Sandia RESEARCH

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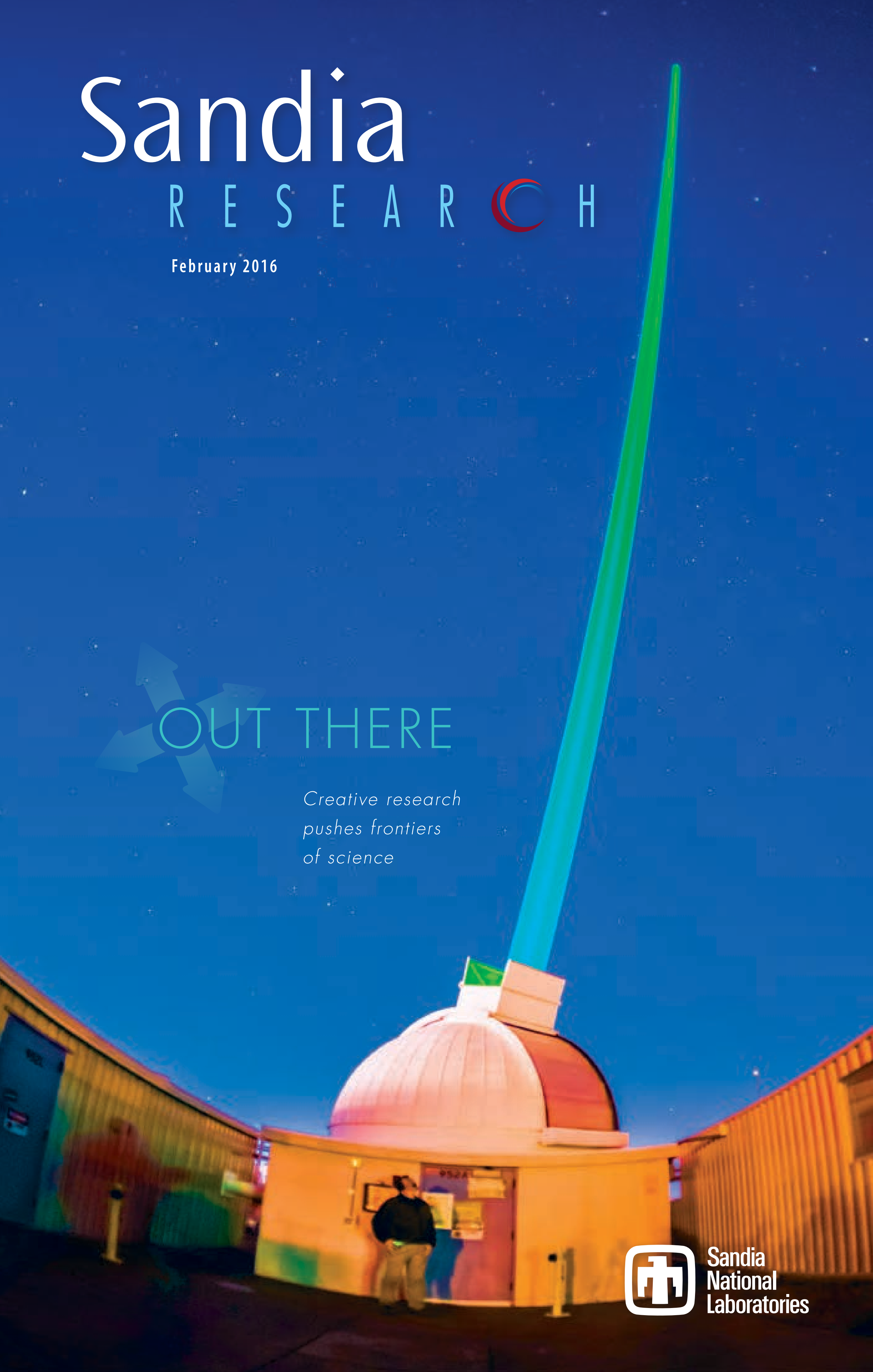

OUT THERE

Creative research pushes frontiers of science

Sandia National Laboratories

Exceptional service in the national interest

Sandia National Laboratories

Sandia Research is a magazine published by Sandia National Laboratories. Sandia is a multiprogram engineering and science laboratory operated by Sandia Corporation, a Lockheed Martin company, for the U.S. Department of Energy. With main facilities in Albuquerque, New Mexico, and Livermore, California, Sandia has research and development responsibilities for nuclear weapons, nonproliferation, military technologies, homeland security, energy, the environment, economic competitiveness and other areas of importance to the nation.

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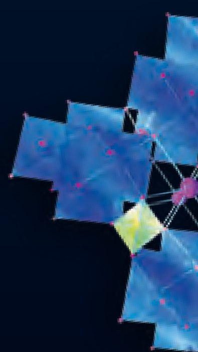
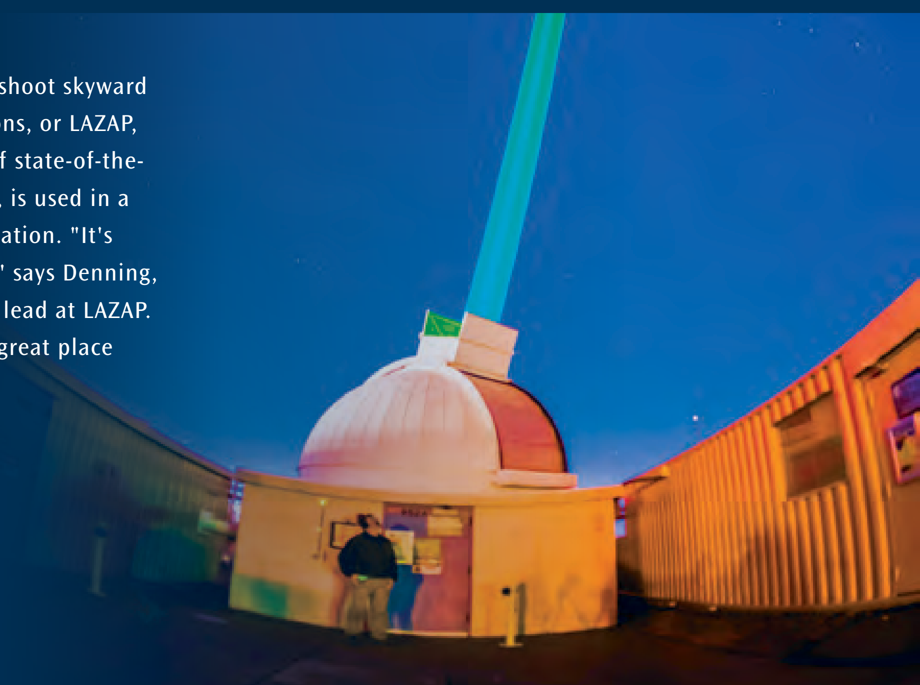
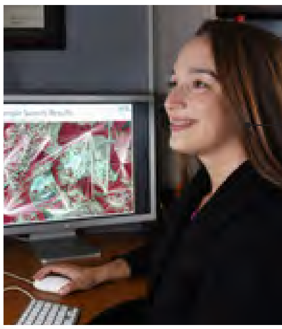


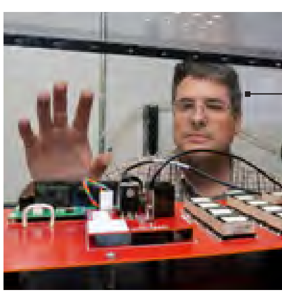
ON THE COVER

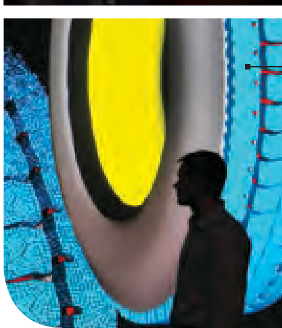
Dave Denning watches a beam shoot skyward at Sandia Labs' Laser Applications, or LAZAP, station. LAZAP, one of dozens of state-of-the-art research facilities at Sandia, is used in a wide variety of scientific exploration. "It's cool to shoot lasers into space," says Denning, a systems engineer and project lead at LAZAP. "We do all kinds of tests. It's a great place to work."

(Photo by Randy Montoya)









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LDRD

TWENTY-FIVE YEARS OF DISCOVERY

This issue of *Sandia Research* marks an important milestone in the history of Sandia and the other Department of Energy national laboratories. On Nov. 5, 1990, President George H.W. Bush signed the National Defense Authorization Act for FY1991, establishing the Laboratory Directed Research and Development (LDRD) program. The act authorized the laboratories to allocate a portion of their budgets toward innovative research and development that serves to maintain their scientific and technical vitality.

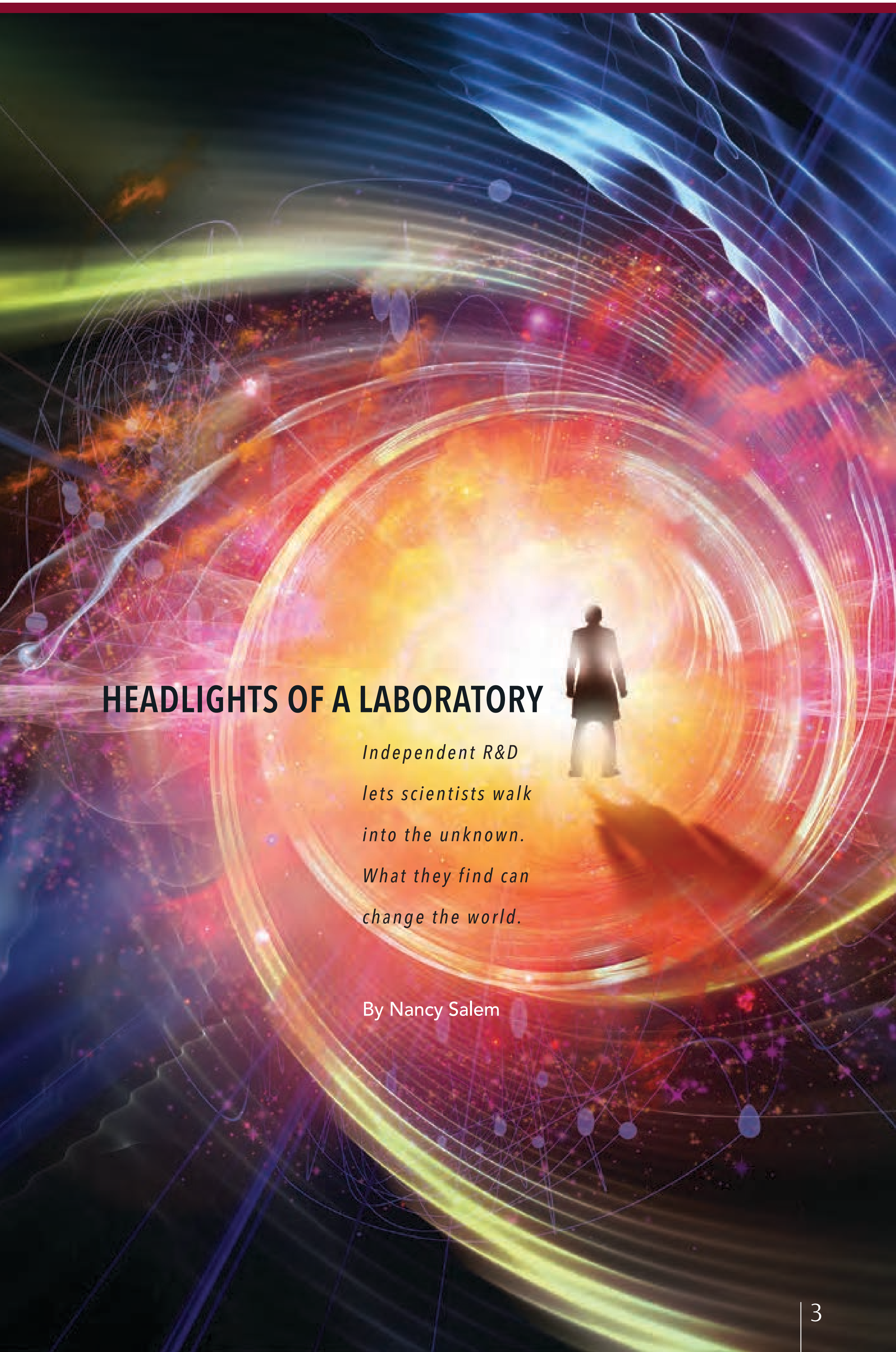
In the ensuing 25 years, the LDRD program has played a vital role in our national security and defense and has led to an impressive array of technological advances, awards, patents and publications.

At Sandia, LDRD-funded work has been a major contributor to scientific understanding and technological advances that help ensure the safety, security and reliability of the U.S. nuclear stockpile. The LDRD program has and continues to play a critical part in Sandia's ability to attract outstanding engineers and scientists, thus allowing us to continually refresh the laboratory staff.

The following stories are intended to give readers a flavor of some of the impacts from LDRD investments. Sometimes the benefits are fairly immediate (see "Stick together," page 20), while in other cases the impacts may not be fully realized for many years (see "Clean sweep," page 18).

As we mark the 25th anniversary of the act that created LDRD, we look forward to the bold discoveries and innovations that the LDRD program will produce in the next 25 years.

Rob Leland
Chief Technology Officer
Vice President, Science & Technology



HEADLIGHTS OF A LABORATORY

Independent R&D lets scientists walk into the unknown. What they find can change the world.

By Nancy Salem

Research at a national laboratory is concrete. It produces scientific and engineering solutions to real-world challenges tied to precise, vital missions. Most of the time.

Someone, somewhere, decades ago looked at the extraordinary talent and brain power collected at the labs and thought, what if?

What if the country turned those super-smart people loose to really explore what they could only imagine. Give them time and money to take science to the frontiers of possibility.

Thus was born Laboratory Directed Research & Development (LDRD), established in 1990 by Congress to let scientists at national laboratories do creative, innovative, independent research. “LDRD has allowed us to stay at the cutting edge of science in our core mission areas,” says Andy McIlroy, deputy chief technology officer and director of Sandia’s Research Strategy and Partnerships Center. “The origin was the realization that national labs, particularly national security labs as opposed to science labs, needed to have a small portion of their budgets directed to forward-looking research.”

At Sandia, LDRD is funded as a percentage of all the programs that come into the labs. Currently at just under 6 percent, or $155 million a year, it is directed toward long-term research that ultimately benefits the national security mission but may be at a lower technological readiness level than core programs can support. “It keeps the technical base fresh and forward looking in ways the core programs might not be able to in the course of usual business, but is of long-term benefit to them,” McIlroy says.

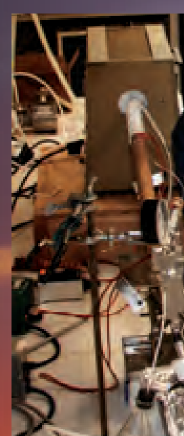
The investment has paid off in 25 years with important scientific advances. LDRD funds much of the work in Sandia’s seven research foundations, each focused on a specific scientific discipline and overseen by the Office of the Chief Technology Officer. “Research helps us to envision things that haven’t been realized yet,” says Rob Leland, Sandia Vice President of Science & Technology and Chief Technology Officer. “We can look broadly across the scientific and engineering community and ask what new and emerging areas of research could have a beneficial impact on the nation, and then develop understanding necessary to bring them to life.”

The seven foundations are Bioscience, Computing and Information Science, Engineering Science, Geoscience, Materials Science, Nanodevices and Microsystems, and Radiation Effects and High Energy Density Science. “The foundations enable the mission and advance the frontiers of knowledge in science and engineering,” Leland says.

Research supports national security in important ways, McIlroy says. “We can look into new and emerging areas that, if mastered by an adversary, could be used to the disadvantage of us and our allies,” he says. “We can position ourselves to counter a threat if it becomes a reality.”

Attract and keep exceptional scientists

LDRD has also helped Sandia attract and keep exceptional scientists. “It offers the freedom to propose and explore your own, mission-relevant ideas and push the state of the art in new ways,” McIlroy says. “When you add in the national security mission, it is very attractive. We attract professionals who are among the smartest people on the planet, who are not afraid



of challenging problems and who believe national service is worthy of a career commitment.”

The LDRD process starts with a set of calls from research and mission foundations. Broad areas are identified that have the potential for strong mission impact in the short or long term. Researchers respond with brief proposals that are reviewed by experts within the laboratory. About a fourth are asked to submit a full proposal. Those get an extensive programmatic and technical review. Roughly half will be funded.

R&D at Sandia takes countless forms and draws in thousands of people.

"We get a lot of ideas," McIlroy says. "There is quite a bit of scrutiny." A typical LDRD project is funded at $200,000 to $600,000 and takes up about a third of the principal investigator's time for up to three years. Typically, researchers work on other projects in addition to an LDRD project.

A significant portion of Sandia's LDRD portfolio is now connected to Research Challenges, long-term, cross-disciplinary projects in 11 designated areas related to national security. "We're looking for big, bold ideas to move the Research Challenges forward," McIlroy says.

Groundbreaking discoveries and innovations

Not all LDRD projects are long and complex. "Some let us explore new areas that might fall outside our expertise with small seed projects to see if it will lead in a new direction," McIlroy says. "This allows us to explore quickly areas that could become important in the future."

McIlroy says LDRD has produced groundbreaking work including discoveries and innovations in microelectronics, microsystems and nanodevices, materials science, defense and advanced radar. "We've stayed at the forefront of radiation-hardened electronics. Sandia is one of the only places in the country that produces them," he says. "It is important in nuclear weapons work but also applies to space-related activities."

Bioscience was a niche at Sandia until LDRD advances led to establishment of a research foundation. The breakthrough was MicroChemLab, a micro-laboratory compact and light enough to fit in a hand. It harnessed the power of a full chemistry lab, detecting and analyzing toxic agents such as bacteria, viruses and protozoa in minutes rather than hours. And it did its work using only minuscule amounts of sample and analytes.

The micro device, created out of Sandia's first Grand Challenge LDRD, was a milestone on a strategic path to establish the lab as a microfluidics authority.

Grand Challenges are larger LDRD projects at around $3 million a year for three years that focus on bold, high-risk ideas with potential for significant national impact. Sandia has enhanced the basic technology behind MicroChemLab, generated a multitude of patents and garnered national recognition, including a 2012 R&D 100 award for an entire integrated system for automated sample preparation and analysis of micro-liter volumes.

And proving that innovation breeds innovation, MicroChemLab has spurred a half dozen startup companies and unanticipated uses such as monitoring for gases released during fracking.

More than a decade after the first prototype was launched, the momentum remains strong as Sandia continues to receive funding for new applications of the microfluidics technology in national security, public health and energy.

"This was an iconic project where an early investment in LDRD planted the seeds of an important national security program," McIlroy says. "LDRD really helps us deliver on our tagline of delivering exceptional service in the national interest. To be exceptional we have to be at the cutting edge, and LDRD is one of the tools that helps us meet the expectations of the country. We have delivered." ■

Sandia's first generation MicroChemLab produced fast microfluidic separations of biological samples with high sensitivity. It miniaturized benchscale analyses using fabricated microchannels in a hand-held, low-power device.

MEET

Adrian Chavez

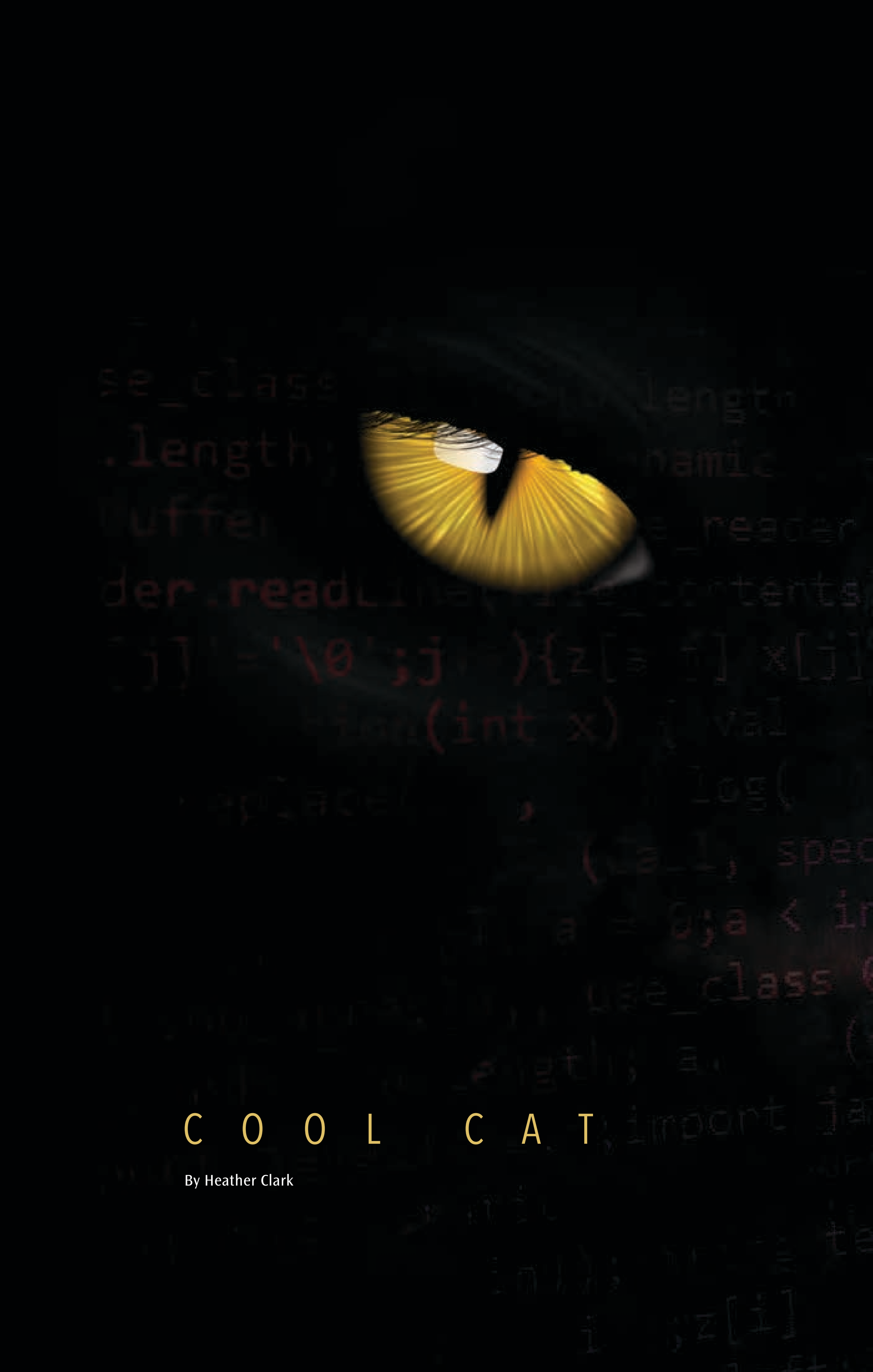
Adrian Chavez likes a good puzzle. When he was growing up in Albuquerque, his mother and grandmother gave him plenty to solve. "They would be busy making lunch at my grandmother's house and they'd give me a puzzle. I was 5 or 6 years old. They had jigsaw puzzles, mechanical puzzles, brain teasers," Chavez says. "They would time me and I would finish before they got lunch done, so they would tell me to do it 10 times instead."

Chavez took a computer programming class his senior year of high school and, with encouragement from his mom, found his calling. "It was a lot like the puzzles, which involved troubleshooting and problem solving," he says. As a University of New Mexico computer science undergrad, Chavez interned for four years starting in 2000 at Sandia's Center for Cyber Defenders. In 2004, he took advantage of the Labs' Master's Fellowship Program to earn a master's degree at the University of Colorado, Boulder. He's now pursuing a doctorate at the University of California, Davis, through Sandia's University Part-Time program.

He has led two Laboratory Directed Research and Development projects and contributed to several others, all with the goal of developing and deploying new cybersecurity technologies for systems like the power grid, oil and gas refineries and water pipelines to make sure responses and protections are in place in the event of a cyberattack. "The vision of each project is to secure the hardware and software of critical infrastructure systems that harness our nation's most critical assets," Chavez says. "The impact our team has made in securing these systems goes beyond Sandia. A couple of our prototypes that started as LDRDs have made their way to the market in more than 10 vendor products that are deployed in several utilities' operational networks around the country."

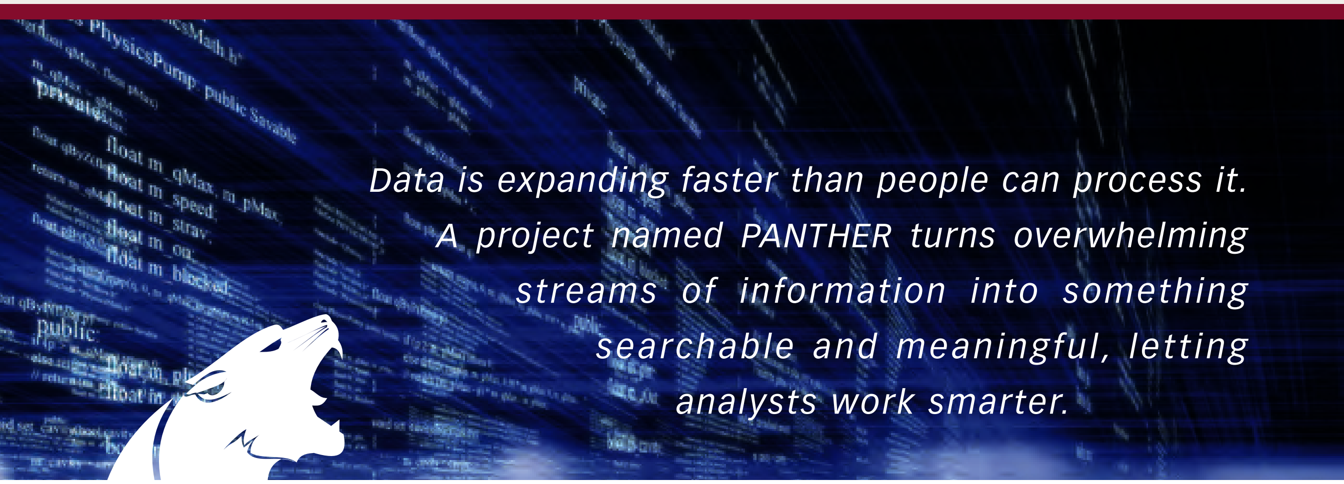
STATS

- Bachelor of Science in computer science from the University of New Mexico
- Master of Science in computer science from the University of Colorado, Boulder
- In 2014, named by President Barack Obama a recipient of the Presidential Early Career Award for Scientists and Engineers (PECASE). PECASE is the highest honor bestowed by the U.S. government on outstanding scientists and engineers who are beginning their careers.



COOL CAT

By Heather Clark



Data is expanding faster than people can process it. A project named PANTHER turns overwhelming streams of information into something searchable and meaningful, letting analysts work smarter.

After a disaster or national tragedy, bits of information often are found among vast amounts of data that might have mitigated or even prevented what happened — if spotted ahead of time.

In this information age, national security analysts often find themselves searching for a needle in a haystack. Data is growing much faster than analysts' ability to observe and process it. Sometimes they can't make key connections and often are overwhelmed by the struggle to use data for predictions and forensics.

The Pattern Analytics to Support High-Performance Exploitation and Reasoning (PANTHER) Laboratory Directed Research & Development (LDRD) Grand Challenge has made progress that will let analysts work smarter, faster and more effectively when looking at huge, complex data sets in real-time, stressful environments where the consequences might be life or death.

Grand Challenges are three-year LDRD projects that focus on bold, high-risk ideas with potential for significant national impact. While a typical LDRD project is funded at $400,000 to $700,000, Grand Challenges are funded at about $3 million a year.

At the conclusion of the PANTHER Grand Challenge in September 2015, PANTHER's 26-member team had made breakthroughs in rethinking how to compare motion and trajectories; developing software to represent remote sensor images, couple them with additional information and present them in a searchable form; and conducting fundamental research on visual cognition, says Kristina Rodriguez Czuchlewski, PANTHER's principal investigator and acting manager of Intelligence, Surveillance and Reconnaissance Systems Engineering and Decision Support at Sandia Labs. The PANTHER team looked at raw data and ways to pre-process and analyze it to make it searchable and more meaningful. The project also studied fundamental research in cognitive science to inform the design of software and tools to help those viewing the data and make information of interest or trends easy to uncover. PANTHER led to strong partnerships within Sandia, "creating seminal technical achievements that are having direct impacts on the Labs' ability to provide solutions for some of our nation's most challenging national security problems," senior manager Steve Castillo says.

PANTHER is providing deeper insights from complex data sets in minutes, instead of months, and covering hundreds of square miles instead of dozens. "PANTHER developed the foundation for transforming how massive, complex data sets can be quickly analyzed to provide the nation's decision-makers with new perspectives on situations and circumstances," says Anthony Medina, director of the Radio Frequency & Electronic Systems Center. "If an analyst is collecting information on a specific location over time and learns that something of interest might be occurring there, they probably don't have the tools they need to quickly gather and analyze information from all relevant data sets that might corroborate the forecast. But PANTHER is probably the nation's best bet right now to get to that point quickly."

Danny Rintoul, a Sandia data scientist, developed the Tracktable code along with Sandia researcher Andy Wilson and others under PANTHER to automate the observation of motion and trajectories. The code could be applied to any problem that examines movement, such as those involving airliners, ships or people.

Current approaches to getting meaningful information from trajectories focus on comparing one trajectory to another. If you have millions of trajectories to consider, that could mean trillions of comparisons, which take a lot of time and computer power, Rintoul says. "We've developed a way to store and represent trajectories so that computers can compare them all at once in a very fast and effective manner," he says. Instead of trillions

MEET

Kristina Rodriguez Czuchlewski

Ask Kristina Rodriguez Czuchlewski about her travels and it's no surprise she works at Sandia Labs. She first visited New Mexico on a college field trip to study geology. "I remember it was really sunny and we were studying for a differential equations test. We were all engineers taking geology and great friends, so we were hiking around New Mexico quizzing each other," she says. "It was super nerd-out time."

Czuchlewski's exposure to science and college came even earlier on family trips when her dad, a high school chemistry teacher, took her to science museums, aquariums and college campuses. "We went to every science museum in the country for fun when we were on vacation," she recalls. "I always knew I was going to be a scientist in some form and I always knew I was going to go to college."

As an undergraduate at Princeton University in the geological engineering program, Czuchlewski was interested in the way the Earth worked and excited about understanding natural disasters, though she had never been in one. In graduate school at Columbia University, she focused on seismology and geophysics, but her natural curiosity led her to work with microwaves and use remote sensing to study natural disasters.

At Sandia she saw a connection between national security and the civil applications she studied in school. "I've been able to keep that theme of understanding the deep technical stuff while applying it to real-world problems that are meaningful," she says.

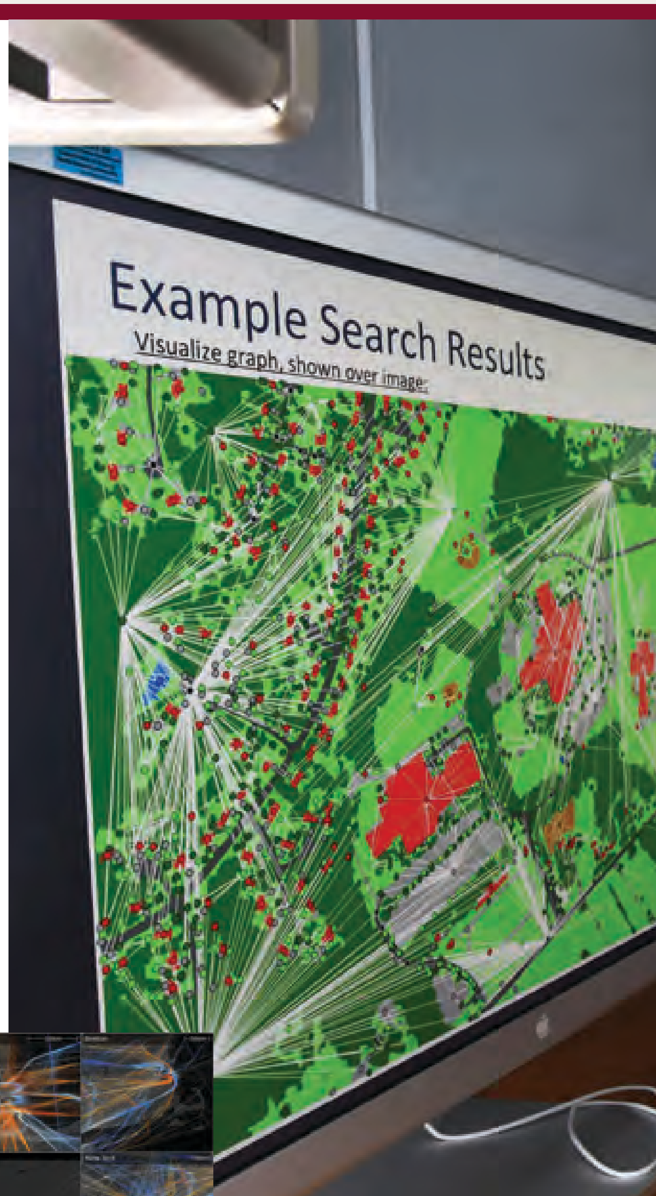
STATS

- Bachelor of Science in civil engineering in the Geological Engineering Program from Princeton University
- Master's and doctorate in earth and environmental sciences from Columbia University
- Postdoctoral research fellow at Columbia University where she addressed the impact of natural hazards and development on low- and medium-income international regions and the benefits of long-term forecasting and planning

of comparisons, the software does the same job in millions of comparisons, which is manageable.

An analyst concerned about the number of airliners stuck in holding patterns could ask Tracktable about aircraft trajectories that made a certain pattern of turns. Tracktable then calculates geometric features, such as the number of 90-degree turns an aircraft flew or the length of a straight line. By associating a type of motion with these features and assigning a number to each one, the computer can quickly group flights that behave in similar ways and show them to the viewer for interpretation. "If you have millions and you're not interested in precise comparisons, but general groupings of them, this is very effective," Rintoul says.

PANTHER also examined the predictive capability of the information buried in data. If an analyst looks at the first half of a flight, considers historical data about similar flight paths and then looks at the second half of the flight, any deviation from the pattern might cue an analyst to take a closer look. Finding that outlier from millions of flights that have flown before takes about



a second with Tracktable, Rintoul says. The analyst is alerted because PANTHER team members are using advances in cognitive science to design visual results that will highlight the odd behavior of the single aircraft. By studying how analysts use visual data, Sandia researchers are figuring out ways to make an outlier pop out of a screen full of detail to demand an analyst's attention.

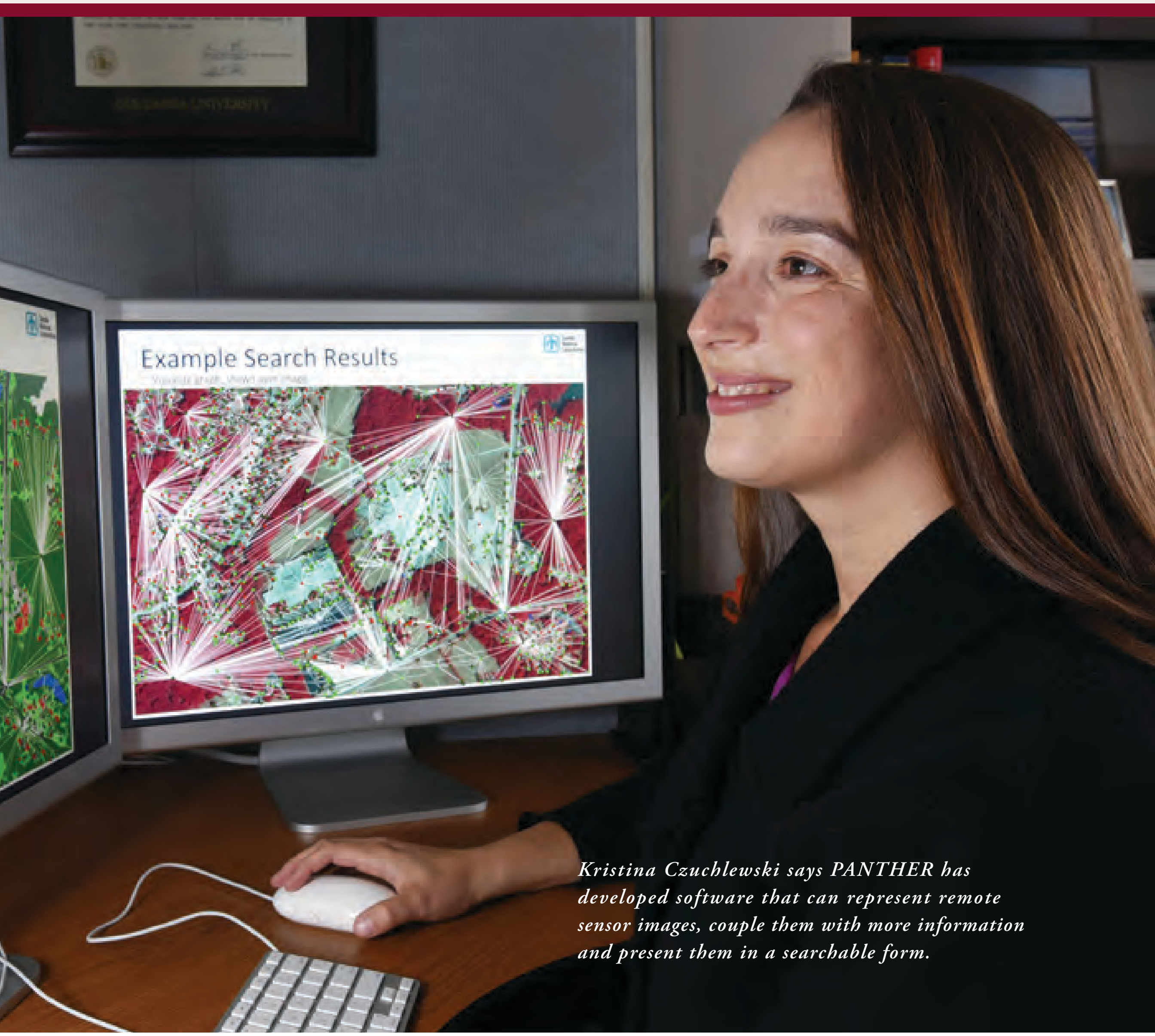
The team is now looking at integrating motion and trajectories into a system called GeoGraphy. Initially funded by the National Nuclear Security Administration, GeoGraphy is a software system that converts remote sensing images expressed in pixels into nodes and edges in a graph to show changes over time and make the data searchable, says Randy Brost, a Sandia computer scientist who led the team that developed the software.

GeoGraphy breaks the images into categories, such as buildings, trees or rivers. This pre-processing creates a graphic like a complex paint-by-number that shows the categories of everything in the image. The program uses nodes and edges — nodes are analogous to the beige hubs in Tinkertoys, while edges are the colored connecting rods — to describe relationships between objects, such as distance or time, Brost and Czuchlewski say.

This award-winning image by Sandia researcher Andy Wilson shows PANTHER's geometric and temporal trajectory analyses of air traffic patterns from 43,000 flights over the U.S. on April 4, 2014. White lines represent level flight, orange lines indicate ascent and blue lines show descent.

In addition to the imagery, the software package could include such information as phone books or county records to produce a single searchable database of all the information together that shows what's changed over time. For example, to find a high school, the analyst tells the program to search for large buildings near regions that look like parking lots, football fields and tennis courts and defines those items. The analyst then can choose from among the results the computer provides.

The system is hierarchical, so once an analyst identifies high schools, the program can be asked to find high



Kristina Czuchlewski says PANTHER has developed software that can represent remote sensor images, couple them with more information and present them in a searchable form.

schools the next time without a description. And if there is doubt that something is a high school, the software makes the raw data available for verification, Brost says.

"The purpose of these codes — GeoGraphy and Tracktable — is to assist humans, not to replace them or to automatically do their jobs. It's to enhance their ability to do their jobs well and to allow them to be more effective in dealing with large sets of evidence," Brost says. "In the end, basically they are suggestion systems that say, 'Hey, based on what you told me you're interested in, you ought to look here, here and here.'"

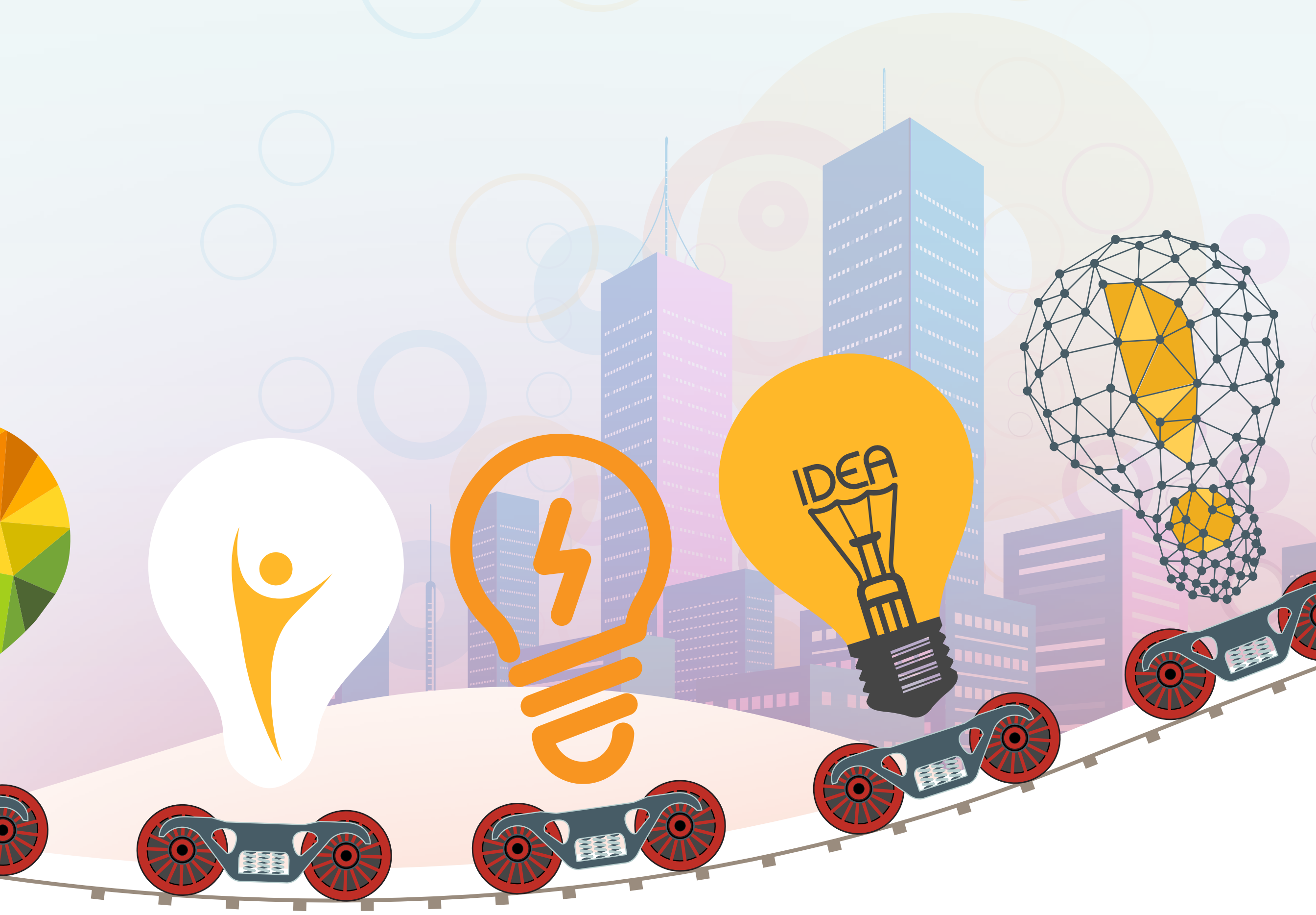
The PANTHER team included researchers focused on enhancing the user experience. Laura Matzen and others are conducting cognitive science experiments to learn how analysts' expertise affects their visual cognition and to create a model of how top-down visual attention — when a user approaches an image with a goal in mind — works. The researchers hope to use the answers to such fundamental cognitive science questions to guide the design of new tools that will improve interactions between humans and computers, Matzen says.

The prototype products and ideas developed under PANTHER are ready for the next step in development: to be tested in real-world environments, Czuchlewski says.

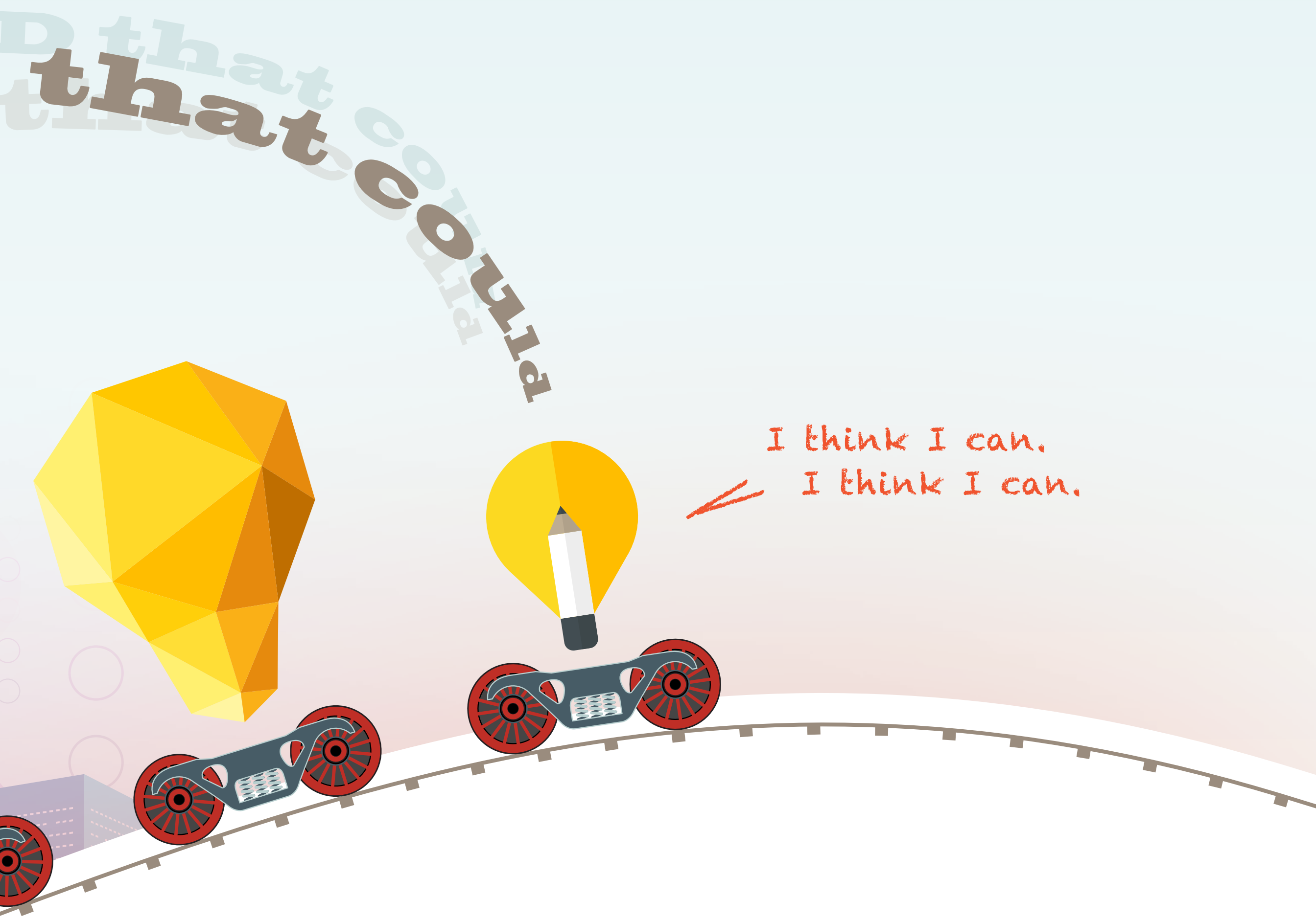
Sandia researchers have proposed looking into new problems illuminated by PANTHER, while other agencies are solidifying the foundation the project has developed. Some projects will use PANTHER's ideas to address real-world problems, researchers say.

"We went into PANTHER thinking we were going to do one thing: we're going to improve the lives of image analysts," Czuchlewski says. "And in the research process we did a whole lot more." ■

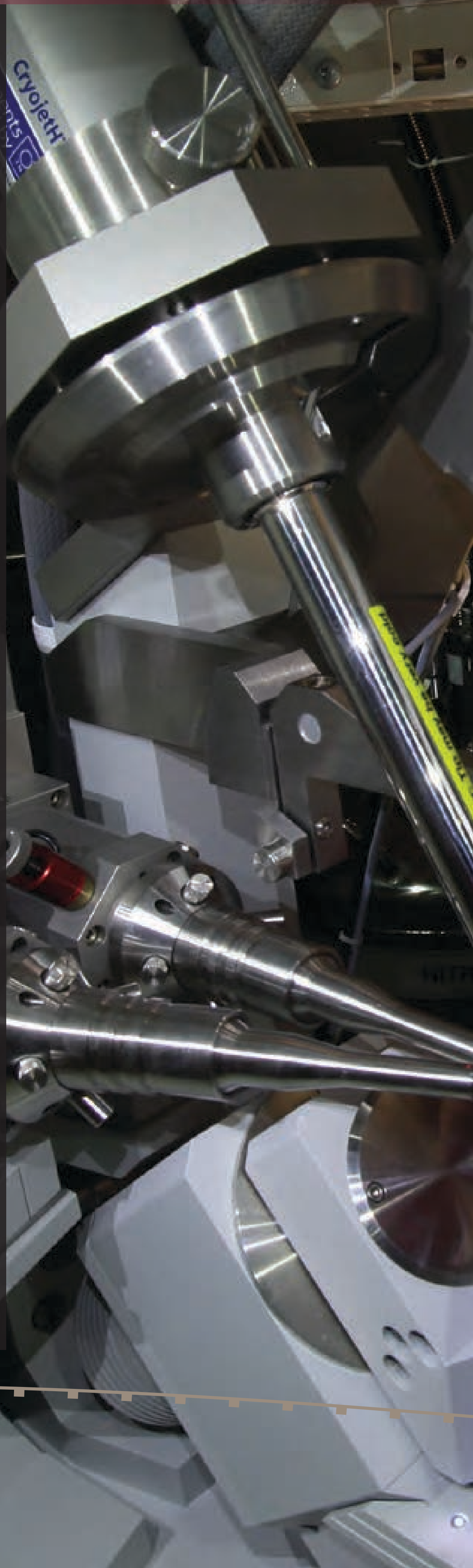
The little LDRD



By Patti Koning



Sometimes it's the small ideas that turn into the greatest successes. One scientist's foray into radiation detection ended up being quite remarkable.



About five years ago, in a one-year Laboratory Directed Research and Development (LDRD) project, Patrick Doty explored the idea of a material that could transform radiation detection. That small investment has paid for itself more than 15 times with a project that keeps going.

Doty's idea — "Use of Metal Organic Fluors for Spectral Discrimination of Neutrons and Gammas" — led to scientific breakthroughs. He addressed a well-known problem with a radiation detection method that relies on light-emitting organic molecules. The method uses scintillating materials, which fluoresce when exposed to ionizing radiation. The light properties yield valuable but limited information about the radiation source.

"This is an energy transport problem," says Doty, a Sandia materials scientist. "My initial idea relied on metal-organic phosphors to convert a portion of the energy normally lost to the scintillation process into useful luminescence."

The LDRD looked at organic scintillators in different testbeds including plastics, oils and metal organic frameworks (MOFs). Patrick Feng, a postdoc assigned to Doty's colleague Mark Allendorf, also worked on the project.

In the LDRD proposal, Doty wanted to test if a heavy metal dopant — a trace impurity that alters electrical or optical properties — could improve the organic scintillator's performance. Dopants had been shown to dramatically increase the brightness of organic light-emitting diodes (OLEDs) by "scavenging" the excited-state energy in the device that was not converted to light. This was the same principle Doty wanted to apply to radiation detection.

The LDRD proved the principle and identified MOFs as an ideal carrier to study the structure-property relationships of energy-transfer. Often described as "molecular tinker toys," MOFs have a crystalline structure that resembles molecular scaffolding, consisting of rigid organic molecules linked together by metal ions. Chemists love MOFs for the empty space within that scaffolding that can be filled with practically any small molecule.

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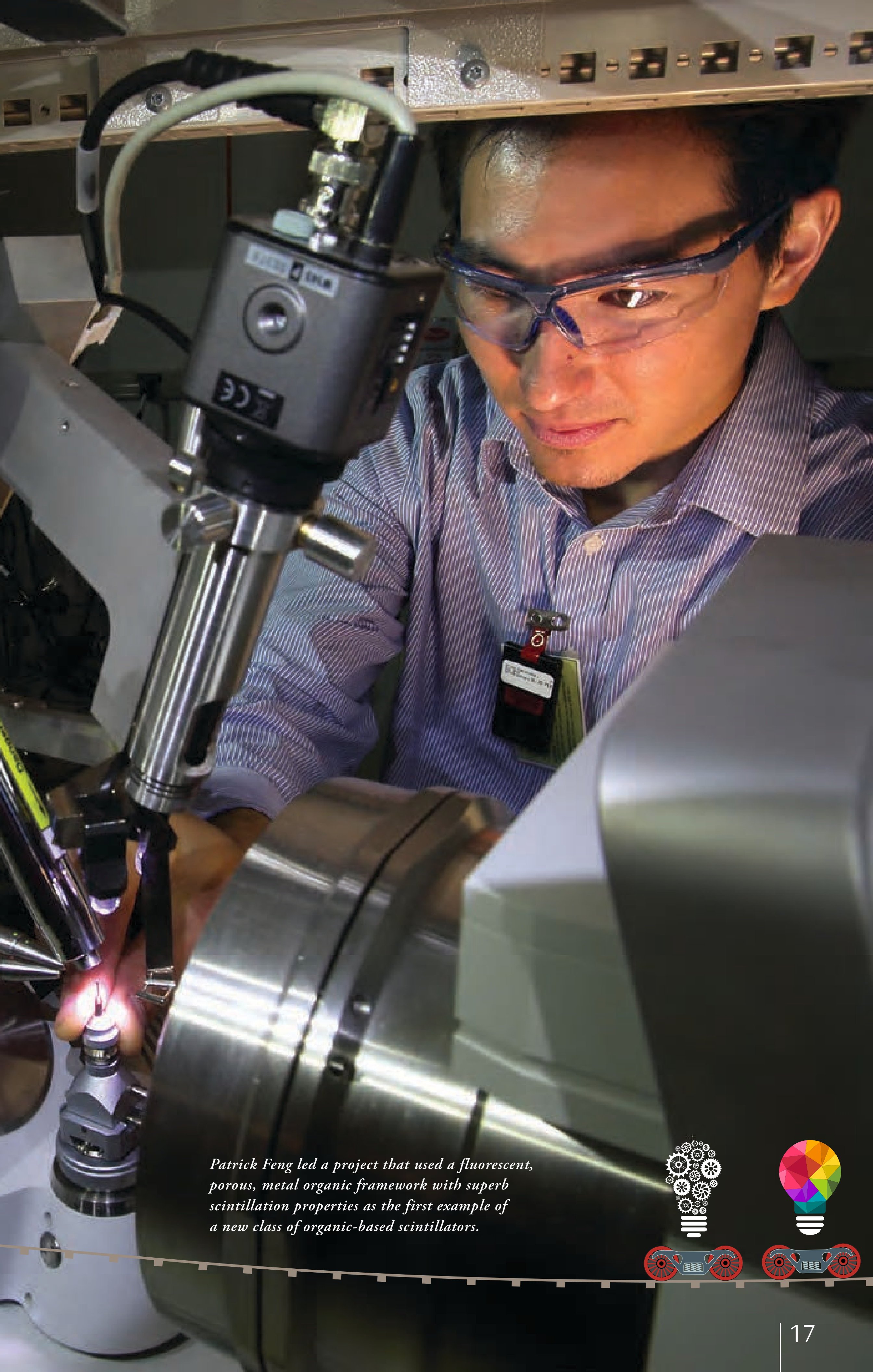


Patrick Feng led a project that used a fluorescent, porous, metal organic framework with superb scintillation properties as the first example of a new class of organic-based scintillators.

SCAN TO SEE VIDEO

CleanSWEEP

CSTs came to the rescue at Fukushima

In the early 1990s, Sandia researchers used Laboratory Directed Research and Development funds to investigate materials that could remove radioactive waste from liquid. They saw that a class of molecular sieves, microporous minerals used as adsorbents and catalysts, was better at capturing cesium ions from water than other technologies.

Chemist Tina Nenoff worked nearly around the clock for days to prove that CSTs outperformed other materials in removing radioactive cesium from seawater.

A team developed and commercialized CSTs, or crystalline silicotitanates, inorganic, molecularly engineered ion exchangers that take high-level radioactive contaminants such as cesium out of wastewater.

CSTs played a role when the Fukushima Dai'ichi nuclear reactor complex was damaged in an earthquake and tsunami on March 11, 2011, and seawater was pumped in to cool the reactors. The water was contaminated with cesium and could not be released back into the ocean.

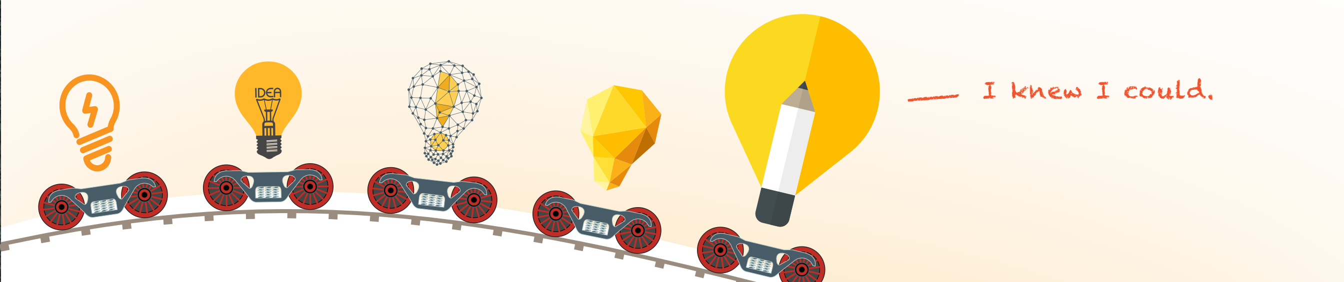
Honeywell UOP licensed the Sandia technology in the mid-1990s and revised the license in 2012 to become the exclusive U.S. manufacturer of CSTs. The company had worked with Sandia through a Cooperative Research and Development Agreement to produce a commercial-scale manufacturing procedure for the technology.

Sandia chemist Tina Nenoff, who had experience developing and working with CSTs in the 1990s, was called upon to test the material for removal of cesium in seawater after the Fukushima disaster. She worked nearly around the clock for 10 days, concluding that CSTs outperformed other materials in removing cesium from seawater.

Since then, Honeywell UOP products with CST technology have successfully treated more than 43 million gallons of contaminated water at Fukushima.

"It's the kind of thing that sends a chill," says Mark Rigali, who was on the Sandia team. "We helped really make a difference in the world. These are the kinds of successes we want to see with all our intellectual property." ■

— ***Nancy Salem***



Continued from page 16

The team won funding from the National Nuclear Security Administration (NNSA) to extend the MOF results to a system based on a bulk polymer matrix. Feng, who became a Sandia employee, led that effort, which leveraged the insights gained from the MOF materials discovered in the LDRD project to create triplet-harvesting plastic scintillators. Triplet-harvesting refers to a process that converts energy from an organic polymer matrix to highly luminescent triplet energy states on organometallic dopant complexes.

Triplet-harvesting was proven to be efficient in MOFs filled with small amounts of OLED dopants to modify the luminescence response to ionizing radiation. The team was then able to extend these results to polymer-based systems to create bulk materials that not only produced more light, but light of another color. This enables more effective detection of neutrons, which is technically challenging due to the difficulty in distinguishing neutrons from ubiquitous background gamma rays.

"Fundamentally, it is easier to monitor the color of light emissions rather than the rate at which that light is emitted," Allendorf says. "That's the crux of this approach."

Distinguishing particles

The trick is to add just the right amount of dopant so that both the scavenged light and fluorescence from the excited matrix itself are emitted. Then the ratio of the intensities at the two wavelengths is a function of the type of high-energy particle interacting with the material. Feng and Doty developed this into a method known as spectral shape discrimination (SSD) that can be used to distinguish one particle from another based on the color of the emitted light.

Because the ratio of neutrons to gamma rays is low — as low as one neutron to 10^5 gamma rays in some environments of interest — the threshold at which current detectors can see neutrons is fairly high. Sandia calculations suggest that the threshold for detecting neutrons produced by fissionable material could be lowered substantially using SSD, perhaps improving the "figure of merit" by a factor of 10 compared to the current standards.

An onslaught of gamma rays

SSD also addresses another radiation detection problem — active interrogation. Using an active source to create a signal from special nuclear material is an effective means for detection, but this causes an onslaught of gamma rays that overwhelms current detectors. The new materials developed at Sandia can be tuned for improved timing performance at high rates, and the new technology also could be used in radiation detectors for treaty verification.

In 2014, this breakthrough research was recognized with an R&D 100 award. Feng also won an Asian American Engineer of the Year award, Most Promising Engineer, in large part for his work on triplet-harvesting plastic scintillators.

Commercialization is a next step. The team is working to further tune the materials. "Scaling up may present separate challenges," Doty says. "There are applications for the smaller-sized detectors that have been demonstrated at Sandia, but to be widely applicable we need to prove we can create this material in large quantities with the same effectiveness."

Feng is also leading a small project with Massachusetts-based Radiation Monitoring Devices Inc. (RMD). "The project seeks to combine neutron discrimination and gamma identification in a single material," he says.

The RMD project leverages the triplet-harvesting plastic scintillators and another project, funded by the Department of Homeland Security's Domestic Nuclear Detection Office, that uses spectroscopy to identify gamma rays and their energy spectrum.

"I think the triplet-harvesting plastic scintillators project exemplifies the potential of LDRD investment," Doty says. "A small amount of money to pursue an offbeat idea has paid off immensely. I needed that space to test the feasibility before I was ready to seek outside funding." ■

STICK TO

Seals that connect the parts of an aircraft or satellite can't leak, ever. But getting some materials to bond for life is a challenge. Research into reliable glass-to-metal seals could have wide use in industrial design.

By Sue Major Holmes


GETHER

Components housed in stainless steel for protection against extreme environments seen in the aerospace and defense industries require paths for electricity to power them and communicate with them. Those paths in turn need a reliable insulation seal to prevent contact with the metal case that could short out the power and communication lines.

Strong bonds between materials for airtight, or hermetic, seals are crucial, and Sandia National Laboratories continues to advance how that's done.

Typically, material used to isolate electrical paths is either glass or a glass-ceramic composite. Work by Steve Dai, principal investigator for a project on bonding glass-ceramic to stainless steel, aims to develop fundamental science in materials and processing for high-performance and high-reliability glass/ceramic-to-metal seals. That scientific foundation then could be used in designing, developing and manufacturing next-generation seals.

Dai's team filed a provisional patent application in November for interfacial bonding oxides for glass-ceramic-to-metal seals.

A durable seal needs a strong chemical bond between the glass-ceramic and the metal and a close match of the coefficient of thermal expansion (CTE) between materials. The CTE defines how an object's size changes as temperatures change. A glass-ceramic with crystalline phases formed inside the original glass increases the CTE to better match the metal housing and reduce thermal stresses.

Since bonded glass-metals must be processed at very high temperatures, "we need to manage the thermal mismatch very carefully to make sure during any stage in the sealing process there's no tensile stress or tension on the glass that will cause a crack or unrecoverable separation from the metal housing," Dai says.

Advantages and disadvantages

A seal that's strong at high temperatures and pressures also has potential industrial uses, such as in fuel cells and aerospace or defense applications that operate in extreme environments.

Pure glass shrinks less in high temperatures than metal does. The mismatch causes metal to crimp, compressing the seal. That has both advantages and disadvantages. "The good thing is you don't have to have very good bonding because there's a lot of compression; the downside is that there could be too much compression, which could crack the glass over time," Dai says.

His team looked at making a chemical bond between metal and glass-ceramics, without adding steps to production, by establishing an interfacial bonding layer, a bridge material that bonds to both steel and glass. "It's very difficult because these are two very dissimilar materials, a piece of steel and a piece of glass-ceramic. They hardly share anything," Dai says.

Glass-to-metal seals are processed in an inert atmosphere devoid of oxygen because metal grabs oxygen from the atmosphere, leading to oxidation and rust. But the process contains an inherent contradiction: A metal bond to a glass-ceramic requires an oxide, so the interfacial bonding layer is really an interfacial oxide layer.

"That's the fundamental challenge, how do we do that?" Dai says. Some processes pre-oxidize the metal, but Sandia wanted to avoid that extra step.

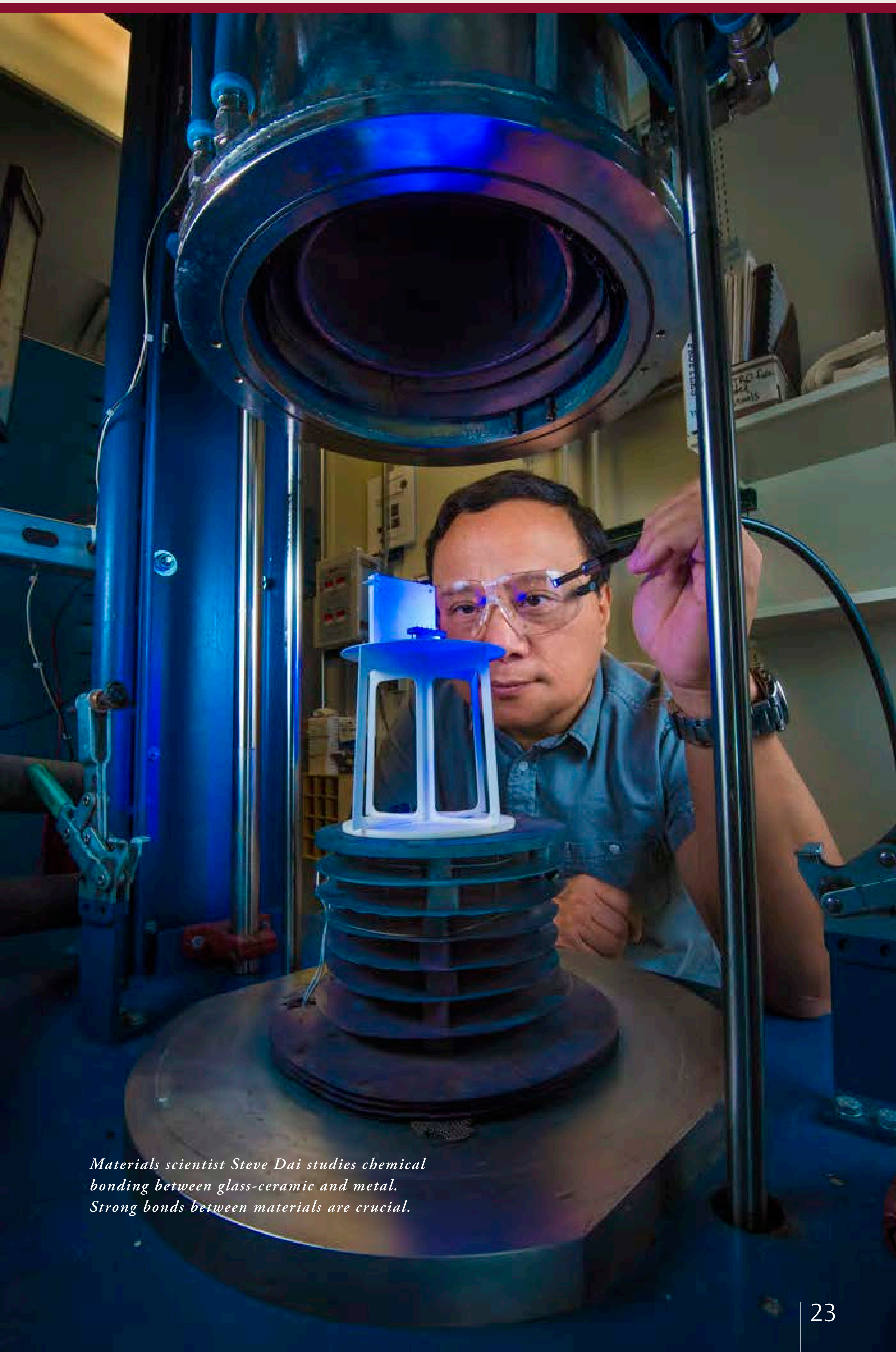
A bond that seals

Dai's thermodynamic approach modified, or doped, the glass-ceramic sealant with an oxidant. That oxidant, serving as a sacrificial metal oxide, decomposes and migrates at high temperatures, providing oxygen to oxidize the metal chromium in the stainless steel. The chromium oxide bond formed at the glass-ceramic and metal interface results in hermetic seals.

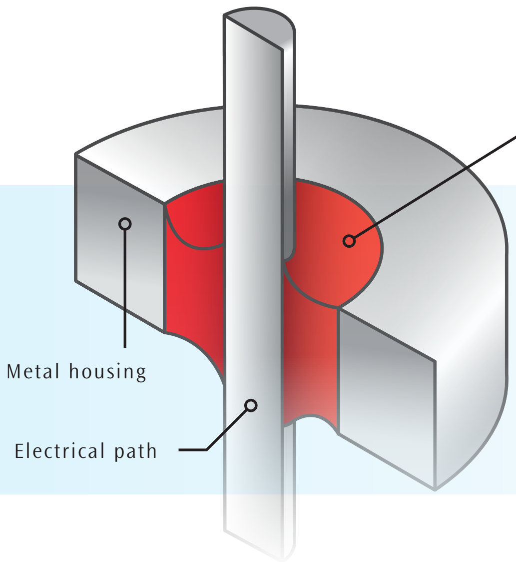
The team made 24 potential modified glass-ceramic compositions using a variety of metal oxides that were non-toxic and reasonably easy to handle, such as cobalt oxide. "Most of the work is really saying, 'OK, how many metals from the periodic table can we use and when we dope our glass with these sacrificial metal oxides, what quantity do we need to dope it?'" Dai says.

Researchers want the doped ceramic-glass material to give up oxygen at the interface, not at the surface of glass-ceramics. "The idea is giving up oxygen in the right place. That's kind of a fine line that has to do with the properties of the materials and the way you process them," Dai says.

The team identified two modified glass-ceramic compositions that worked best. Dai says they're not perfect, but they're a big step forward. "Basically we see a chemical bond between the glass-ceramic and the metal, and it's a very strong bond," he says. "If we break it, we break the glass."



Materials scientist Steve Dai studies chemical bonding between glass-ceramic and metal. Strong bonds between materials are crucial.



Electrical paths in components need a reliable insulation seal to the metal case that surrounds them. Sandia is working on a new glass-ceramic with linear expansion that is a better thermal match to the expansion of the metal case.

Sandia also developed a way to test both whether interfacial bonding is established and, if so, whether it's strong enough to ensure the glass won't break.

Thermodynamic competition

Other factors have to be considered. Without careful processing, the glass sticks to other surfaces as well as to the metal housing. To prevent that, the bonding process uses graphite for the fixtures that hold metal and glass-ceramic pieces while the bond is formed.

But graphite, like stainless steel, fights for oxygen.

"Essentially, that's a kind of competition thermodynamically," Dai says. "If my metal housing gets that oxygen to form the bond oxide, that's all I want. If the graphite grabs that oxygen, it doesn't do any good. That delicate balance of the reaction is very challenging."

The first two years of Dai's three-year Laboratory Directed Research and Development (LDRD) project centered on the bonding process. The final year studied how to control glass-ceramic crystallization to ensure the best thermal match. LDRD funding has ended, but the work continues with other funds because of its potential to aid production. Although the project wasn't aimed at an immediate application, researchers found a near-term opportunity to help a weapons production team with a better thermal match between glass-ceramic and metal.

Crystallization and temperature change

During sealing, glass-ceramic goes through a crystallization phase, which allows formation of a high-expansion crystalline phase, increasing the CTE of the glass-ceramic to better match high-CTE metals like stainless steel. However, because of the abrupt volume change associated with that crystalline phase, the glass-ceramic expansion is not well distributed over the temperature change that occurs during processing. Thus, the rate of thermal strain between the metal and glass-ceramic doesn't match.

The team was interested in managing the crystallization process by breaking it to form two or three high-expansion crystalline phases, with the abrupt volume changes in each phase occurring at temperatures several hundred degrees apart. The concept requires understanding what temperatures produce certain crystalline phases.

"We try to do two or more multiple crystallizations to smooth the thermal strain of the glass-ceramic," Dai says. "As a result, you no longer have this nonlinear, almost step-like strain change in the glass-ceramic. It's a more near-linear strain curve and matches a lot better to the metals."

Managing multiple crystallization phases at very high temperatures is challenging. "We need to learn that part of the process is to make sure we have a good balance of all the phases, have them all crystallize in the right sequence and ideally in the right proportion," Dai says. He believes the effort will result in a consistent way to improve hermetic seals.

His team is developing verification methods to see if the process works for production applications. Then researchers will study whether the process consistently produces the desired results.

"Once we reach that point," Dai says, "we will make sure the right specifications are in place and that the processed parts have certain properties so that the production agency can do the process on a continual basis using their equipment." ■

MEET Steve Dai

Steve Dai wants to play the guitar someday. He has always enjoyed music but never had the chance to learn an instrument. Guitar-playing along with his daily science and engineering "will get both sides of my brain going," he says.

Dai worked on a memorable project shortly after joining Sandia in 2009. The Early Career Laboratory Directed Research and Development (LDRD) program funded him to create a temperature-stable, low-temperature co-fired ceramics (LTCC) dielectric. LTCC boards are widely used to build radio frequency circuits. But LTCC dielectric properties change as operating temperatures change, causing circuit parameters to drift and require temperature compensation. The LDRD project formulated compensating dielectrics that were compatible with existing LTCC dielectrics and processes. The compensating dielectrics, when added to LTCC boards, led to temperature-stable microcircuits. A patent has been awarded for the innovative technology.

STATS

- Bachelor's in physics from East China Normal University
- Ph.D. in materials science and engineering from the University of Illinois, Urbana-Champaign
- Won Sandia "Up and Coming Innovators" award in 2014
- Spent 14 years with Motorola Labs in research and development on enabling ceramic technologies for wireless communication, microfluidics and haptics. Haptics is studying the sense of touch to provide realistic ways to interact. Dai won Motorola's 2005 Distinguished Innovator Award for having 10 U.S.-issued patents and was inducted into the company's Science Advisory Board Associates to the chief executive officer

Software simulates how things are made

By Neal Singer

Consider plastic wrap, certainly a humble enough kitchen item. Yet if you had to create it, how would you determine the force needed to coax the sheet into existence, and from exactly what bulk-material base so that the result would be transparent, unroll smoothly with no lumps or bumps and be strong enough not to tear when pulled (but not so strong it can't be cut)?

Without a computer program to do the heavy lifting of deciding among chemical and physical alternatives, you could be in for months, if not years, of trial-and-error testing.

Enter Goma 6.0, open-source software that simulates a wide variety of manufacturing processes. The creation of plastic wrap involves modeling an intricate interplay between energy, fluid flow and complex material response that helps determine the force needed to pull the wrap into existence. For this and other materials-processing problems, such as making flat-panel glass, producing reinforced materials for power lines and drying polymers, Goma 6.0 solves the underpinning equations of mass, momentum, energy and chemical transport.

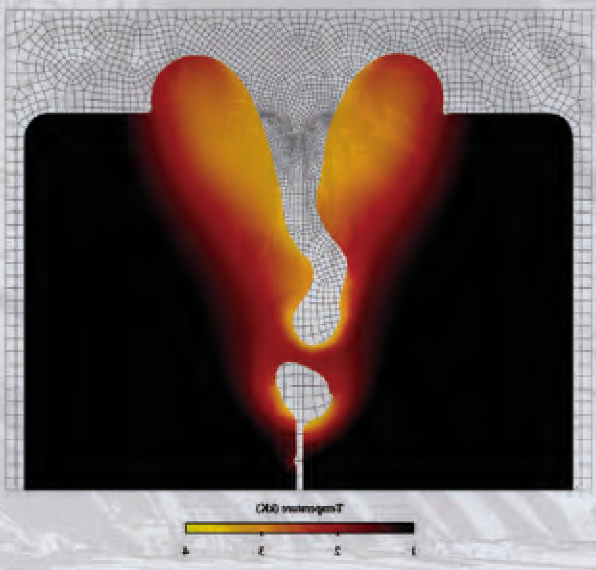
Goma has a long history of performing two- and three-dimensional analyses for a variety of applications, primarily in the coating and manufacturing industries, and was recently released as open-source software. The flexible program excels at problems in capillary hydrodynamics such as coating flows and liquid absorption by a porous material. The program also provides extensive models for polymer and metal processing.

Goma's ease of use makes it valuable to graduate students learning the benefits of code development for research. High-end analysts use it in topical manufacturing and related industries. "Goma 6.0 has a unique feature for those who need to add new physics, equations and material models to evaluate their process or product," says Sandia researcher Rekha Rao, one of the code originators. "Goma's source code is available, allowing easy exploration of new algorithms, physics and verification. And Goma takes advantage of parallel processing architectures."

The Goma team has developed collaborations with University of New Mexico; University of Texas; University of Illinois; University of Vermont; University of California, Berkeley; and Texas Tech University. Goma 6.0 attracted three new Cooperative Research and Development Agreement (CRADA) projects with industry, adding to the number of potential developers and users.

Goma capability development has been funded by a number of sponsors, including the Laboratory Directed Research and Development program, the National Nuclear Security Administration, the National Science Foundation, CRADA partners and others.

"Through open-sourcing Goma, we plan to help create the next generation of computational mechanics experts through a hands-on development process, and to educate the next generation of computational mechanics experts," Rao says. ■



Above, Goma produced a two-dimensional rendering of a laser keyhole weld showing areas where the microstructure of a part's metal is affected by the laser's heat. Laser keyhole welding helps weapons engineers create deep penetrating welds in heat-sensitive components with minimal damage to neighboring materials. The Goma simulation resolved a few hundred thousand unknowns. Below, Goma solves underpinning equations of mass, momentum, energy and chemical transport in materials-processing problems such as making flat-panel glass, shown here in a television screen.

Radiation-hardened circuits toughen up nuclear weapons

The microsystems fabrication complex at Sandia Labs draws on years of research to produce the radiation-hardened electronics critical to everything from nuclear weapons to satellites.

Ionizing radiation like that encountered in space interferes with the functioning of microchips found in such devices as automobile electronics, computers, satellites and nuclear weapons. Sandia has worked for decades to reduce the damaging effect of radiation on components.

Laboratory Directed Research and Development (LDRD) funded projects helped those efforts. "Everything we develop in the LDRD projects keeps our neurons going and then we have an 'ah-ha' moment in which we perceive ways to make our radiation-hardened technologies better," says Advanced Microelectronics and Radiation Effects manager Fred Sexton.

LDRD projects dating back to the 1990s helped position Sandia's Microsystems and Engineering Sciences Applications (MESA) complex to begin producing base wafers in 2014 for radiation-hardened Application-Specific Integrated Circuits (ASICs) for the B61-12 Life Extension Program, W88 Alteration 370 and W87 Mk21 Fuze Replacement nuclear weapons. MESA had produced and delivered more than 700 ASICs by September 2015. Sandia is slated to provide more than 25,000 radiation-hardened integrated circuits between fiscal years 2016 and 2025 for U.S. weapons modernization programs.

LDRD projects had a common goal: allow MESA to make better products, Sexton says. Projects between 1996 and 2007 analyzed a variety of materials to understand how to limit the damage from ionizing radiation and ensure weapons would survive over their life cycle. That led to two complementary approaches to protect microchips — designing radiation-hardened characteristics into the chip and applying special techniques during processing to mitigate radiation's damaging effects. The investments helped create ASICs technology for the W76-1 Life Extension Program and reduced development costs by more than $30 million.

"One of the things that made technologies hard enough to survive these huge amounts of radiation is the fact we moved from bulk wafers to a Silicon-On-Insulator wafer," Sexton says. A bulk wafer is the same all the way through, while a Silicon-On-Insulator wafer sandwiches a silicon dioxide layer between two silicon layers. Sexton says keys to hardening the wafer lie in the structure and in the silicon dioxide layer that cuts down on the charge generated when a cosmic ray, a proton or a neutron hits a part. "So those give us some immunity to single-event upsets where a high-energy particle comes into a circuit," he says.

Sexton says Sandia's success in producing strategic radiation-hardened components was fueled by a need to ensure the deterrent value of the nuclear weapon stockpile. "As we continue to modernize the stockpile and develop new microsystem technologies, Sandia will need new ways to mitigate the threat caused by man-made and natural radiation environments," he says. ■

— Sue Major Holmes

MEET

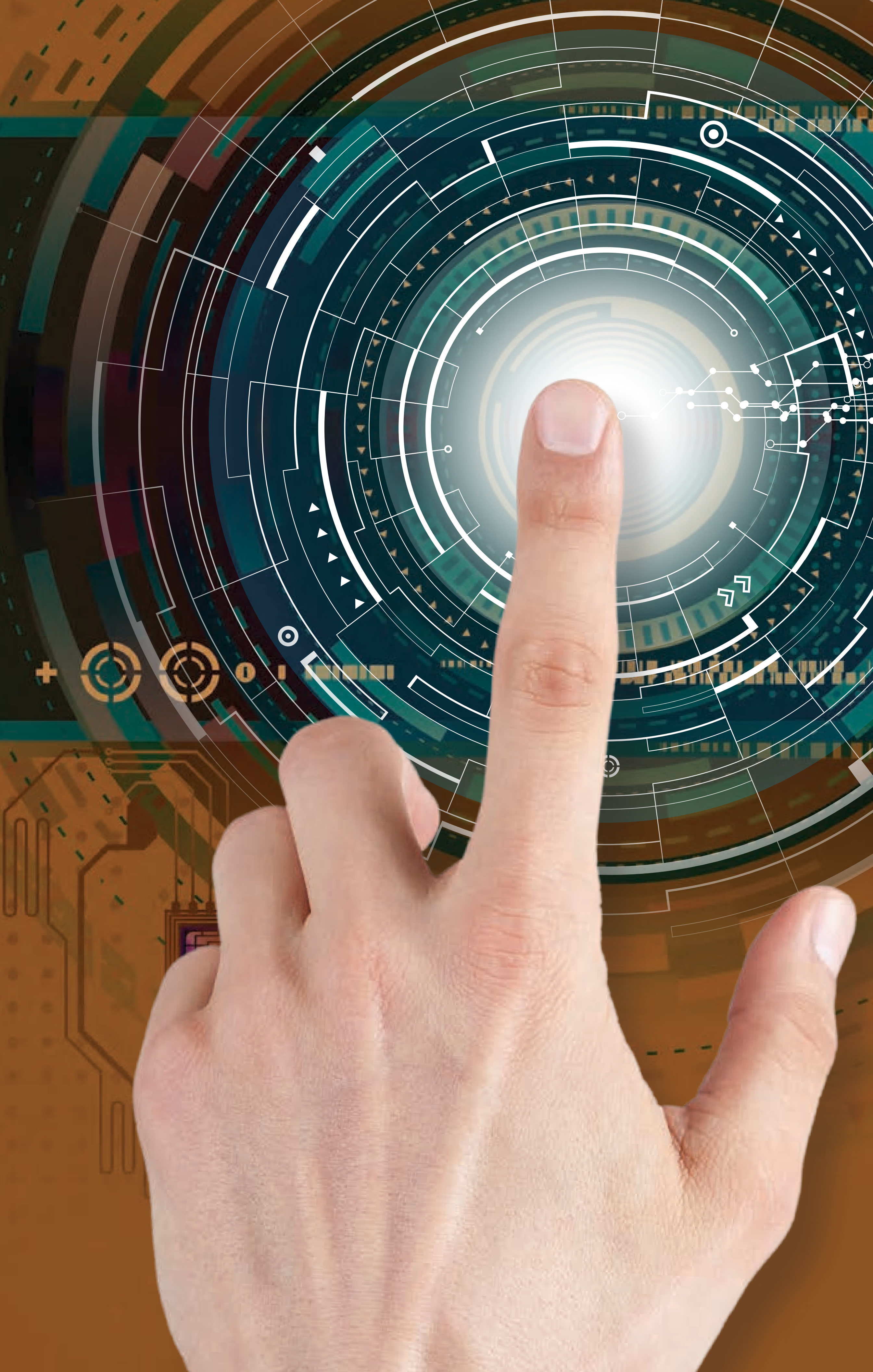
Nedra Bonal

As a high school junior in Houston, Texas, Nedra Bonal, unlike her classmates, had no idea what she wanted to do in life. Then her physics teacher assigned the class to research physics-based careers. "I saw geophysics and was interested because I'd always liked rocks," Bonal says. "It got me thinking." She went to a community college with an undeclared major and heard about the New Mexico Institute of Mining and Technology in a geology course. She transferred there as a geology major but wasn't sure she was up to the challenge of geophysics. "I was intimidated," she says. "It's tough." But she forged into the field and graduated with a geophysics degree. Bonal worked in industry in Texas a couple years then returned to school for a doctorate in geophysics. Marriage brought her back to New Mexico and to a postdoc position at Sandia. She was hired in 2007.

Bonal got an Early Career Laboratory Directed Research and Development (LDRD) project looking at the effects of saturation in the pore spaces around tunnels on seismic waves. She's now working on an LDRD project using muons, elementary particles similar to electrons, to see inside the Earth, like an X-ray, an emerging technology that also has the potential to improve identification of clandestine underground activity. "It has been an exciting project and totally different from other areas I've worked in," says Bonal, who in her spare time promotes STEM (Science, Technology, Engineering and Math) education to young girls through Expanding Your Horizons. "It's fun and educational. I like that my work at Sandia has an impact on national security."

STATS

- Bachelor of Science in geophysics from New Mexico Institute of Mining and Technology
- Ph.D. in geophysics from the University of Texas, Austin
- Member of the American Geophysical Union and the Engineering and Environmental Geophysics Society



SWITCHED ON

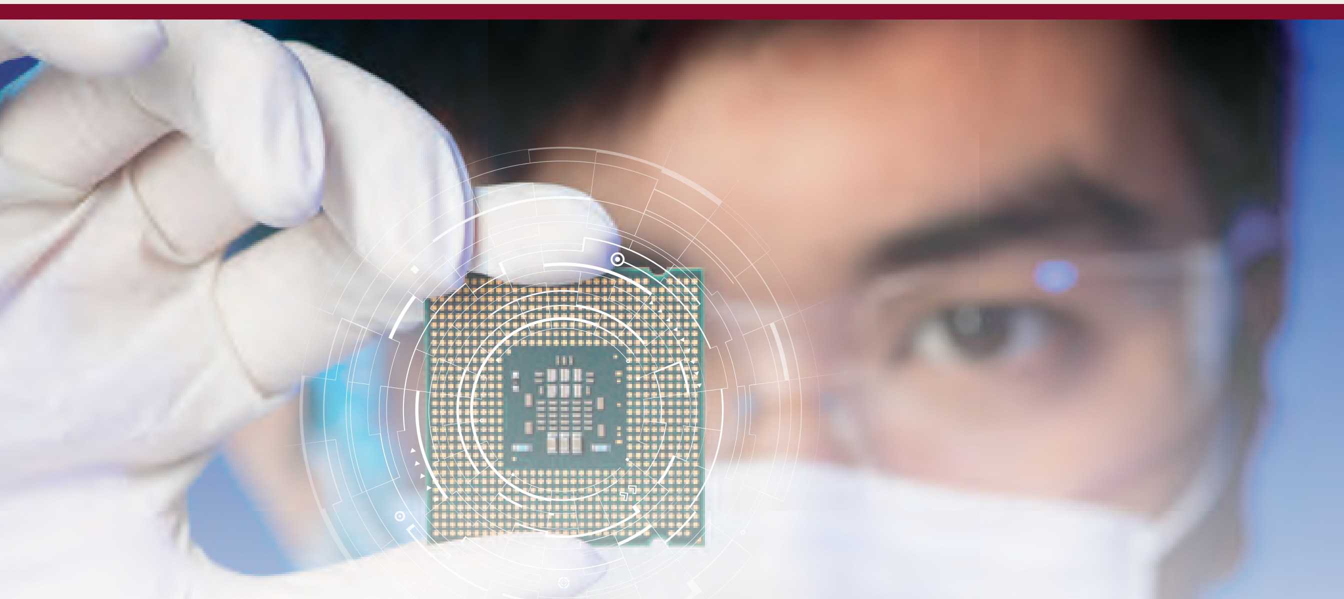
BY NANCY SALEM

Silicon has long been the go-to material for semiconductors that power the electronic world. Now scientists are looking far beyond that omnipresent element to materials that could make everything from computers to power grids to electric cars more mighty and energy efficient.

Electrical power doesn't travel a one-way street. In a technology called power electronics, it is converted from one form to another when you plug in a computer, drive a car or flip on a light.

"Power electronics use semiconductor devices such as transistors, diodes and thyristors to control the flow of electrical energy by switching electronic circuits," says Sandia electrical engineer Bob Kaplar, who is leading a Laboratory Directed Research and Development project exploring new, more powerful and energy-efficient semiconductor materials. "If you want to convert a direct current, or DC, signal into an alternating current, or AC, signal, the actual circuit that does that is complex. But the basic idea is to turn the DC signal on and off."

Semiconductor devices are switching systems that convert voltages and currents. The switches have been made of silicon since about the 1950s when semiconductors were first developed, replacing in many applications power conversion that uses



transformers, or coils of wire around magnetic cores. Silicon is at the center of all microprocessors, computer chips, cell phones and more. “Silicon is the core material that the device that functions as a switch is made of,” Kaplar says. “When semiconductor devices were invented, people started making big transistors that could handle large amounts of power.”

Because power electronics process substantial amounts of electrical energy, and energy is lost when power is converted, there has been a move over the past decade to replace silicon with other materials that would be more energy efficient. “The more you can reduce the loss, the better the energy efficiency,” Kaplar says. “Power electronics had been viewed as a not-so-exciting area in the past. But now there is a resurgent interest in it.”

Bandgaps and energy

The new semiconductor materials are referred to as wide bandgap. Bandgap, a fundamental materials property, is an energy range in a solid where no electron states can exist. In the electronic band structure of solids, the bandgap generally refers to the energy difference in electron volts between the top of the valence band and the bottom of the conduction band in insulators and semiconductors. If the valence band is full and the conduction band is empty, electrons cannot move in the solid. But if some electrons transfer from the valence to the conduction band, then current can flow. So bandgap is a major factor determining the electrical conductivity of a solid.

Wide bandgap refers to higher-voltage electronic bandgaps significantly larger than one electron volt (eV), typically at least three eV. The bandgap of silicon is 1.1 eV and gallium arsenide, another common semiconductor material, is 1.4 eV. Wide bandgap semiconductor materials such as silicon carbide (SiC) and gallium nitride (GaN) allow devices to operate at much higher voltages, frequencies and temperatures than the conventional materials, so more powerful, cheaper and more energy-efficient electrical conversion systems can be built.

Wide bandgaps have already revolutionized lighting, particularly in the area of light-emitting diodes, or LEDs, which are widely available and are replacing incandescent and fluorescent bulbs. 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 for elevators and HVAC systems, and even computer power supplies. Smaller, faster switches mean less loss of power. “Faster switching also means you can make other parts of the circuit smaller, such as capacitors and inductors,” Kaplar says.

Wide bandgap has the potential to substantially reduce the estimated 10 percent energy loss between generating electricity and transmitting it into a home or business. “In a decade or two, the giant transformers in your neighborhood distributing power from the electric grid to homes, which now weigh 10,000 pounds, could be replaced by things the size of a suitcase that weigh 100 pounds,” says Sandia Fellow and materials scientist Jerry Simmons.

And if electric vehicles could tap the potential for wide bandgap 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. “There are non-civilian applications as well,” Kaplar says. “The military wants small power converters on unmanned aerial vehicles, and the Navy is interested in electric ships. You want as much power as you can get in a confined space. These advantages are pretty universal.”

Sandia is researching SiC and GaN, but it's also working to leapfrog over these next-generation materials to the generation-after-next, ultra-wide bandgap materials such as aluminum nitride (AlN), which has a bandgap of 6.2 eV. The Ultra-Wide Bandgap Power Electronics Grand Challenge LDRD project that Kaplar is leading is at the end of its first year. Grand Challenges are three-year LDRD projects that focus on bold, high-risk ideas with potential for significant national impact.

Taking small steps

"Potential benefits like shrinking system size and high-temperature operation become even greater with ultra-wide bandgap materials," Kaplar says. "We're also interested in other harsh environments. There the challenges become greater."

AlN and GaN are compatible enough to be mixed. That allows researchers to take small steps toward developing AlN by gradually increasing the amount of AlN versus GaN to study behavior and the effect of lattice mismatch between the semiconductor and the material it's grown on, Kaplar says.

Estimates predict SiC could perform 100 times better than silicon for power switching, GaN could be 1,000 times better than silicon, and AlN could be 10,000 times better than silicon. However, their potential can't be tapped until researchers better understand how the materials work, develop mature techniques to process them and address reliability concerns, particularly for high-consequence uses.

Lots of energy in a small package

The Ultra-Wide Bandgap Grand Challenge is the flagship LDRD project for Sandia's Power on Demand Research Challenge aimed at developing electrical power systems with the smallest size and weight, while handling the largest possible amount of energy. The research challenge tackles underlying fundamental science questions, engineering applications and technical challenges for devices, materials growth and power systems.

The Grand Challenge covers three areas: materials growth; device design, fabrication and testing (including demonstration of efficient switching); and defects and radiation resistance. It's exploring ways to grow ultra-wide bandgap materials with fewer defects and different device designs to exploit the properties of materials other than silicon.

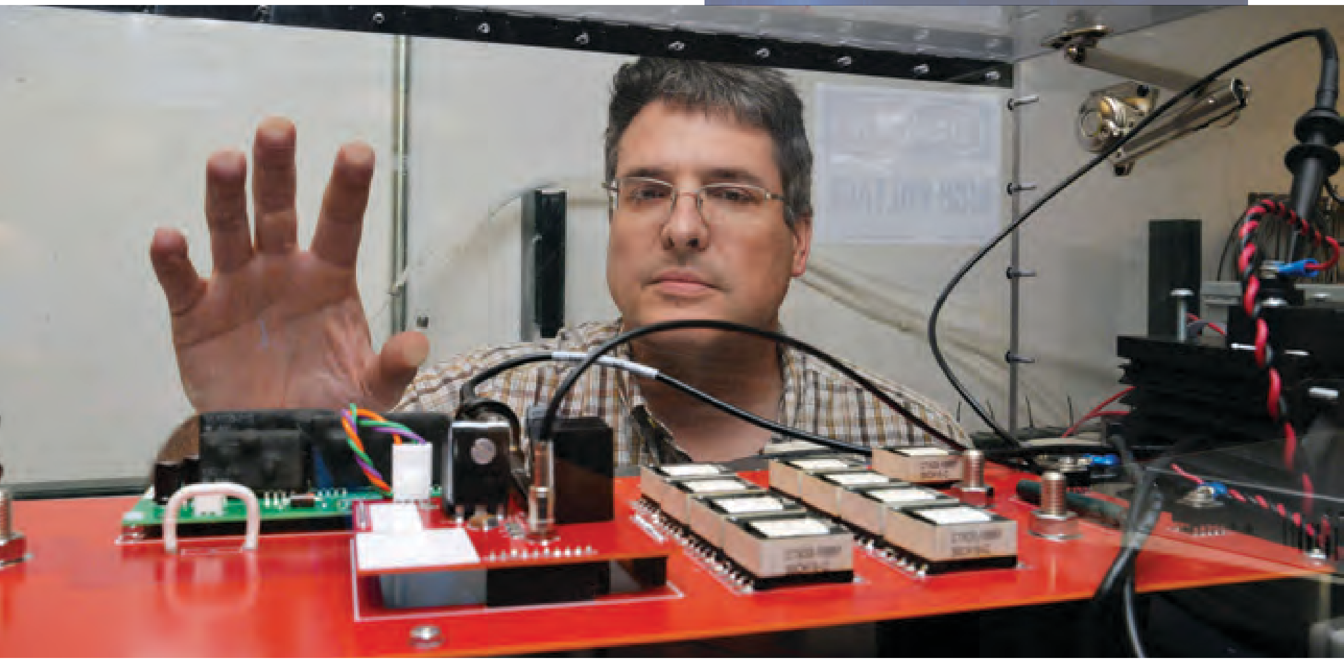
Although some devices using SiC and GaN are on the market, thorny problems remain, Kaplar says. Common performance issues include defects, incompatibility with the microelectronics substrates on which the materials are grown and the impact of integrating a device into a larger system. Sandia researchers can evaluate those problems impartially, building on expertise from decades of nuclear weapons work.

The downside to wide and ultra-wide bandgap technology is that it is not as mature as the silicon industry, which has a huge manufacturing infrastructure. "It's easy to control the properties of silicon and related materials," Kaplar says. "People know how to process those really, really well."

Researchers are not at the point of making a power converter out of ultra-wide bandgap materials but envision such a device several years down the road.

WHY SWITCH?

Different methods exist to convert electrical energy from one form to another. For example, direct current (DC, or constant) voltage can be converted to a lower DC voltage by connecting two resistors in a series arrangement known as a voltage divider. But that method of conversion is inefficient and wastes much of the power as heat. An alternative approach is to switch the DC voltage on and off, and take the average of the resulting on-off-on signal. That switching approach is known as power electronics and is much more efficient, so that little power is wasted as heat. The switching approach also allows for a wider variety of types of power conversion, for example, from a lower DC voltage to a higher DC voltage, from DC to alternating current (AC), from AC to DC or from one AC frequency to another.



Electrical engineer Bob Kaplar checks out a test circuit built under a Grand Challenge Laboratory Directed Research and Development project to evaluate the switching performance of wide bandgap and ultra-wide bandgap power semiconductor devices.

"At the circuit level we're characterizing the devices, measuring how much voltage we can put across before it goes into breakdown and how fast the switching transient is when we turn it on and off," Kaplar says. "We have voltage targets for the devices we're building. We can see all the pieces fitting together and moving toward the devices and circuit demonstrations."

About 50 scientists are working on the Ultra-Wide Bandgap Power Electronics Grand Challenge, and Kaplar hopes the research will continue when the challenge ends. "This is forefront materials science," he says. "This is a brand new field to go beyond the wide bandgap materials, and not many people are working on it. The impact potential is huge."

MEET Kathy Simonson

Kathy Simonson is the rare applied scientist who went to a liberal arts college. "There aren't many of us at Sandia," she laughs. "But it was great because it encouraged me to learn a broad spectrum of things." At Middlebury College in Vermont, Simonson majored in math and had to pick a minor in a different educational division. She went with modern literature. "I have found throughout my career as a scientist that all the writing courses I took for the literature minor have been tremendously helpful," she says.

Simonson, who grew up in a small New England town, went on to Princeton University where she earned a master's and doctorate in statistics. She envisioned a life on the East Coast, and had a job offer in Cambridge, Massachusetts, but a Sandia recruiter invited her to Albuquerque. She jumped at the chance to see the West — and pick up airline miles. "I didn't know much about it," she says. "I got here and absolutely loved it."

Twenty-six years later, Simonson's Sandia research focuses on developing statistical and mathematical techniques for analyzing data from a variety of sources for national security applications such as intrusion detection and military surveillance, looking for interesting patterns. "It's puzzle-solving," she says. Simonson has worked on five Laboratory Directed Research and Development (LDRD) projects involving techniques of automated image registration with uncertainty assessment, detecting anomalies in fast-framing video data, working with synthetic aperture radar data, and researching advanced data analytics. She's now heading an LDRD project looking at hybrid classifiers using statistics and machine learning. "The variety of work here has been amazing," she says. "It's been a fascinating career."

STATS

- Bachelor of Arts in math from Middlebury College
- Master of Arts and Ph.D. in statistics from Princeton University
- Patents for her work in automated image registration with uncertainty assessment and detecting anomalies in fast-framing staring video data

WeaselBoard sends cyberattackers packing

By Stephanie Holinka

When you own or manage a critical infrastructure or component of one, such as a power plant or oil refinery, a day with a zero-day exploit is a horrible, no good, very bad day.

It means someone has compromised the most fundamental level of your system, allowing a potential evildoer access to all the things you've been attempting to protect, such as your manufacturing machinery, solar array, microgrid or nuclear power plant. And you have zero days to fix it before it's too late.

In other words, it's already too late. Sandia's WeaselBoard, developed in a Laboratory Directed Research and Development project, helps critical infrastructure owners protect their systems against zero-day exploits. It is a small card that plugs into the backplane of an industrial controller, where a computer's main circuit boards connect, to detect illicit traffic. WeaselBoard creates an assurance platform for responding to attacks as systems network together and scale up in the future.

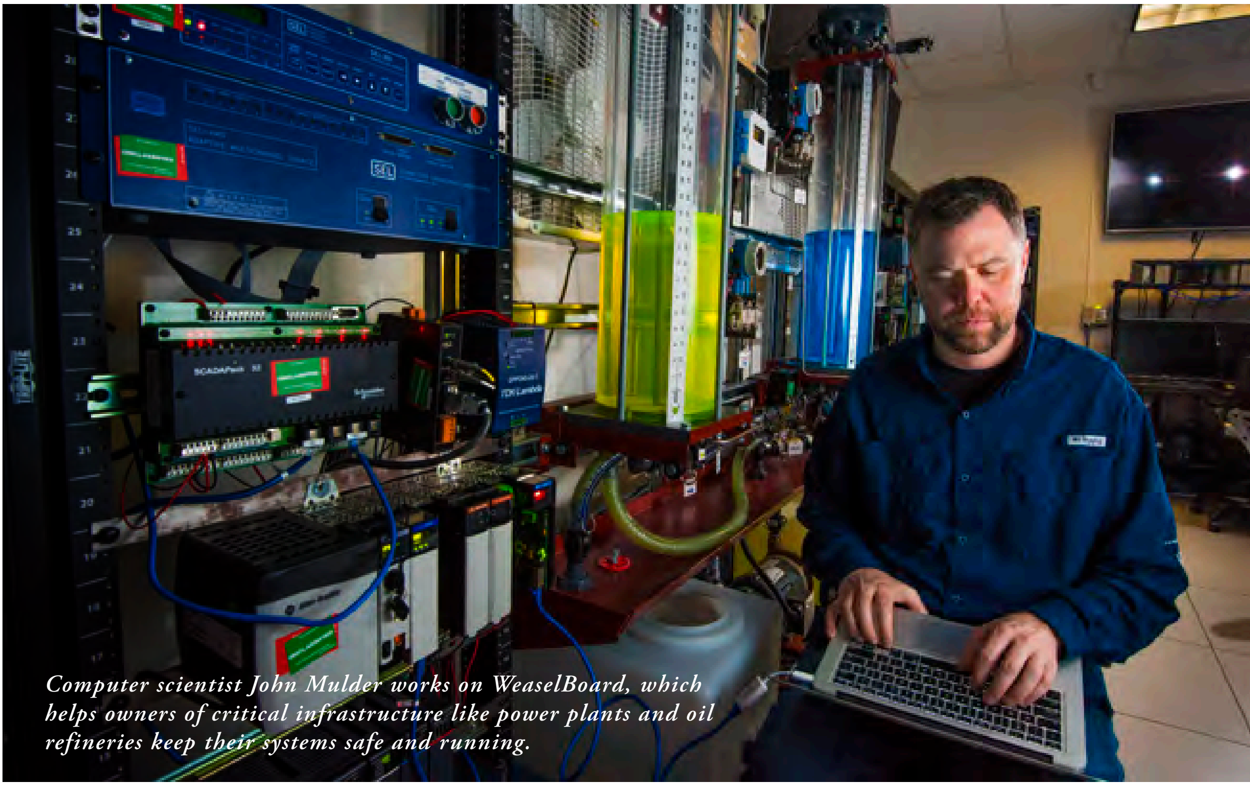
To regulate essential processes, critical infrastructures like those including electric power plants and oil refineries rely on industrial controls, referred to as a primary logic controller (PLC) in industry and supervisory control and data acquisition (SCADA) in government systems.

PLCs and SCADA systems control billions of dollars of production, manufacturing and utility equipment in the United States. They must be always accessible, and any cyberattack could result in lost uptime, costly equipment damage and even casualties among operating personnel. And most industrial control processes are unprotected.

“Most machines weren’t initially designed to be networked together, so industrial control systems were not designed with security in mind,” says Sandia principal investigator John Mulder.

firmware updates and process control program (logic) updates. It forwards inter-module traffic to an external analysis system that detects changes. The analysis workstation then extracts fields at each protocol layer.

These fields are tested using mechanisms to identify malicious behavior — a rule set and a machine-learning algorithm. The rules-based mechanism causes an alert when predetermined behavior is seen, and can be customized to process-specific limits.



Computer scientist John Mulder works on WeaselBoard, which helps owners of critical infrastructure like power plants and oil refineries keep their systems safe and running.

Most attacks on control systems focus on network communications and computer software, so industrial control systems, which are at the hardware or firmware level, are not often monitored for security compromise.

“Because industrial control systems aren’t monitored routinely, current industry practice forces critical infrastructure owners to wait for the zero-day exploit before they know something is wrong. This means that owners can only react to malicious attacks after the damage has occurred,” Mulder says.

WeaselBoard works by detecting changes in the controllers and its processes, such as control settings, sensor values, module configuration information,

“WeaselBoard allows operators to detect compromises as they are in progress because it alerts on the effects of the attack in progress and not on signatures of previously catalogued attacks,” Mulder says. “This allows zero-day exploits to be detected, unlike systems using signature-based detection methods.”

Highlighting WeaselBoard’s potential use for many types of cyber-physical systems, Juan Torres, a senior manager for Renewable Energy Technologies, took the technology to Capitol Hill as part of the Grid Modernization Lab Consortium discussion on security and resilience.

“WeaselBoard is an example of cyber technology that Sandia developed with potential application to energy systems,” Torres said. ■

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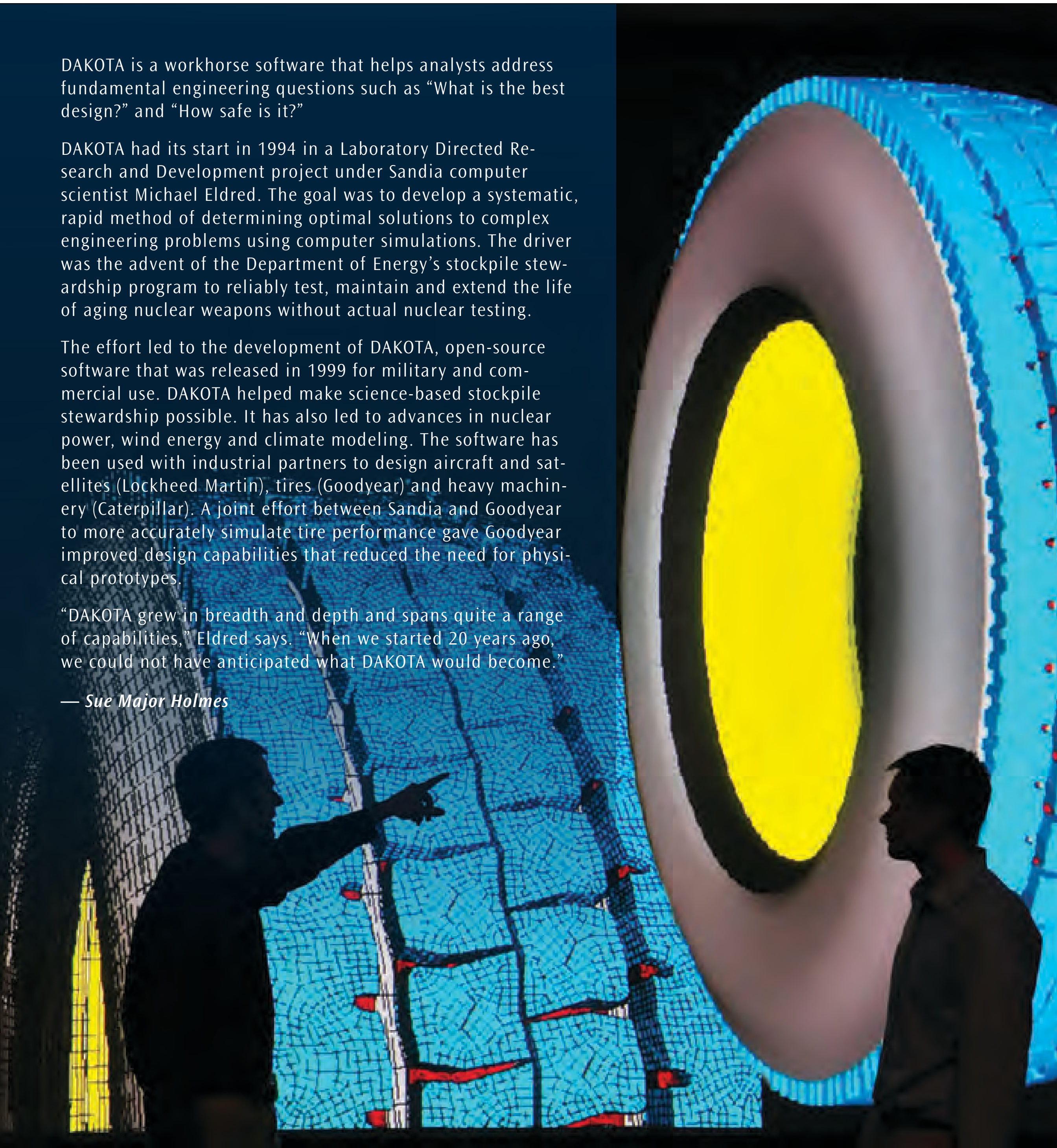

DAKOTA is a workhorse software that helps analysts address fundamental engineering questions such as "What is the best design?" and "How safe is it?"

DAKOTA had its start in 1994 in a Laboratory Directed Research and Development project under Sandia computer scientist Michael Eldred. The goal was to develop a systematic, rapid method of determining optimal solutions to complex engineering problems using computer simulations. The driver was the advent of the Department of Energy's stockpile stewardship program to reliably test, maintain and extend the life of aging nuclear weapons without actual nuclear testing.

The effort led to the development of DAKOTA, open-source software that was released in 1999 for military and commercial use. DAKOTA helped make science-based stockpile stewardship possible. It has also led to advances in nuclear power, wind energy and climate modeling. The software has been used with industrial partners to design aircraft and satellites (Lockheed Martin), tires (Goodyear) and heavy machinery (Caterpillar). A joint effort between Sandia and Goodyear to more accurately simulate tire performance gave Goodyear improved design capabilities that reduced the need for physical prototypes.

"DAKOTA grew in breadth and depth and spans quite a range of capabilities," Eldred says. "When we started 20 years ago, we could not have anticipated what DAKOTA would become."

— ***Sue Major Holmes***