughly 10 instruments in the world that can introduce an ion beam into a TEM,” says Sandia manager Jon Custer. “Ours is the only one that can insert two ion beams down the same path.” The alteration to allow two beams to enter the I3TEM without damaging critical parts of the microscope was designed at Sandia by Khalid Hattar. One beam provides heavy ions that go through TEM samples



Chemical engineer Bernadette Hernandez-Sanchez studies nanomaterials in Sandia’s Advanced Materials Laboratory.



MEET

Blythe Gore Clark

Clark played **scrum half** — the equivalent of **quarterback in football** — on the first Northwestern University women's rugby team, and was the first female player to score. As a post-doc she won two first-place prizes from the Materials Research Society in the "science as art" category. One image, a colorized transmission electron microscope shot of a deformed shape-memory alloy, looks like trees in a forest; another, a scanning electron microscope collaboration, resembles spaghetti and meatballs.

Clark is co-captain of The Penultimates ("Our goal is not to finish in last place."), a cycling team that raised more than \$30,000 last year for the National Multiple Sclerosis Society through raffles, a trivia night and donations for Bike MS, a two-day, 150-mile ride through the pueblos of northern New Mexico.

STATS

- Bachelor's degree in materials science and engineering from Northwestern University.
- Ph.D. in materials science and engineering from the University of Illinois at Urbana-Champaign.
- Post-doc at the Max Planck Institute for Metals Research in Stuttgart, Germany, on a Humboldt fellowship.
- Member of the Materials Research Society, American Nuclear Society and the Microscopy Society of America.
- Volunteer judge for MESA Day, the New Mexico Regional Science Fair and FIRST LEGO League Robotics competitions.

"like a bowling ball through pins," Custer says. The other drives helium or hydrogen ions too light and unenergetic to pass through a TEM foil. Instead the ions implant there. What happens when they implant and then a heavy ion barges through? Both beams, acting separately or together, allow observations in real time of interactions critical to nuclear research.

To do the critical materials science, the PPM, or Predicting Performance Margins project, must use both microscopes above, as well as tools like the RoboMET, which dissects and takes pictures of welds, one micron at a time. Led by Sandia manager Amy Sun and principal investigator Brad Boyce, the group also has developed in-situ scanning electron microscopy (SEM) experiments in materials under strain that are

coupled with electron backscattered diffraction and digital image correlation to understand plastic (i.e., permanent) deformation and microstructural evolution in tantalum.

This involves void formation, coalescence and ultimately fracture during deformation of that element. Results are then compared with predictions from crystal plasticity codes to improve the fidelity of predictive simulations for mechanical behavior of tantalum and other structurally similar metals.

Clark says advanced experiments and simulations, and the insights they provide into the behavior of materials, will shed light on such issues as the reliability and long-term viability of materials for applications ranging from airplanes to alternative energy.

"Projects with this structure could potentially impact everything that relies on the performance of a material," she says. ■



Hydrogen may be small, but it can ROUGH UP TOUGH

Hydrogen embrittlement knows no boundaries. No matter how it's used and what was its source, hydrogen affects the properties of materials, creating many engineering challenges. The small and highly mobile hydrogen molecule can penetrate structural materials, break down ductility and other key properties and cause structural failure.

Chris San Marchi, a hydrogen and metallurgy researcher, is on a team studying how hydrogen and materials interact and how that affects the mechanical properties of materials. The research has important applications in energy, nuclear weapons and other areas.

"One reason Sandia has such a strong energy program is because of the institutional expertise developed to support gas transfer system (GTS) components of nuclear weapons," he says. "Because of those decades of work, we are ideally situated to study the effects of gaseous hydrogen. This expertise helped the development of hydrogen energy programs supported by the president's 'all of the above' energy strategy. We have what is probably the most comprehensive effort anywhere in the country studying embrittlement from gaseous hydrogen, in particular high-pressure hydrogen."

San Marchi and colleague Brian Somerday develop codes and standards for hydrogen fueling stations and other energy-related uses of gaseous hydrogen in partnership with organizations such as the Society of Automotive Engineers, the Canadian Standards Association (CSA Group) and the American Society of Mechanical Engineers.

In the Hydrogen Effects in Materials Laboratory, materials immersed in high-pressure gaseous hydrogen, often at pressures more than 1,000 atmospheres, are put through fracture and fatigue tests. "We seek to validate and improve test methodologies as well as develop new ones for quantifying the adverse effects of hydrogen," San Marchi says. The goal is to build robust codes and standards on a foundation of proven science while capturing all the insidious effects of hydrogen.

There is a need for global coordination of codes and standards driven mainly by the automotive industry. In the past year San Marchi has given seminars and discussed collaborations in Korea and France and spent two weeks at Japan's National Institute of Advanced Industrial Science and Technology as a visiting researcher.

The energy program has invigorated Sandia's hydrogen research in nuclear weapons. "Even with all of our experience, there is still a lot that is not well understood about uncertainty and margins for design-

MEET

Chris San Marchi

San Marchi is a Southern California native whose two young children keep him busy. He enjoys cooking, gardening and spending time in the Mediterranean, where he learned a little Greek. He describes his Sandia work in the Hydrogen and Metallurgy Science Department as challenging and significant. “We have access to unique capabilities that allow our work to be truly impactful. That’s an aspect I enjoy,” he says. “There’s also an excellent team who keep me motivated.”

STATS

- San Marchi has two bachelor of science degrees from the University of California, Irvine (UCI), one in mechanical and aerospace engineering and another in chemistry.
- The decision to return to UCI for a fifth year to get the chemistry degree set the stage for his career in materials science.
- San Marchi earned a Ph.D. in materials science from the Massachusetts Institute of Technology.
- He did an extended postdoc at the École Polytechnique Fédérale de Lausanne, Switzerland.
- After a year at Northwestern University in Chicago, San Marchi joined Sandia in 2002 as a member of the materials science community.

METALS

By Patti Koning

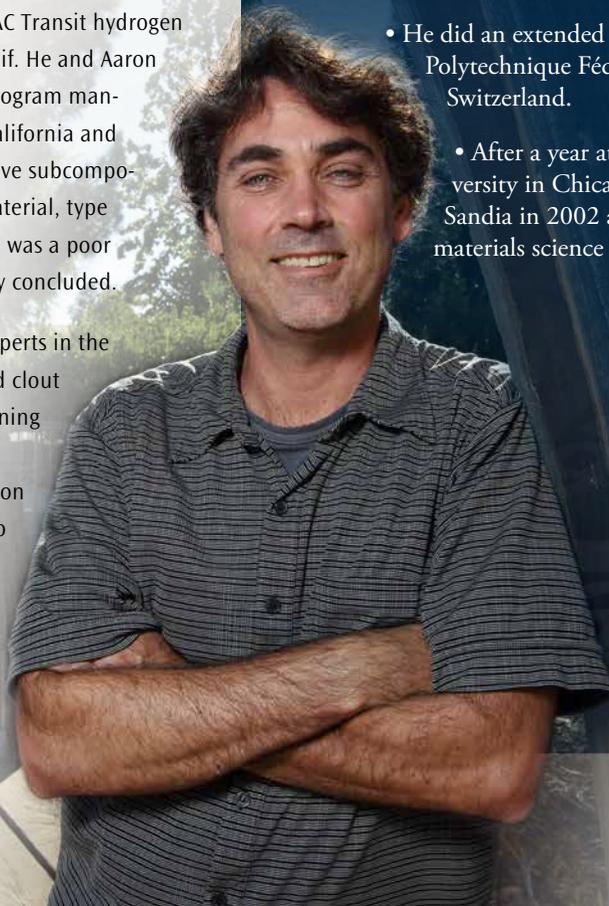
ing GTS components,” San Marchi says. “The tools we develop through energy research are allowing us to investigate materials more deeply. And in some cases, similar materials are used by both programs, which allows us to further leverage each area.”

Better defined margins for GTS components could give engineers more design flexibility. For example, they might be able to reduce weight and volume, both of which are at a premium.

Last year San Marchi was on a team that investigated a hydrogen release at an AC Transit hydrogen fueling station in Emeryville, Calif. He and Aaron Harris, a Sandia engineer and program manager, worked with the state of California and others to investigate why the valve subcomponent failed. The construction material, type 440-C martensitic stainless steel, was a poor choice for hydrogen service, they concluded.

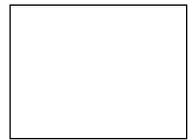
“We were viewed as impartial experts in the field. This gave us credibility and clout to aid, in a small way, the reopening of the station,” San Marchi says.

“We want to share our expertise on hydrogen with the community to help overcome roadblocks and setbacks to the deployment of hydrogen energy technologies.” ■



Sandia

R E S E A R C H



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LOOKING BACK

Simple ideas can have big impact. The simplest subjects sometimes offer the widest applications. Such was the case with lead-free solder, a modest product that became the highest-grossing patent at Sandia Labs.

Senior manager Mark F. Smith says U.S. patent 5,527,628, granted in 1996 to Sandia, Ames Laboratory and Iowa State University, came about because government tests showed that lead-based solder in discarded materials “oxidized, turned to powder, was driven into the ground by rain and snow, and found its way to local aquifers.”

But lead-free solders of the time put electronic fabrication techniques at risk because they required melt temperatures higher than industry could tolerate.

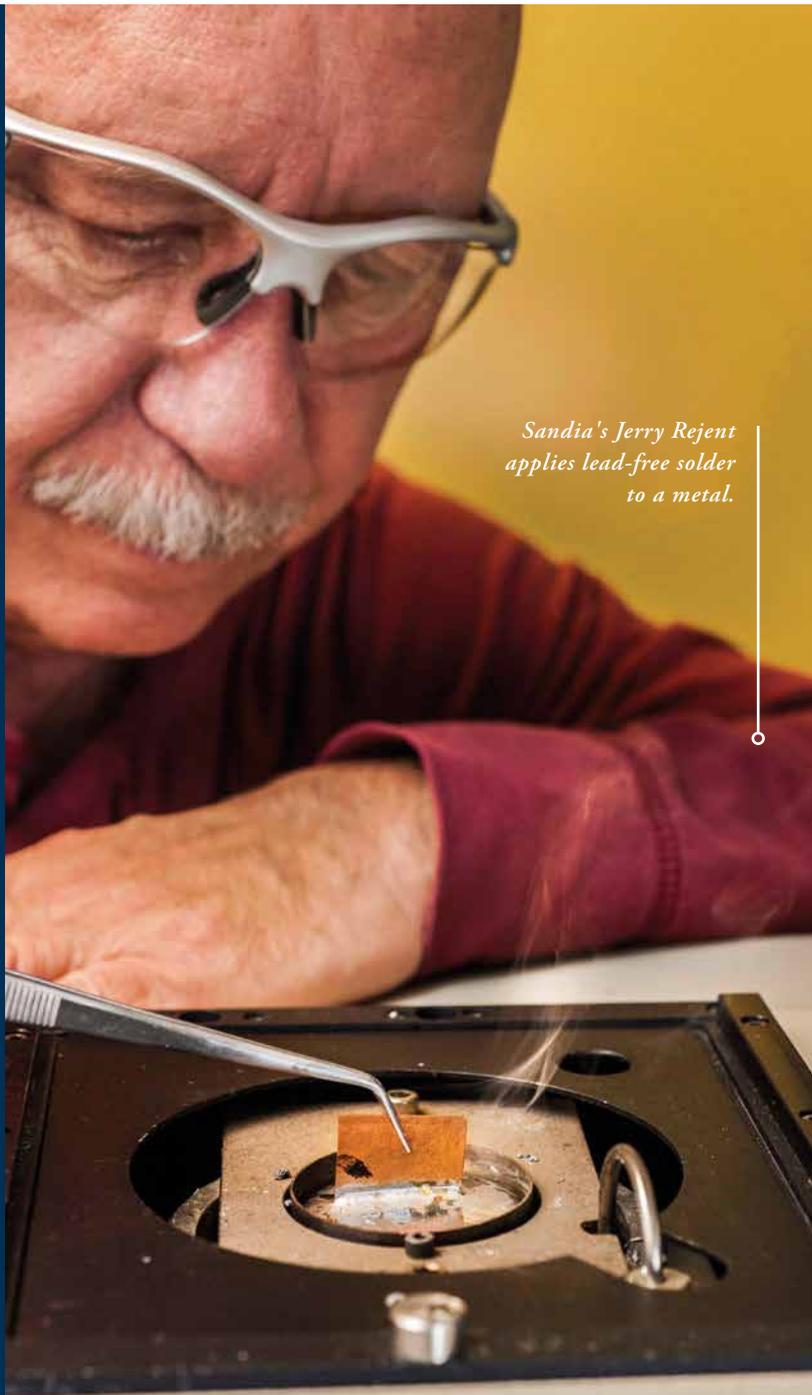
Sandia researcher Fred Yost mentioned the problem to his former Ph.D. adviser, ISU professor J.F. Smith, Mark Smith’s father, who was visiting Sandia on a consulting contract. The elder Smith said there was a region of the tin-silver-copper phase diagram that “looked funny” to him, and asked Iver Anderson at Ames to collect more data on the alloy. Their investigation revealed a melting point only slightly higher than that of the traditional leaded solder, 217°C vs. 188°C.

Sandia tested properties of the new solder.

When it appeared on the market — hardy, environmentally safe and low-temperature — it was bought all over the world.

The patent, which returned millions of dollars to taxpayers, ran out in July.

— Neal Singer



Sandia's Jerry Rejent applies lead-free solder to a metal.