OAK RIDGE NATIONAL LABORATORY

Review

Smile!

OAK RIDGE National Laboratory

Vol. 50 | No. 3 | 2017
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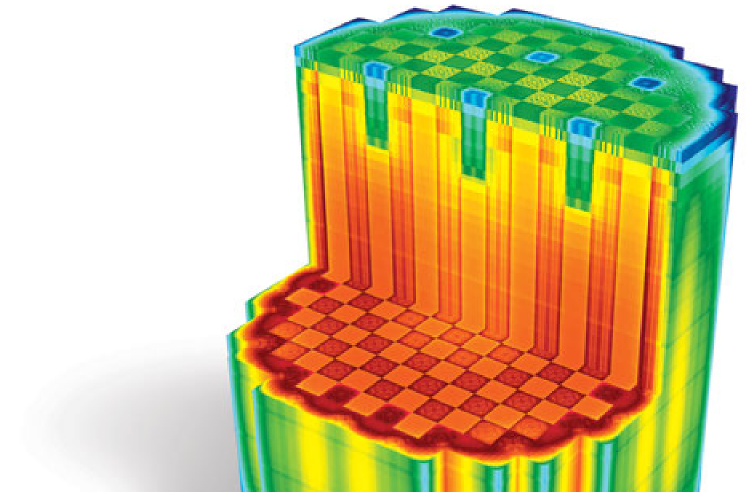


On the Cover

Hector Santos-Villalobos of ORNL's Imaging, Signals, and Machine Learning Group is working on photo technologies to advance identity science.

Science and security

The science of national security is not fundamentally different from science applied to other mission needs.

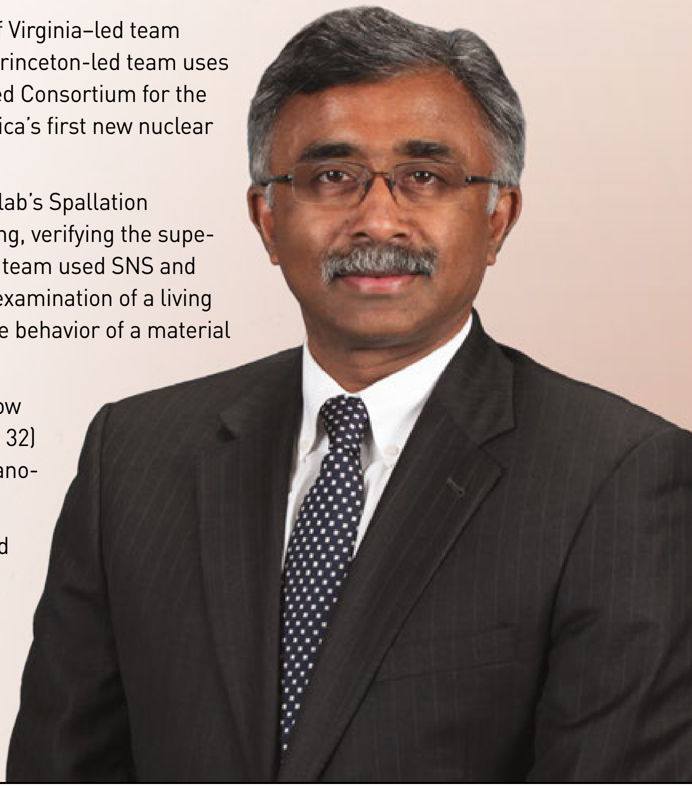
Nuclear science paves the way for abundant electricity, but it also provides tools to stop the production and smuggling of dangerous materials. Advances in data analysis open the way to more productive physical experiments, but they also strengthen cybersecurity and protect the nation's power grid.

Indeed, the biggest difference may simply be the stakes that necessarily accompany national security applications. The development of new materials to better cool consumer electronics is desirable, but that same improvement applied to military equipment can easily mean the difference between life and death for soldiers in a desert war zone.

Because fundamental science is at the core of ORNL's broad research portfolio, the laboratory has been the source of a variety of applications that make our nation more safe and secure. In this issue of *ORNL Review*, we look at ways our expertise in areas such as materials research, genetics, computing and nuclear science is translated into innovations that protect service members and citizens alike (Page 8).

We also look at technologies that can identify individuals from photographs taken under a wide variety of challenging circumstances (Page 13), other technologies that re-create a person's facial structure based on nothing more than a DNA sample (Page 15), and a sophisticated range of approaches to keep the electric grid secure (Page 24).

ORNL's national security programs also have a strong educational element; in this issue we introduce you to four active service members who have come to the lab to further their educations and learn about the work we do here (Page 9).



Supercomputing is well represented in this issue. In one story a University of Virginia–led team pushes the boundaries of laser-modified materials (Page 18). In another a Princeton-led team uses earthquake data to map the Earth's interior (Page 16). In a third the ORNL-led Consortium for the Advanced Simulation of Light Water Reactors simulates the startup of America's first new nuclear power reactor in two decades (Page 20).

We focus on neutron science in several stories. ORNL researchers used the lab's Spallation Neutron Source to analyze an internal combustion engine while it was running, verifying the superiority of a cerium-aluminum alloy developed here (Page 26). Another ORNL team used SNS and ORNL's High Flux Isotope Reactor to provide the first-ever direct nanoscale examination of a living cell membrane (Page 30). And a third used neutron scattering to examine the behavior of a material that could enable advanced quantum computing (Page 28).

Materials research takes the lead in two other stories, one demonstrating how earlier research into ceramic matrix composite materials is paying off (Page 32) and another describing work that advances our understanding of polymer nanocomposites (Page 34).

Also in this issue we hear from award-winning *New York Times* columnist and author Thomas Friedman on the impact that technology has and will have in our lives (Page 36) and meet a few of the grad students and postdocs at ORNL who represent the future of science and innovation (Page 38). Finally, our look back at a chapter in ORNL's past details our relationship with Adm. Hyman Rickover, the father of the nuclear Navy (Page 40).

I hope you enjoy this issue of *ORNL Review*.

Thomas Zacharia
Laboratory Director

Zacharia takes over as director of ORNL

Thomas Zacharia, who built ORNL into a global supercomputing power, became the laboratory's director July 1 after being selected for the position by UT-Battelle, the partnership that operates ORNL for DOE.

He replaces Thom Mason, who has joined Battelle Memorial Institute after 10 years leading ORNL.

"Thomas has a compelling vision for the future of ORNL that is directly aligned with the U.S. Department of Energy's strategic priorities," said Joe DiPietro, chair of the UT-Battelle Board of Governors and president of the University of Tennessee.

"He has led many of the innovative research and development initiatives that ORNL has successfully pursued over the past decade. His background in materials and computing positions him well to strengthen ORNL's signature research capabilities in computational, neutron, materials, and nuclear science. His vision of ORNL playing a prominent role in advancing U.S. national and energy security reflects his leadership strengths. He has been key to the success of developing joint academic programs with UT. Finally, he embraces diversity and has a passion for developing and strengthening the workforce at the laboratory."

Zacharia came to ORNL in 1987 as a postdoctoral researcher after receiving his Ph.D. in engineering science from Clarkson University in New York. When UT-Battelle became ORNL's management and operating contractor in April 2000, Zacharia was director of the Computer Science and Mathematics Division.

In 2001 he was named associate laboratory director for the new Computing and Computational Sciences Directorate, and over the next eight years he built a scientific enterprise that brought more than 500 new staff to Oak Ridge and opened the nation's largest unclassified scientific computing center, the Oak Ridge Leadership Computing Facility, a user facility of DOE's Office of Science.

ORNL Laboratory Director Thomas Zacharia. Image credit: Jason Richards, ORNL

Zacharia was named ORNL's deputy for science and technology in 2009, responsible for the lab's entire research and development portfolio. During his tenure the lab strengthened its translational energy programs, establishing the Nuclear Science and Engineering Directorate and the Energy and Environmental Sciences Directorate.

"Thomas represents the very best of Oak Ridge National Laboratory: scientific excellence, a willingness to tackle tremendous challenges for the benefit of the nation, and the vision to find innovative solutions and make them reality," said Jeff Wadsworth, president and CEO of Battelle and director of ORNL from 2003 to 2007. "His whole career shows that he knows how to apply ORNL's unique breadth of expertise to our most important priorities in science, energy, national security, and economic competitiveness."

In 2012 Zacharia took a leave to serve as executive vice president of the Qatar Foundation for Education, Science and Community Development, overseeing research in energy and the environment, information and computing technology, life sciences and biomedical research, and social sciences, as well as leading the country's science and technology park, which is home to more than 40 multinational companies including GE, Microsoft and Siemens. He returned to ORNL in 2015.—*David Keim*

For more information: https://go.usa.gov/xNerp

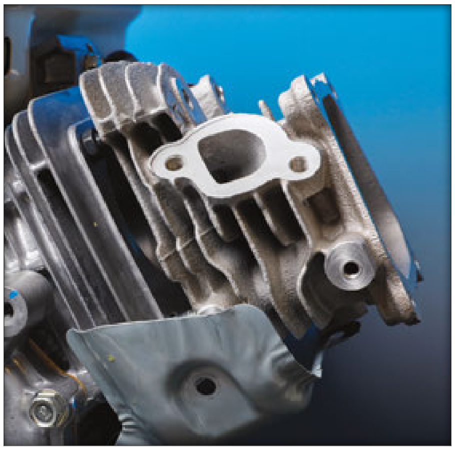
Eck Industries licenses promising new alloy

Wisconsin's Eck Industries has signed an exclusive license for the commercialization of a aluminum-cerium alloy codeveloped by ORNL that is ideal for creating lightweight, strong components for advanced vehicles and airplanes.

The patent-pending alloy was developed as part of DOE's Critical Materials Institute and makes use of cerium, the most abundant rare earth element. Cerium makes up as much as half of mined rare earths, yet has less value than other rare earth elements such as neodymium and dysprosium that are in high demand for advanced energy technology applications. Creating new uses for cerium supports both domestic rare earth mining operations and the U.S. manufacturing sector.

Scientists at ORNL, working with Eck Industries and researchers at DOE's Ames and Lawrence Livermore national laboratories, developed the Ce-Al alloy, which is easy to work with, lightweight, corrosion-resistant, and exceptionally stable at high temperatures—making it ideal for automotive, aerospace, power generation, and other applications.

Testing has shown the Ce-Al alloy is stable at 500 degrees Celsius. Withstanding higher temperatures means, for instance, that engines made using the



The cerium–aluminum alloy developed by scientists at ORNL, Eck industries and Ames and Lawrence Livermore national laboratories is ideal for automotive and other applications. Image credit: Carlos Jones, ORNL alloy can run hotter with more complete fuel combustion while being lighter in weight, which advances fuel efficiency.

Ce-Al does not require additional thermal processing during the casting process and takes advantage of abundant, low-cost cerium, said ORNL materials scientist Orlando Rios. Casting with the alloy can be accomplished using standard aluminum foundry practices and without a protective atmosphere.

"The alloy is thermodynamically stable," Rios said. The cost of heat treatment and the additional machining required due to thermal distortion can make up some 50 to 60 percent of the cost of casting traditional alloys. Energy costs could potentially be reduced by 30 to 60 percent compared with traditional casting processes, he noted. The Ce-Al alloy's potential marks a significant departure from post-casting heat treatment and age-hardening approaches developed over some 100 years and can significantly advance manufacturing competitiveness as a result, Rios added.—*Stephanie Seay*

For more information: https://go.usa.gov/xNzDK

ORNL, UT launch Ph.D. data program

The Tennessee Higher Education Commission has approved a new doctoral program in data science and engineering as part of the Bredesen Center for Interdisciplinary Research and Graduate Education.

The Bredesen Center combines resources and capabilities from the University of Tennessee and ORNL to promote advanced research and to provide innovative solutions to global challenges in energy, engineering and computation.

The new program is the brainchild of ORNL Computational Sciences and Engineering Division Director Shaun Gleason, UT Business Analytics Associate Professor Russell Zaretzki, and Bredesen Center Director Lee Riedinger. It will bring new doctoral students from some of the world's top institutions to East Tennessee for an in-depth education in data science as it applies to specific scientific domains.

The massive amounts of data gathered via cellphones, tablets, sensors and other devices, along with the enormous datasets generated at leading scientific facilities such as ORNL's Spallation Neutron Source, Manufacturing Demonstration Facility, and Oak Ridge Leadership Computing Facility pose a unique set of challenges and opportunities for researchers across the scientific spectrum. Creating a new generation of graduates with an enhanced understanding of how to manage and analyze this data could greatly expedite research breakthroughs and provide novel solutions to long-standing problems. For example, electronic health records, when analyzed en masse, could reveal better and cheaper ways to treat patients, and the combination of cell phones, GPS technology and traffic sensor data will allow researchers to optimize traffic flow and assist city planners in responding to emergencies more quickly and effectively. Researchers who use scientific facilities such as SNS, which provides the most intense pulsed neutron beams in the world for research and industrial development, will benefit from the ability to analyze data on the fly.

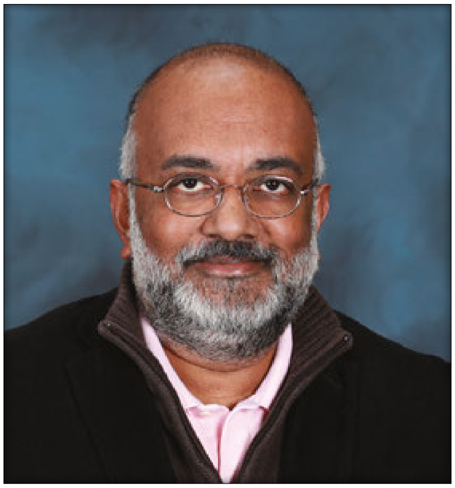
The curriculum will seek to integrate candidates' data science education with seven scientific domains: health and biological sciences, advanced manufacturing, materials science, environmental and climate science, transportation science, national security, and urban systems science. Candidates will work alongside ORNL and UT researchers and earn a doctorate tied to a specific scientific specialty.—*Scott Jones*

For more information: https://go.usa.gov/xNzNX

ORNL-UT welcome new Governor's Chair

Easo George, one of the world's foremost authorities on advanced alloy development and theory, has been named the 15th Governor's Chair of ORNL and the University of Tennessee.

George comes from Ruhr University Bochum in Germany, where he was professor of materials design and director



UT Governor's Chair Easo George. Image credit: Jason Richards, ORNL

of the Center for Interface Dominated High Performance Materials since November 2014. Prior to that he had a nearly three-decades-long career at ORNL, where he was a distinguished research staff member and head of the Alloy Behavior and Design Group. He was also a professor of materials science and engineering at UT.

"I am honored to have been chosen for this position," George said. "There is already tremendous synergy between ORNL and UT in advancing materials research, and I cannot wait to help build even more momentum."

George's research areas include high-entropy alloys, small-scale mechanical behavior of crystalline and amorphous materials, refractory and precious metals for space power applications, mechanical behavior at extremes of temperature and strain rate, and environmental effects on microstructure and mechanical properties.

His hiring is the latest sign of the growing emphasis on materials research at ORNL and UT. His expertise in advanced alloys is critical to the understanding and development of new materials that could be used in everything from energy programs to flight applications. As manufacturers continue to focus on stronger, lighter materials, they will also increasingly rely on research done by scientists like George.—*ORNL staff*

For more information: https://go.usa.gov/xNeY4

Buchanan named ORNL deputy for science and tech

Michelle Buchanan, an accomplished scientific leader and researcher, has been appointed ORNL's deputy for science and technology by new lab Director Thomas Zacharia. Her appointment is effective Oct. 1.

"Dr. Buchanan's research accomplishments, programmatic expertise, and reputation for achievement support ORNL's role as a premier research institution that provides scientific expertise and breakthroughs that are critical to national priorities in energy, industry, and national security," said Zacharia, who served in the deputy position until becoming lab director on July 1.

Buchanan has been associate laboratory director for the Physical Sciences Directorate since 2004, with responsibilities including the lab's Chemical Sciences, Physics, and Materials Science and Technology divisions, as well as its Center for Nanophase Materials Sciences, a DOE Office of Science user facility. The lab will conduct an international search for her replacement.

Buchanan's responsibilities as deputy for science and technology will cover the range of ORNL research—computing and computational sciences, neutron science, nuclear science and engineering, the physical sciences, energy and environmental science, and national security—as well as the lab's leadership role in U.S. ITER, the Exascale Computing Project, and ORNL research centers and institutes.

"The scientific challenges and impact of Oak Ridge's research have compelled me for many years," said Buchanan, who came to the lab as a chemist in 1978. "It is a great privilege to be entrusted with shaping our future as a laboratory. My focus will be on strengthening collaborations across our diverse disciplines and promoting scientific achievement among ORNL staff, as well as the world-leading scientists who use ORNL facilities and benefit from our expertise."

Buchanan is a fellow of the American Chemical Society and the American Association for the Advancement of Science.

Michelle Buchanan. Image credit: Jason Richards, ORNL

She has written or contributed to more than 100 scientific publications and reports, holds two patents, edited a book on Fourier transform mass spectrometry, and worked extensively at the national level helping shape research directions for DOE as well as the National Science Foundation.

She earned her bachelor's degree in chemistry from the University of Kansas and her doctorate in chemistry from the University of Wisconsin at Madison. Her research focused on the development of mass spectrometry for trace detection of materials related to energy, health, and the environment for multiple DOE offices and other federal agencies.—*David Keim*

Bacteria breaks down toxic methylmercury

An ORNL-led team has identified a novel microbial process that can break down toxic methylmercury in the environment, a fundamental scientific discovery that could potentially reduce mercury toxicity levels and support health and risk assessments.

Methylmercury is a neurotoxin that forms in nature when mercury interacts with certain microbes living in soil and waterways. It accumulates at varying levels in all fish—particularly large predatory fish such as tuna and swordfish—and when consumed in large quantities can cause neurological damage and developmental disorders, especially in children.

A previous ORNL-led study, published in *Science* in 2013, unlocked the genetic code that led scientists to accurately identify microbes responsible for methylmercury production in the environment. Following this finding, the ORNL team has now discovered which bacteria perform the reverse process, called demethylation. Details were published in *Science Advances*.

"Much attention has focused on mercury methylation or how methylmercury forms, but few studies to date have examined microbial demethylation, or the breakdown of methylmercury at environmentally relevant conditions," said Baohua Gu, co-author and a team lead in ORNL's Mercury Science Focus Area.

Bacteria called methanotrophs feed off methane gas and can either take up or break down methylmercury, or both. Methanotrophs are widespread in nature and exist near methane and air interfaces, and methane and methylmercury are usually formed in similar anoxic, or oxygen-deficient, environments.

To single out how and which methanotrophs perform demethylation, the

Environmental scientist Carrie Miller, now an assistant professor at Alabama's Troy University, samples groundwater for mercury in 2012. Image credit: Jason Richards, ORNL

ORNL-led team—along with methanotroph experts from the University of Michigan and Iowa State University—investigated the behavior of many different ones and used sophisticated mass spectrometry to analyze methylmercury uptake and decomposition by these bacteria. They discovered that methanotrophs such as *Methlyosinus trichosporium OB3b* can take up and break down methylmercury, while others such as *Methylococcus capsulatus* Bath only take up methylmercury.

In either case, the bacteria's interactions can lower mercury toxicity levels in water.

"If proven environmentally significant through future studies, our discovery of methanotrophs' behavior could be a new biological pathway for degrading methylmercury in nature," Gu said. This approach differs greatly from a previously recognized enzymatic pathway, which is effective only at very high mercury concentrations.—*Sara Shoemaker*

For more information: https://go.usa.gov/xNzBY

Simulation tackles nanoparticle magnetism

With the potential to increase storage capacity and density, magnetic nanoparticles are promising materials for next-generation recording and storage devices like hard drives. But before developing new devices, scientists must understand how magnetism works at the atomic level.

Using new data from researchers at the University of California, Los Angeles and Lawrence Berkeley National Laboratory who traced the positions of 23,000 atoms in an iron–platinum nanoparticle, ORNL computational scientists Markus Eisenbach and Paul Kent used the Titan supercomputer at the Oak Ridge Leadership Computing Facility to simulate magnetism atom by atom from a region of the nanoparticle. The study, published in *Nature*, is the first to model the magnetic properties of a nanoparticle using real experimental data.

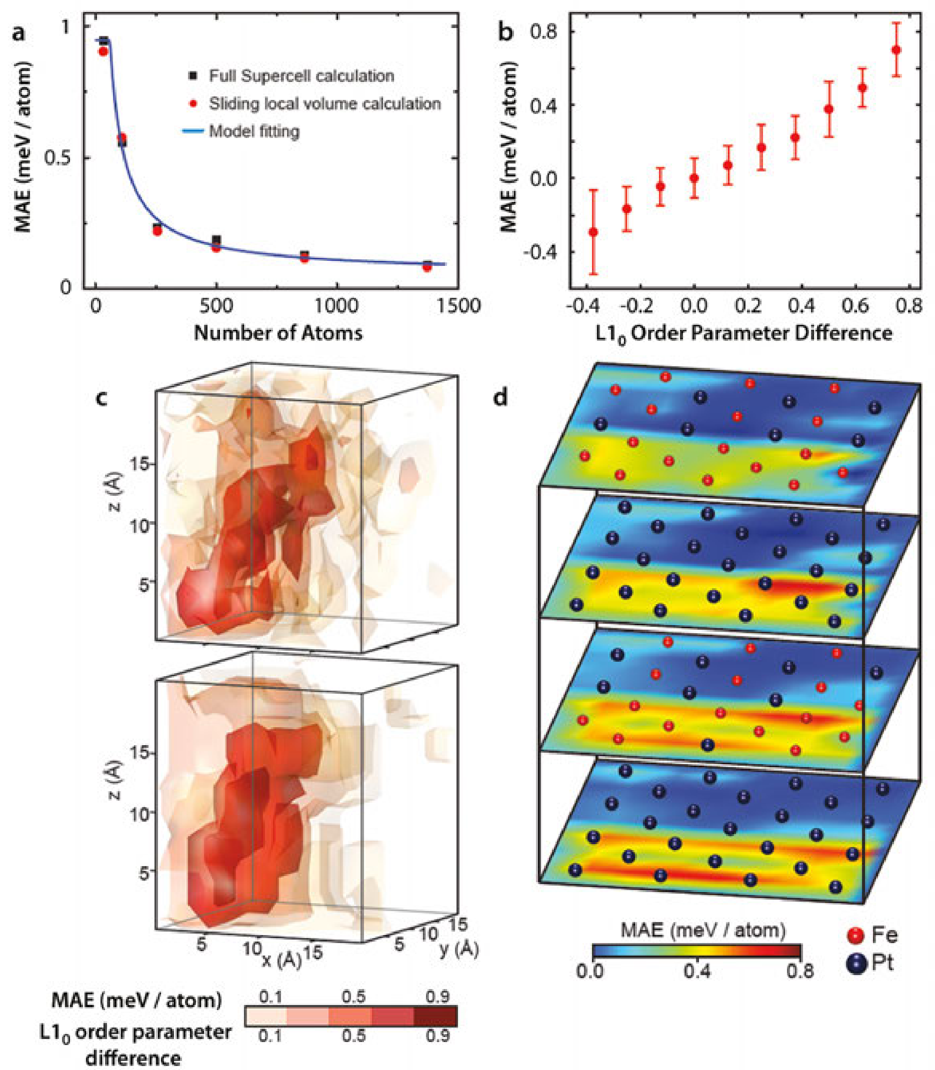
"These types of calculations have been done for ideal particles with ideal crystal structures but not for real particles," Eisenbach said.

Eisenbach and Kent simulated a supercell of about 1,300 atoms from strongly magnetic regions of the nanoparticle using the award-winning Linear Scaling Multiple Scattering (LSMS) code—a first-principles density functional theory code developed at ORNL.

The unprecedented simulations revealed that the energy associated with magnetic anisotropy—or the direction magnetism favors from atom to atom—suddenly transitions at boundaries created by different configurations of iron and platinum particles, an important result for focusing future studies.

Although first-principles calculations are currently too intensive to solve small-scale magnetism for regions larger than a few thousand atoms, researchers hope that computing advances will make a full-particle simulation possible in the future. More computationally-intensive simulations could also show how different fabrication processes, such as the temperature at which nanoparticles are formed, influence magnetism and performance.—*Katie Elyce Jones*

For more information: https://go.usa.gov/xNeCy



For the first time, researchers have simulated local magnetic anisotropy at the atomic level in a magnetic material based on experimental data. This figure shows changes in magnetic energy across individual iron and platinum atoms from an iron–platinum nanoparticle. Image courtesy Markus Eisenbach and *Nature*

Global Security names Peery chief scientist

James Peery, who has led critical national security programs at Sandia National Laboratories and Los Alamos National Laboratory, has been selected as the chief scientist of ORNL's Global Security Directorate.

"James brings more than two decades of experience in creating successful national security initiatives for the U.S. Department of Energy," said Brent Park, associate laboratory director of global security at ORNL. "In particular, his leadership in cybersecurity, data analytics and high-performance computing will enable him to lead the laboratory's cybersecurity initiative for the electric grid and beyond."

Next-generation cybersecurity for the electric grid is a multidirectorate, multiprogram effort at ORNL that supports the DOE cybersecurity program for critical energy infrastructure. The initiative aims to enable electric utilities and other components of the nation's energy supply to defend against emerging and previously unseen cyberattacks.

Peery also will help ORNL researchers draw on the lab's distinctive capabilities to develop scientific and technological solutions aligned with national security policies and strategies.

"As the lab's chief scientist for national security challenges, James will lead our talented and passionate staff—with their incredible breadth of capabilities from computing to materials to nuclear science and technology to neutron sciences—with the sense of purpose that comes from serving the country in the compelling mission of national security," ORNL Director Thomas Zacharia said.

Peery, who is a member of the U.S. Air Force's Scientific Advisory Board, began his career at Sandia in 1990, the year he graduated from Texas A&M University with a doctorate in nuclear engineering. In one of his first assignments at Sandia, he developed first-generation massively parallel algorithms and tools for use in high-energy physics applications in support of national security.—*Morgan McCorkle*

James Perry. Image credit: Sandia National Laboratories

For more information: https://go.usa.gov/xRpaw

Neutron scattering finds elusive quantum state

An ORNL-led team has used sophisticated neutron scattering techniques to detect an elusive quantum state known as the Higgs amplitude mode in a two-dimensional material.

The Higgs amplitude mode is a condensed matter cousin of the Higgs boson, the storied quantum particle theorized in the 1960s and proven experimentally in 2012. It is one of a number of quirky, collective modes of matter found in materials at the quantum level. By studying these modes, condensed matter researchers have recently uncovered new quantum states known as quasiparticles, including the Higgs mode.

These studies provide unique opportunities to explore quantum physics and apply its exotic effects in advanced technologies such as spin-based electronics, or spintronics, and quantum computing.

"To excite a material's quantum quasiparticles in a way that allows us to observe the Higgs amplitude mode is quite challenging," said Tao Hong, an instrument scientist with ORNL's Quantum Condensed Matter Division.

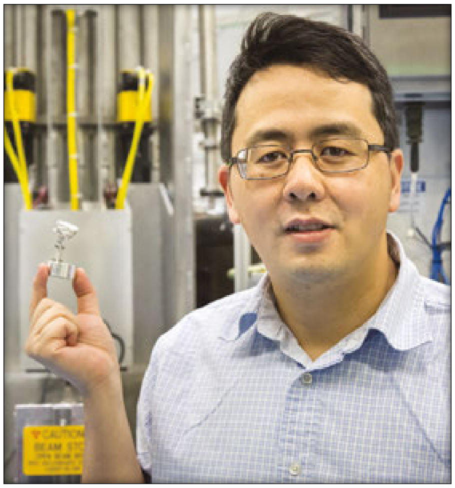
Although the Higgs amplitude mode has been observed in various systems, "the Higgs mode would often become unstable and decay, shortening the opportunity to characterize it before losing sight of it," Hong said.

The ORNL-led team offered an alternative method. The researchers selected a crystal composed of copper bromide, because the copper ion is ideal for studying exotic quantum effects, Hong explained. They began the delicate task of "freezing" the material's agitating quantum-level particles by lowering its temperature to 1.4 Kelvin, which is about minus 457 degrees Fahrenheit.

The researchers fine-tuned the experiment until the particles reached the phase located near the desired quantum critical point—the sweet spot where collective quantum effects spread across wide distances in the material, which creates the best conditions to observe a Higgs amplitude mode without decay.

With neutron scattering performed at ORNL's High Flux Isotope Reactor, the research team observed the Higgs mode with an infinite lifetime: no decay.

"There's an ongoing debate in physics about the stability of these very delicate



ORNL's Tao Hong analyzed a copper bromide compound's low-energy behavior during a neutron scattering experiment at the lab's High Flux Isotope Reactor that yielded the elusive Higgs amplitude mode in two dimensions with no decay. Image credit: Genevieve Martin, ORNL

Higgs modes," said Alan Tennant, chief scientist of ORNL's Neutron Sciences Directorate. "This experiment is really hard to do, especially in a two-dimensional system. And, yet, here's a clear observation, and it's stabilized."—*Sara Shoemaker*

For more information: https://go.usa.gov/xRpac

ORNL tech wins innovation award

A novel material invented by an ORNL researcher has won an award from the TechConnect National Innovation Summit.

TechConnect, a global innovation prospecting company, gave a 2017 National Innovation Award to "Hybrid Hollow Silica Particles with Unprecedentedly Low Thermal Conductivity," a material invented by Jaswinder Sharma, a scientist in ORNL's Energy and Transportation Science Division.

The material is made of hollow silica particles and a coating that provides insulation properties similar to state-of-the-art aerogels. Current thermal insulation materials use expensive synthesis precursor materials with a relatively low yield, driving up production costs. The hybrid hollow silica particles utilize a unique combination of low-cost precursors and material structure to reduce production costs up to 50 percent.

The price reduction and thermal insulation properties of the silica particles make them ideally suited for applications in building and automotive technology, space shuttle and aerospace components, hydrogen storage and waste-heat energy conversion systems.

The TechConnect Corporate and Investment Partner Committee ranks submissions to the National Innovation Summit based on the technology's potential positive impact on its industrial sector, and technologies in the top 15 percent receive National Innovation Awards.

The hybrid hollow silica particles technology was featured at a showcase booth at the TechConnect National Innovation Showcase in Washington D.C.—*Sean Simoneau*

ORNL researcher Jaswinder Sharma. Image credit: Image credit: Carlos Jones, ORNL

Four ORNL researchers win early career awards

Four ORNL researchers specializing in nuclear physics, fusion energy, materials science and environmental science are among 59 recipients of the DOE Office of Science Early Career Research Program awards.

The program, now in its eighth year, supports the development of individual research programs of outstanding scientists early in their careers and stimulates research careers in the disciplines supported by the Office of Science. The 59 selectees for fiscal year 2017 were chosen based on peer review of about 700 proposals.

"Our effectiveness in solving big problems of national importance over the long term relies directly on the vitality of our early-career staff—their creativity, talents and new ideas," ORNL Director Thomas Zacharia said. "DOE's investment in these promising young researchers is a recognition of their talents and evidence of the importance of their work."

Kelly Chipps, a Liane B. Russell Fellow working in ORNL's Physics Division, will receive funding for her proposal "Next-Generation Particle Spectroscopy at FRIB: A Gas Jet Target for Solenoidal Spectrometers," selected by the Office of Nuclear Physics.

David Green, of ORNL's Fusion and Materials for Nuclear Systems Division, proposed a project titled "Scale-Bridging Simulation of Magnetically Confined Fusion Plasmas," which was funded by the Office of Fusion Energy Sciences.

Thomas (Zac) Ward's proposal "Designing Metastability: Coercing Materials to Phase Boundaries" was selected by the Office of Basic Energy Sciences. Ward works in ORNL's Materials Science and Technology Division.

David Weston of ORNL's Biosciences Division submitted a proposal titled "Determining the Genetic and Environmental Factors Underlying Mutualism within a Plant-Microbiome System Driving Nutrient Acquisition and Exchange," which will be funded by the Office of Biological and Environmental Research.

National lab recipients will receive at least $500,000 per year to cover annual salary plus research expenses over a planned five years. The final details for each project award are subject to final grant and contract negotiations between DOE and the awardees.—*Sara Shoemaker*

Kelly Chipps

David Green

David Weston

Zac Ward

The science behind national security

by Amy Reed
reedac@ornl.gov

ORNL carbon researcher James Klett demonstrates the heat transfer rate of high-conductivity graphite foam using an ice cube.
Image credit: Jason Richards, ORNL

Standing in his lab nearly two decades ago, carbon researcher James Klett used a pair of tweezers to press an ice chip against a chunk of newly created material he held in his palm. The dark grey material, looking much like a hardened sponge, whisked heat up from his warm palm and melted the ice.

"In that moment I realized we had discovered a new material, a lightweight material that is not insulating but extremely thermally conductive," said Klett, who made the serendipitous discovery while experimenting with his ORNL team on new carbon composites for lightweight aerospace components.

Made from carbon that has undergone multiple processes, the porous, bricklike foam felt cool to the touch. It owed its high thermal conductivity to an unusual graphite crystal structure peppered with miniscule air pockets. "Once the effect was apparent, the ideas blossomed and they've continued evolving ever since," Klett said.

Characteristic of ORNL's dual application of scientific discoveries, nearly every idea that followed for harnessing the foam's unique capabilities soon transitioned into a national security application. Its use in cooling personal computers led to prevention of heat damage in military satellites and electronics carried by soldiers in the Middle East. Applications for civilian cars and trucks led to cooling of military vehicles and weapons. Prolonging the life of energy-efficient lights at college sports arenas (including at the University of Tennessee and Virginia Tech) may lead to more cost-effective lighting in cavernous military facilities such as airplane hangars.

"This is the nature of scientific discoveries at Oak Ridge National Laboratory," explained physicist Brent Park, associate lab director for global security. "For every civilian use of a scientific discovery made here at our lab, there is a parallel national security application."

The translation of basic scientific discoveries into real-world national security applications has been ongoing since the first researchers arrived at the Oak Ridge site in the midst of World War II. The work carried out by scientists and engineers grew from one generation to the next, evolving to meet new demands.

See THE SCIENCE BEHIND NATIONAL SECURITY, page 10

New marching orders:

Fast-attack submarine officer and F-35 test pilots among those with one-year assignments at lab

by Amy Reed
reedac@ornl.gov

Despite being landlocked in the hills of East Tennessee, fast-attack submarine Lt. Eric Stromme of the U.S. Navy found himself engrossed in his work at ORNL.

During a one-year assignment at the lab, his most memorable project was a groundbreaking experiment that tested an engine made from an aluminum-cerium alloy developed by ORNL. The alloy both improves the energy efficiency of engines and expands the market for cerium, an underused product often discarded during the mining of rare earth minerals.

"The national lab brought all the pieces together in one place to tackle this challenge," said Stromme, noting that the research team created an alloy, 3-D-printed the mold for the engine, and then conducted neutron analysis on the running engine to test the alloy's performance.

The test results verified that the alloy could indeed be used to make a lighter-weight internal combustion engine that can withstand high temperatures, allowing more complete fuel combustion. Stromme, who worked under the guidance of ORNL scientist Orlando Rios on the project, was on deck at the lab when ORNL announced that Wisconsin-based manufacturer Eck Industries had decided to license the alloy for commercial applications.

"One of the goals the Navy had for me was to learn how the lab applies technology so that I could suggest ways that the Navy can deploy new technology more quickly into the fleet," said Stromme, whose degree is in mechanical engineering. "The aluminum alloy project is a great story in that regard. From the time the scientists had the idea until it was licensed with a manufacturer took only three years."

He credited ORNL's research culture.

"The lab is good at promoting a collaborative environment, not just between researchers and leadership but also between departments, other labs, and industry," Stromme said, noting that ORNL partnered with Ames and Lawrence Livermore national labs as well as an industry partner on the project. "At the lab there is an awareness that you are competing for top talent; people make sure to let others know that their opinions are valued."

Stromme's assignment at the lab was part of the Navy's Tours with Industry program, in which Navy personnel are placed with organizations such as Amazon, Apple, and Lockheed Martin for one-year assignments. Also on board at ORNL was Navy machinist's mate Michael D. Garner, who worked at the lab's High Flux Isotope Reactor.

The Air Force has two similar programs. Air Force Col. Michael Starr, an F-22 and F-16 experimental test pilot, and Maj. Christopher Nations, an F-16 and F-35 experimental test pilot, were at the lab during the past year as part of the Air Force's fellowship program. Capt. Trung Nguyen, a space lift engineer, participated in the Air Force Education with Industry program.

ORNL has hosted 45 military and civilian defense personnel for temporary work assignments since its military education and outreach program began in 2002.

David Landguth of ORNL's Global Security Directorate, who has managed the program since 2012, pairs visiting military personnel with a research experience tailored to the individual's expertise and interests.

"He connected me with researchers and engineers at the vehicle security lab," said Starr, whose next Air Force assignment will be as an F-35 experimental test pilot. "I did a deep dive into cyber-physical research that directly related to aircraft security and an issue near and dear to my heart, which is the ability of a vehicle operator to be alerted at the onset of a hack."

Starr worked closely with ORNL engineers at the lab's National Transportation Research Center on a project designed to detect, intercept, and prevent cyberattacks on moving vehicles.

See NEW MARCHING ORDERS, page 11

THE SCIENCE BEHIND NATIONAL SECURITY, from page 8

"People come to us for operational solutions because of basic science research and technological expertise that we've built up over many, many decades," said nuclear physicist Larry Satkowiak, director of the lab's Nonproliferation, Safeguards, and Security Programs.

Inquisitive scientists at ORNL in the 1950s began unraveling the mysteries of the genetic code in cells. That work provided the foundation for current ORNL experiments that are exploring how microorganisms in soil and water, which show genetic changes when exposed to radioactive materials, can be used as sensors to detect illicit nuclear or radiological activity. The lab's pioneering work in the 1940s led to the production of radioactive isotopes. Today ORNL still produces isotopes for medicine, industry, and research and is the only known producer of nickel-63, which is used in airport detectors to identify high-risk materials.

> *"If the military comes to us with a problem, and I can envision how to develop this basic science discovery for a specific application that saves the life of a soldier on the battlefield, how could I not follow through?"*
>
> — ORNL carbon researcher **James Klett**

Pressing national security needs create a sense of urgency that can accelerate scientific progress.

"A deep sense of commitment, purpose, and passion was pervasive at the time of the birth of this lab, as scientists labored to help win the war," said Thomas Zacharia, ORNL's new lab director. "As I embark on this journey as lab director, I want to harness that same sense of being part of something that is bigger than yourself and apply it to today's national security challenges, which are broad and deep and complex."

ORNL researchers such as computer engineer Hector Santos-Villalobos, who specializes in computational imaging, have turned down job offers in the private sector because of this sense of purpose.

"I chose to come to the lab because here I can make science better. My contributions to science help make society better. On top of that, I am helping make the world a safer place for my child when my work benefits national security," says Santos-Villalobos, who recently became a father.

Roughly one-third of ORNL's staff directly engage in national security work.

"A common misunderstanding is that national security is mainly about fighting wars," noted Rick Raines, director of the Data and Cyber Analytics Initiative in ORNL's Global Security Directorate. "It is also about protecting our nation's intellectual properties, making critical infrastructure more resilient, and keeping the electric grid up and running."

Data analytics and cybersecurity are critical focus areas for the lab's national security work. Defense and intelligence agencies rely on ORNL's expertise to triage overwhelming volumes of data into actionable information based on in-depth analysis, often in real time. They also turn to ORNL for the creation of specialized cybersecurity platforms. These cybersecurity tools protect military resources as well as other enterprises such as the banking industry and the electric power grid.

"The combination of our lab's powerful computing resources and our team's unique talents and capabilities allows us to rapidly transition from brainstorming early concepts to producing operational solutions for national security challenges," said Raines, who directed cyberspace research for the Air Force before joining ORNL.

Computer scientist Justin Beaver, who worked at NASA for a decade before joining ORNL, is on a team that has been working for several years to develop next-generation cybersecurity technology.

"We've developed something different from any tool that currently exists," Beaver said, explaining that ORNL combined site-specific network data, threat data relevant to the defending organization, and advanced machine-learning algorithms to more quickly detect intruders in a network.

"We identify these in real time so that security analysts can verify and respond before damage is done—reducing the reaction time for new and novel threats from weeks to minutes."

ORNL is also solving big data issues for national security databases, which amass huge amounts of information.

"Essentially what we are doing is optimizing the role of the human analyst," Beaver said. "The sheer volume of data that must be analyzed is impossible for a team of people to digest. Our data analytic tools scour the massive volume of data, categorize and prioritize the data based on an analysis of the threat severity, and then visualize the information so that it is easily understood by analysts."

With the arrival of ORNL's next supercomputer, Summit, the lab's capabilities in a related area, artificial intelligence, will also expand.

"What many people don't yet realize is that Summit will very likely be the most powerful artificial intelligence machine in the world because of its unique chip set, which was specifically designed to enhance deep learning and data analytics capabilities," Zacharia said. "The opportunity to use these capabilities in the national security space is broad."

Around the world, ORNL is perhaps best known for its leadership in the science and technology that undergirds nuclear nonproliferation efforts. The lab fulfills an international role in advancing scientific and technical capabilities to detect illicit nuclear activities, secure fissile and radiological materials, and counter the threat of weapons of mass destruction. Areas of expertise include nuclear forensic science, knowledge of the uranium fuel cycle, and best practices in safeguarding and securing high-risk materials.

"When government regimes or rogue groups start pursing avenues to develop nuclear weapons, we have the capabilities to

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NEW MARCHING ORDERS, from page 9

"This research has direct application within the Defense Department as well as for civilians," Starr said. "We're demonstrating that bringing the vehicle operator into the loop at the earliest point of detection can prevent a catastrophic event, whether for a commercial airliner or a transport truck carrying toxic chemicals."

When space lift engineer Nguyen came to ORNL, he switched gears from launching rockets for the Air Force to working with the latest flying platforms—drones and other unmanned aerial vehicles.

"I assisted the Unmanned Vehicle Development Lab with a new system that improves communication between operators and remotely piloted vehicles," said Nguyen, an aerospace engineer whose previous assignment with the Air Force involved launching satellites into orbit from Cape Canaveral, Florida. "Coming from a military background, I gained a new perspective in problem-solving by working with the UAV technical team. That by far is the greatest takeaway from my time at Oak Ridge."

The one-on-one interaction of the lab's researchers with defense personnel is the heart of the lab's military education and outreach program, said retired Navy Vice Admiral Kendall Card, who is the director of intelligence programs in the Global Security Directorate.

"Perhaps the greatest benefit to having these military folks here at the lab is that they are our eyes and ears in helping us translate our basic science research into military applications that meet real needs out in the field, air, and sea," Card said. "We pair them up with researchers, and the resulting collaboration is good for the military and good for the lab. They learn about the lab's capabilities and methods of operation, and we learn about the military's current, most pressing needs where we could be the greatest help."

During one assignment at the lab, the Air Force's Chris Nations teamed with carbon researcher James Klett, inventor of a lightweight graphite foam with high-thermal conductivity that the military uses in multiple applications.

"He and I sat down and brainstormed," Klett said. "Here I was with an F-35 experimental test pilot who had a degree in astronautical engineering and who understood the potential for the application of the graphite foam. He suggested a specific idea that we hadn't tried yet. We helped him put together a test rig, and he was able to demonstrate results."

Forty-five military and civilian defense personnel have taken on work assignments with ORNL's military education and outreach program since 2002. Pictured, from left, are the most recent participants: Air Force Capt. Trung Nguyen, Navy Lt. Eric Stromme, Air Force Maj. Christopher Nations and Navy Petty Officer 1st Class Michael Garner. Image credit: Carlos Jones, ORNL

THE SCIENCE BEHIND NATIONAL SECURITY, from page 10

detect that activity," said analytical chemist Paula Cable-Dunlap, who helped establish ORNL's Ultra Trace Forensic Science Center.

Over decades the lab has built the scientific capabilities needed to detect and trace the origins of illicit, high-risk radiological and nuclear materials that appear in places where they shouldn't be—ideally intercepting and identifying them before an event occurs. The lab's scientists have improved the speed, quality, and capabilities of nuclear forensic analysis and have advanced the technologies required to collect and analyze samples.

solid piece of uranium of the size needed cost $60,000. He found that colleagues at other labs faced the same issue. Some had devised thin sheets of uranium foil, some had created discs in the shape of hockey pucks, some used whatever scraps they had on hand. The result was inconsistent testing results that didn't fully capture the effectiveness or weaknesses of the detectors being tested.

Blessinger began brainstorming. Working with chemists, machinists, engineers, and others across the lab and at the Y-12 National Security Complex, he created several prototypes. The final design was a 3-D-printed hollow sphere made of titanium. Slightly

"ORNL and other DOE national laboratories are the only places where you can get a combination of decades of experience in the nuclear fuel cycle coupled with state-of-the-art basic science research into everything imaginable, from materials science to interactions of biological materials. It is these two things together that allow us to develop ways to detect attempts at nuclear weapons and to verify international treaties."

— ORNL analytical chemist **Paula Cable-Dunlap**

"ORNL and other DOE national laboratories are the only places where you can get a combination of decades of experience in the nuclear fuel cycle coupled with state-of-the-art basic science research into everything imaginable, from materials science to interactions of biological materials," Cable-Dunlap said. "It is these two things together that allow us to develop ways to detect attempts at nuclear weapons and to verify international treaties."

When the International Atomic Energy Agency sought a mechanism for monitoring uranium enrichment processes to help verify that nuclear nonproliferation treaties were being followed, the agency turned to ORNL to lead a multilab effort to develop the technology.

"IAEA is now using this technology to verify that Iran follows the rules of the 2015 international nuclear treaty," said Cecil Parks, director of ORNL's Nuclear Security and Isotope Technology Division. "Building on past technology, we developed a system called an online enrichment monitor, which houses sensors and detectors inside a sealed, tamperproof container. It continuously monitors a key process involved in uranium enrichment to ensure that levels stay within the limits needed for peaceful purposes such as research and nuclear power."

Another recent example is the work of ORNL nuclear physicist Chris Blessinger to solve a problem that had bedeviled researchers in the radiation detection field for some time.

"I was testing radiation detectors used to prevent high-risk materials from being illegally transported across borders," Blessinger explains. "To test the detectors and get accurate, consistent measurements, we needed large and uniform samples of uranium and plutonium."

One problem was that federal security, criticality safety, radiological safety, and transportation regulations created significant inconveniences and made this type of testing cost prohibitive; shipping a

larger than a softball, its surface is made of metal-encapsulated ceramic tiles loaded with uranium or plutonium. Because he carefully designed the device to comply with numerous regulations, it can be shipped commercially and handled more freely within the laboratory. The result is better test results, greatly reduced costs, and, in the end, more effective detectors that help prevent the smuggling of high-risk materials that could be used to make nuclear weapons.

The lab has enhanced nuclear nonproliferation efforts in more than 109 countries by developing next-generation technology, conducting training, and setting standards in security culture and best practices.

One team of ORNL and Y-12 scientists and engineers has been deployed twice to Iraq to retrieve dangerous nuclear materials using the lab's Mobile Uranium Facility. The team, which has jokingly referred to itself as the "Uranium National Guard," trains every couple of years in various geographical environments to prepare for future deployments.

"In one situation, not only were we preventing the materials from falling into the wrong hands, but we were protecting the townspeople. Families had begun taking contaminated equipment from an abandoned facility into their homes," said mechanical engineer Jim Radle, who leads the team.

A common thread in discussions with ORNL scientists and engineers is the sense of purpose they feel in their life's work as they support national security through scientific and technological endeavors.

Nineteen years after his initial discovery, Klett continues materials science research and development of the graphite foam for emerging military needs in extreme environments. "What gives me purpose and direction is seeing the endgame. If the military comes to us with a problem, and I can envision how to develop this basic science discovery for a specific application that saves the life of a soldier on the battlefield, how could I not follow through?"

Eye of the beholder:

Identity science comes of age

by Stephanie Seay
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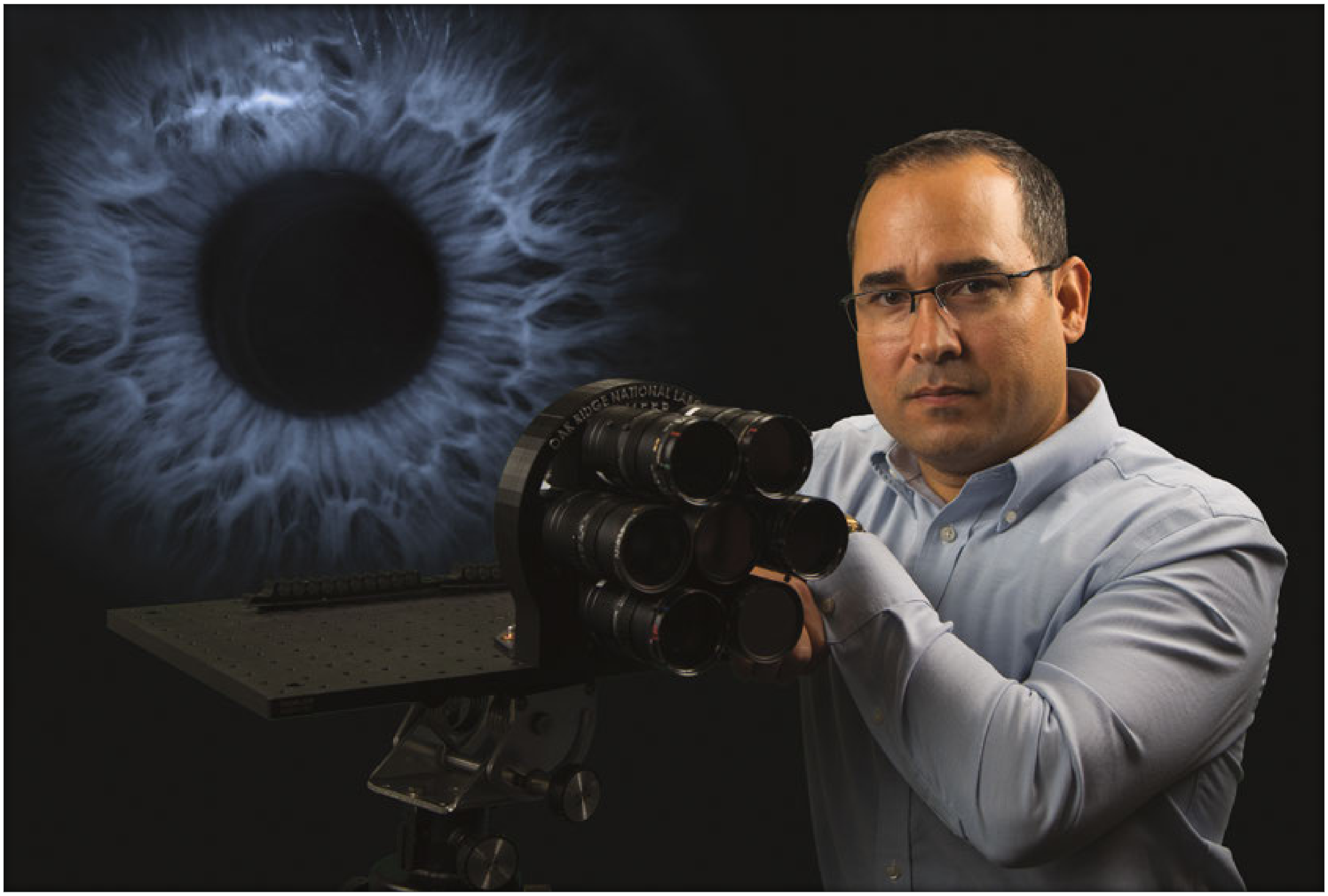
While cameras are seemingly everywhere these days, identifying individuals using images is still a challenge. Traditional camera techniques are often complicated by poor lighting and unfocused scenes with fast-moving subjects.

Today, identity science is shifting toward scenarios in which individuals can be identified in less than optimal conditions—photographed from the side or while moving, for instance. The techniques can be deployed to save time at border crossings and to ensure proper access to secure facilities. Scientists at ORNL are using algorithms and advanced optics to make these advancements a reality.

See EYE OF THE BEHOLDER, page 14



ORNL researcher Hector Santos-Villalobos and colleagues use an array of microlenses and a ray-tracing algorithm to capture the iris of subjects even under challenging conditions. Image credit: Carlos Jones, ORNL

EYE OF THE BEHOLDER, from page 13

The iris, or colored portion of the eye, is second only to DNA in identifying individuals. The complex patterns of the iris can be easily photographed at a distance and are unique to each person, distinct even between the left and right eye. Moreover, the iris is a protected, internal organ that is externally visible and does not change over time the way fingerprints can.

It can be difficult to capture a perfect image of the iris, however. People are unlikely to be looking straight into a camera with eyes wide open, even when instructed to do so. (Think driver's license photos.)

With traditional imaging methods, accurate iris recognition drops if a subject is photographed as little as 15 degrees off center, said Hector Santos-Villalobos, a scientist who leads the work in the Imaging, Signals, and Machine Learning Group in ORNL's Electrical and Electronics Systems Research Division. To correct an off-axis iris image, Santos-Villalobos and his colleagues created a model of the human eye and used a ray tracing algorithm to render the iris from the front.

The model, called the ORNL Eye, takes into account the effect of the eye's limbus on iris recognition. The limbus is an area of tissue that can obscure regions of the iris, which impacts the correction of some off-axis iris images to a frontal iris image. Santos-Villalobos calls it the "limbus effect." Adding that effect into calculations was critical to successfully matching off-axis iris images to individuals.

The ORNL Eye and ray tracing methods resolve light refraction distortions that can compromise the finer details of an off-angle iris image. Ray tracing maps the path of light rays from the off-angle camera to the eye model iris; then the synthetic iris can be rendered from any viewpoint, including frontally.

The ORNL method demonstrated a frontal rendering of the iris in images that were as much as 50 degrees off axis. Another plus is that the process can be integrated into existing iris recognition technology, avoiding the expense of creating new systems, Santos-Villalobos noted.

Light-field studies have led to more research at ORNL, including methods to improve facial recognition by capturing images of individuals viewed from the side or through the windshield of a moving vehicle.

Getting good images from these scenarios is difficult due to light conditions and the need to focus and capture images of someone in motion. To quickly render images and reduce the "noise" of refraction and other challenges, Santos-Villalobos's team is employing a light-field camera—also known as a plenoptic camera.

"With traditional imaging you can create a blur, but you can't fix it. With the plenoptic approach you are guaranteed an in-focus image. That gives you more freedom in subject positioning or distance to the camera. We can identify someone 50 degrees off angle or wearing glasses or cosmetic contact lenses designed to change eye color and pattern, for instance."

— ORNL imaging researcher **Hector Santos-Villalobos**

By capturing vast amounts of information on a scene's light field, a plenoptic camera can compute an image with focus on any point in a scene. This compares to traditional cameras that can bring only one portion of a scene into focus at a time.

The method likewise relies on the increasing availability of inexpensive computational power. Applying novel computational methods to the resulting light field allows the researchers to generate a high-quality composite facial image, Santos-Villalobos noted.

"With traditional imaging you can create a blur, but you can't fix it," Santos-Villalobos said. "With the plenoptic approach you are guaranteed an in-focus image. That gives you more freedom in subject positioning or distance to the camera. We can identify someone 50 degrees off angle or wearing glasses or cosmetic contact lenses designed to change eye color and pattern, for instance."

The ultimate goal is to create a system that makes it easier to capture images and make quick, accurate correlations to a database. "In identity science, creating a user-friendly, less-intrusive system is as important as being able to make a good match," Santos-Villalobos said.

Have you seen these genes?

by Stephanie Seay
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ORNL researchers are a step closer to creating a facial image from a DNA sample, using a novel method that assesses facial scans and compares them to genetic markers.

The technology could improve identification at national borders and help local law enforcement identify crime suspects and unknown remains. ORNL's DNA2Face project has as its long-term goal the ability to predict facial structure using genetic data such as a small blood or tissue sample.

> *"You might put that image on the news and ask, 'Have you seen this person?' You really can't say, 'Have you seen these genes?'"*
>
> — ORNL investigator **Ryan Tokola**

"These days if you get a genetic sample from a crime scene, basically all you can do is apply it to some databank of samples, and we don't have a lot of those. But if you can take that genetic material and make a face prediction, then you can run it against a database of faces, which we have a lot more of," said Ryan Tokola, principal investigator in ORNL's Imaging, Signals, and Machine Learning Group.

Researchers first defined a reference, average face mapped with tens of thousands of 3-D points. The reference face was then aligned with a similarly mapped facial scan. Comparing the two created correspondence vectors—essentially a measure of the differences between the reference face and the scanned face.

Once the correspondence vectors were established, the researchers applied a statistical technique called principal component analysis that transformed each correspondence vector into a relatively small set of numbers, which provided a very compact representation of the face. They then performed a genome-wide association study—a statistical approach to finding genomic variations that are associated with a particular trait—using DNA samples obtained from the subjects of facial scans. The results of the study showed several strong connections between DNA and facial features by comparing principal component analysis scores to DNA markers.

The ORNL researchers found 30 significant mutation locations and more than 5,000 locations that are potentially significant. In comparison, an earlier study without ORNL's statistical method found only five significant locations.

Demographic characteristics such as ethnicity, gender, and age were taken into account for the subjects included in the research. The most significant cluster of variations was found on chromosome 3 on the RAF1 gene, which is known to affect craniofacial shape. Analyzing select portions of the face could result in the discovery of more genes that directly influence facial shape, Tokola noted.

"If you're trying to identify someone, it's a lot easier to do with an image of their face, which you can then feed into a face recognition database or crowdsource," Tokola added. "You might put that image on the news and ask, 'Have you seen this person?' You really can't say, 'Have you seen these genes?'"

ORNL researchers identify facial components useful in predicting faces from DNA samples. Image credit: Ryan Tokola, ORNL

Titan digs deep

with 3-D map of Earth's interior

by Jonathan Hines
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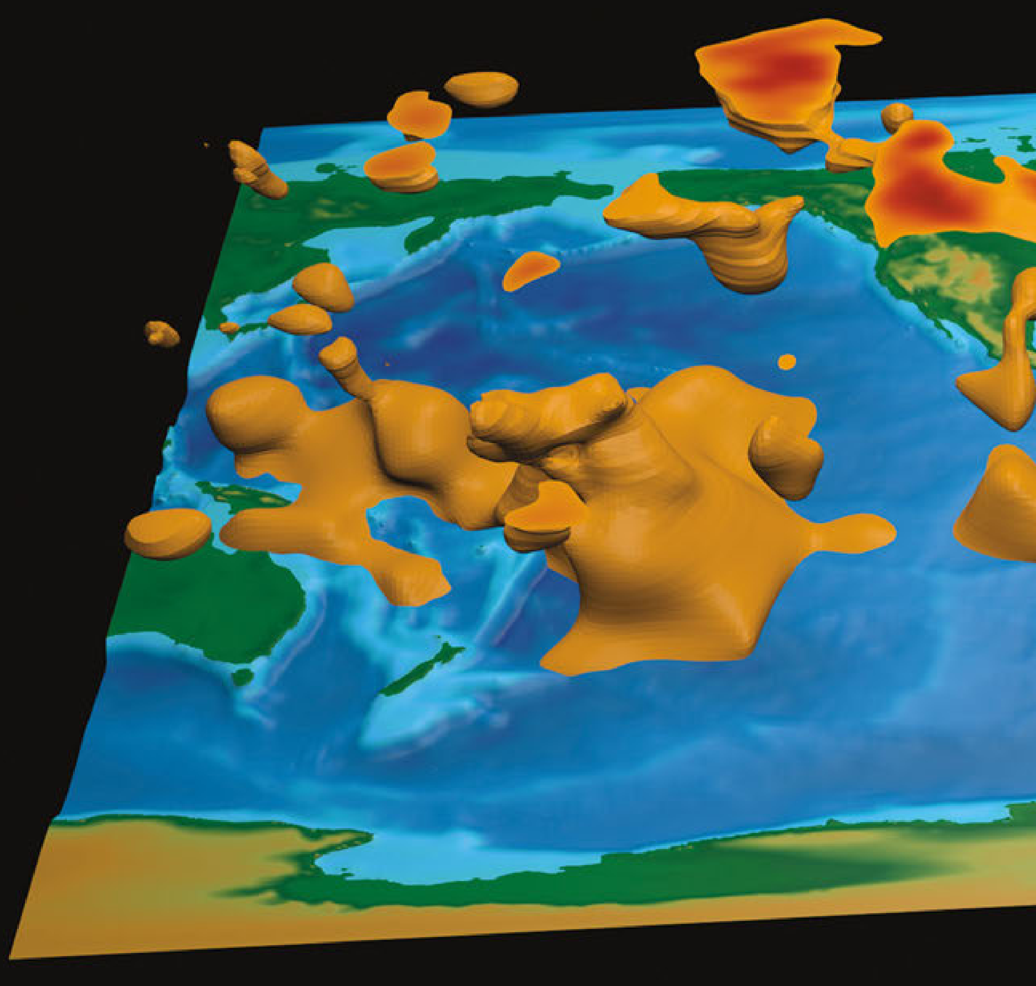
When an earthquake strikes, the release of energy creates seismic waves that often wreak havoc for life at the surface. Those same waves, however, present an opportunity for scientists to peer into the subsurface by measuring vibrations passing through the Earth.

Using advanced modeling and simulation, seismic data generated by earthquakes, and ORNL's Titan supercomputer, a team led by Jeroen Tromp of Princeton University is creating a detailed 3-D picture of Earth's interior. Currently the team is focused on imaging the entire globe from the surface to the core–mantle boundary, a depth of 1,800 miles.

These high-fidelity simulations add context to ongoing debates related to Earth's geologic history and dynamics, bringing prominent features like tectonic plates, magma plumes, and hotspots into view. In 2016 the team published its first-generation global model. Created using data from 253 earthquakes captured by seismograms scattered around the world, the team's model is notable for its global scope and high scalability.

"This is the first global seismic model where no approximations—other than the chosen numerical method—were used to simulate how seismic waves travel through the Earth and how they sense heterogeneities," said Ebru Bozdag, a coprincipal investigator of the project and an assistant professor of geophysics at the University of Nice Sophia Antipolis. "That's a milestone for the seismology community. For the first time we showed people the value and feasibility of running these kinds of tools for global seismic imaging."

The project's genesis can be traced to a seismic imaging theory first proposed in the 1980s. To fill in gaps within seismic data maps, the theory posited a method called adjoint tomography, an iterative full-waveform inversion technique. This technique leverages more information than competing methods, using forward waves, which travel from the quake's origin to the seismic receiver, and adjoint waves, which



are mathematically derived waves that travel from the receiver to the quake.

The problem with testing this theory? "You need really big computers to do this," Bozdag said, "because both forward and adjoint wave simulations are performed in 3-D numerically." In 2012 just such a machine arrived in the form of the 27-petaflop Cray XK7 Titan.

As quake-induced seismic waves travel, seismograms can detect variations in their speed. These changes provide clues about the composition, density, and temperature of the medium the wave is passing through. For example, waves move slower when passing through hot magma, such as mantle plumes and hotspots, than they do when passing through colder subduction zones, locations where one tectonic plate slides beneath another.

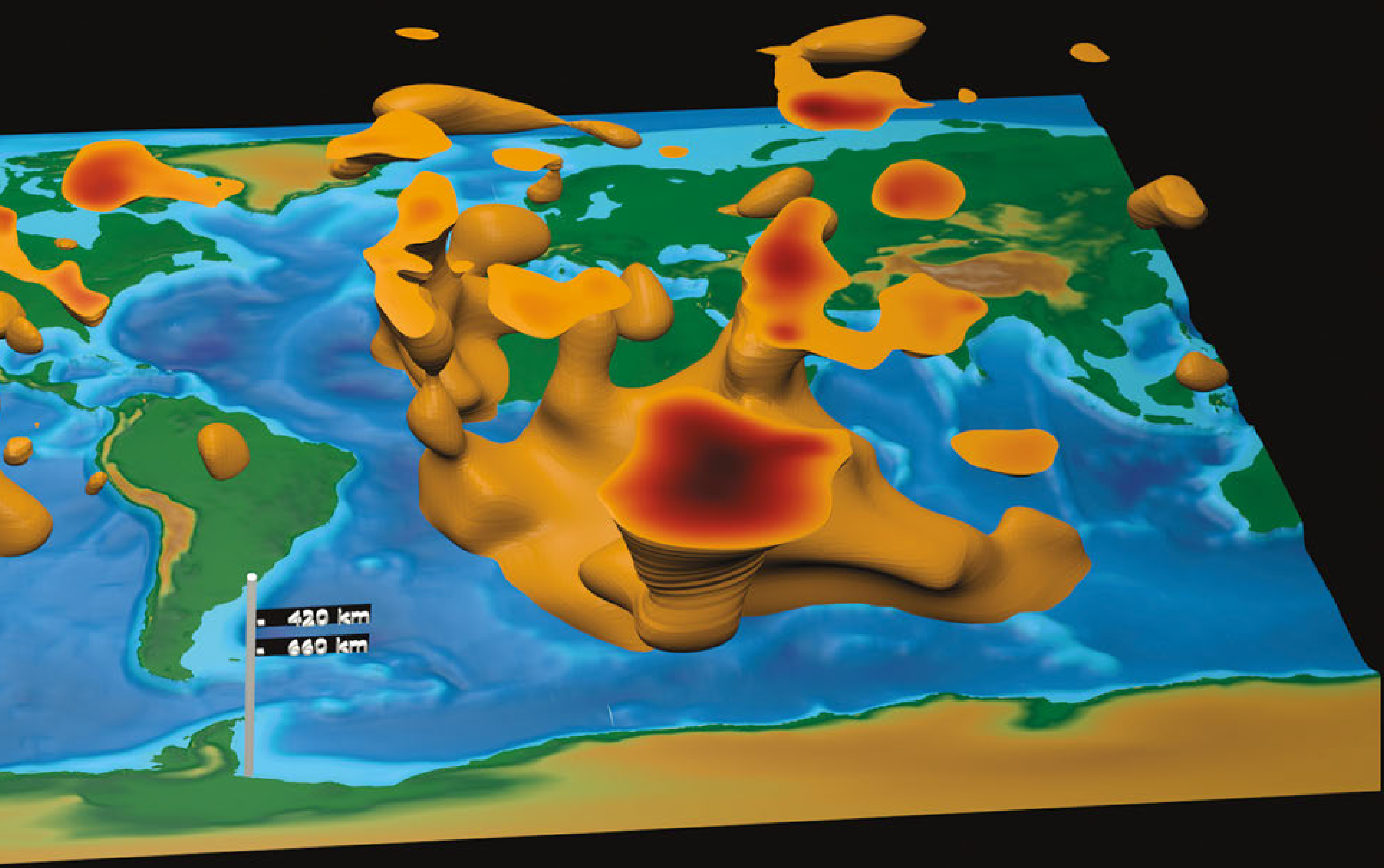
Each seismogram represents a narrow slice of the planet's interior. By stitching many seismograms together, researchers can produce a 3-D global image, capturing everything from magma plumes feeding the Ring of Fire that circles the Pacific Ocean, to the hotspots of Yellowstone National Park, to subducted plates under New Zealand.

This process, called seismic tomography, works in a manner similar to imaging techniques employed in medicine, where 2-D X-ray images taken from many perspectives are combined to create 3-D images of areas inside the body.

To improve its global model further, Tromp's team is experimenting with model parameters on Titan. For example, the team's second-generation model will introduce anisotropic inversions, which are calculations that better capture the differing orientations and movement of rock in the mantle. This new information should give scientists a clearer picture of mantle flow, composition, and crust–mantle interactions.

"Our methods are expensive—we need a supercomputer to carry them out—but our results show that these expenses are justified, even necessary," Bozdag said.

For more information: https://go.usa.gov/xNEBh



A visualization from the first global model constructed using adjoint tomography, an iterative full-waveform inversion technique. The model captures continental-scale features within the Earth's mantle. Image credit: David Pugmire, ORNL

Virtual laser lab

simulations create new insight

by Eric Gedenk
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With the advent of laser technology in the 1960s, materials scientists gained a new tool to both study and modify materials. Today lasers allow researchers to manipulate materials on atomic and subatomic levels, leading to new materials and a host of other applications.

For instance, by controlling laser wavelength, intensity, and pulse duration, researchers can modify metals to exhibit useful new properties for a broad range of applications. Until recent years they relied on experimental trial and error to achieve the desired properties, but in the era of supercomputing, experiments can be done in a virtual laboratory.

The University of Virginia's Leonid Zhigilei and colleagues have created such a virtual laboratory with ORNL's Titan supercomputer, using the system to gain deeper insights into laser interactions with metal surfaces.

"Rapid expansion of practical applications of ultrashort pulse laser processing, including engineering of new materials, requires understanding of fundamental mechanisms of laser-induced structural and phase transformations," Zhigilei said.

"Experimental probing of these transformations, which takes place on the picosecond timescale [one-trillionth of a second], is difficult, expensive and often not even feasible. Performing 'virtual experiments' on a supercomputer provides an attractive alternative."

By combining virtual and real-world experiments, the team is gaining a fundamental understanding of the mechanisms for material interactions induced by lasers.

Laser beams are a collection of coherent light waves. The amount of energy they carry, however, can vary widely, and both low- and high-energy lasers have made huge impacts on modern life. Low-energy lasers helped usher in the era of CDs and DVDs, whereas high-energy lasers have simplified countless medical procedures and enabled a wide range of material design applications.

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— University of Virginia researcher **Leonid Zhigilei**

Zhigilei's team has focused on understanding the ultrafast phase transitions triggered by laser irradiation, or the pathways the material takes to go from one state of matter to another, such as ice melting and becoming water.

If a heat source hits an ice cube, for instance, it begins melting at the heating point. Heat then transfers to the colder regions behind, melting the whole cube essentially from front to back. The intense energy of lasers, though, makes it possible for that same ice cube to melt from the inside or melt in various regions simultaneously.

In the case of an ice cube, of course, the entire solid ultimately turns to water, but when researchers are trying to catalog metallic surface changes at the nanoscale, the picture becomes more complex.

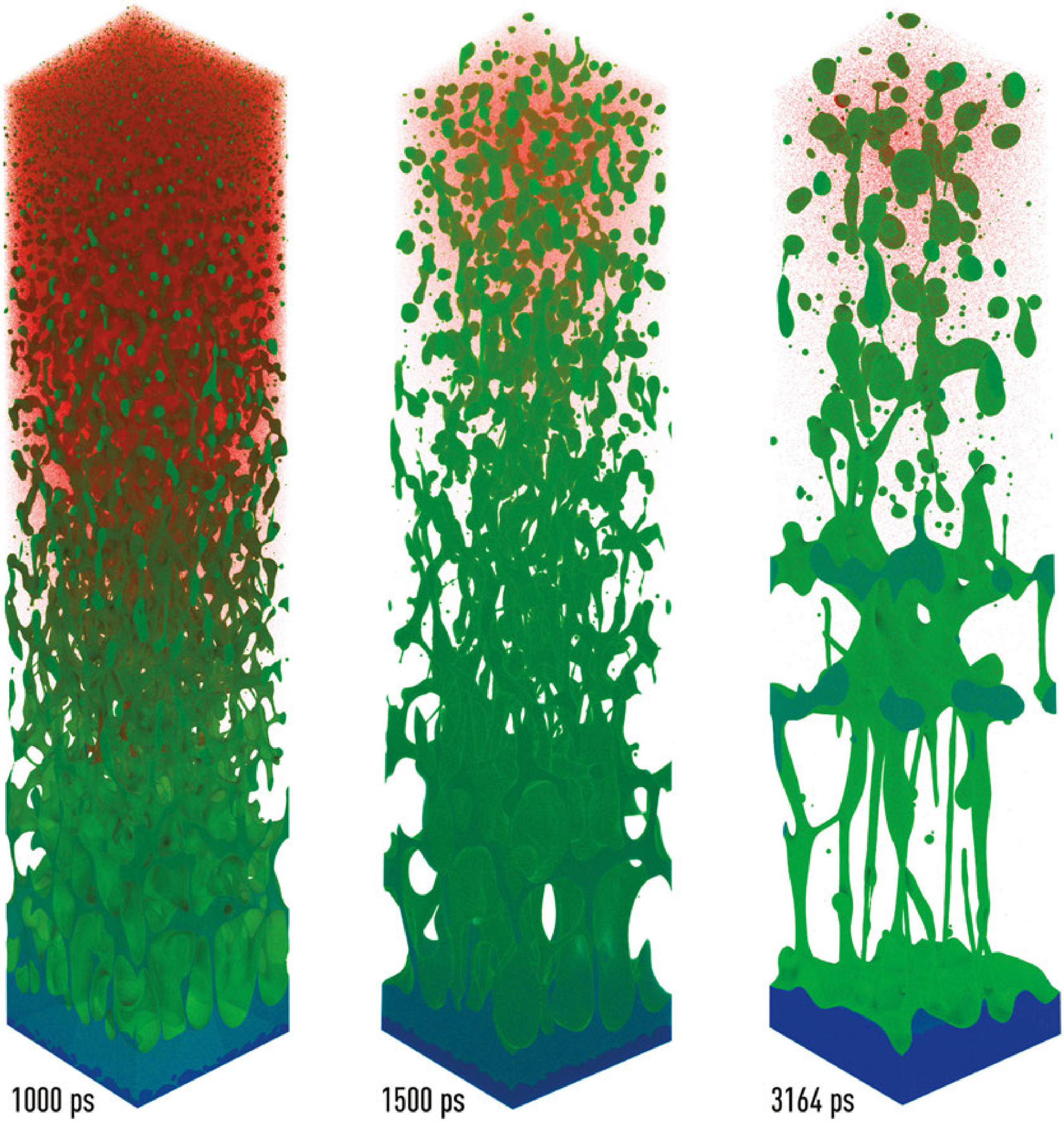
Zhigilei's team uses supercomputers to simulate these phase transformations at atomic scales. To create meaningful simulations, though, the team needs to simulate millions or, in some cases, billions of atoms. They can then watch how atoms move over a sequence of very brief moments called time steps.

By running long simulations consisting of millions of time steps, researchers may be able to observe all the processes happening during a laser–metal interaction during a total time of several nanoseconds (each nanosecond being one-billionth of a second). The team recently ran a 2.8-billion-atom simulation of silver for 3.2 nanoseconds, allowing it to compare for the first time the frozen surface's morphology—its surface structure—to experimental data.

Lasers can imbue metals with many novel properties. One way to do this is to use laser ablation, or the process of selectively removing small amounts of material, thus changing the surface morphology and microstructure. While often invisible to the human eye, this process can make major changes to a metal's characteristics.

A surface can be modified to force water to roll off in a certain direction, for example, or a metal can be given a black surface without paint. Short laser pulses can also locally modify the hardness of metals, allowing engineers to increase flexibility by creating a hard outer shell while leaving the inside of the material softer.

For more information: go.usa.gov/xNEZp



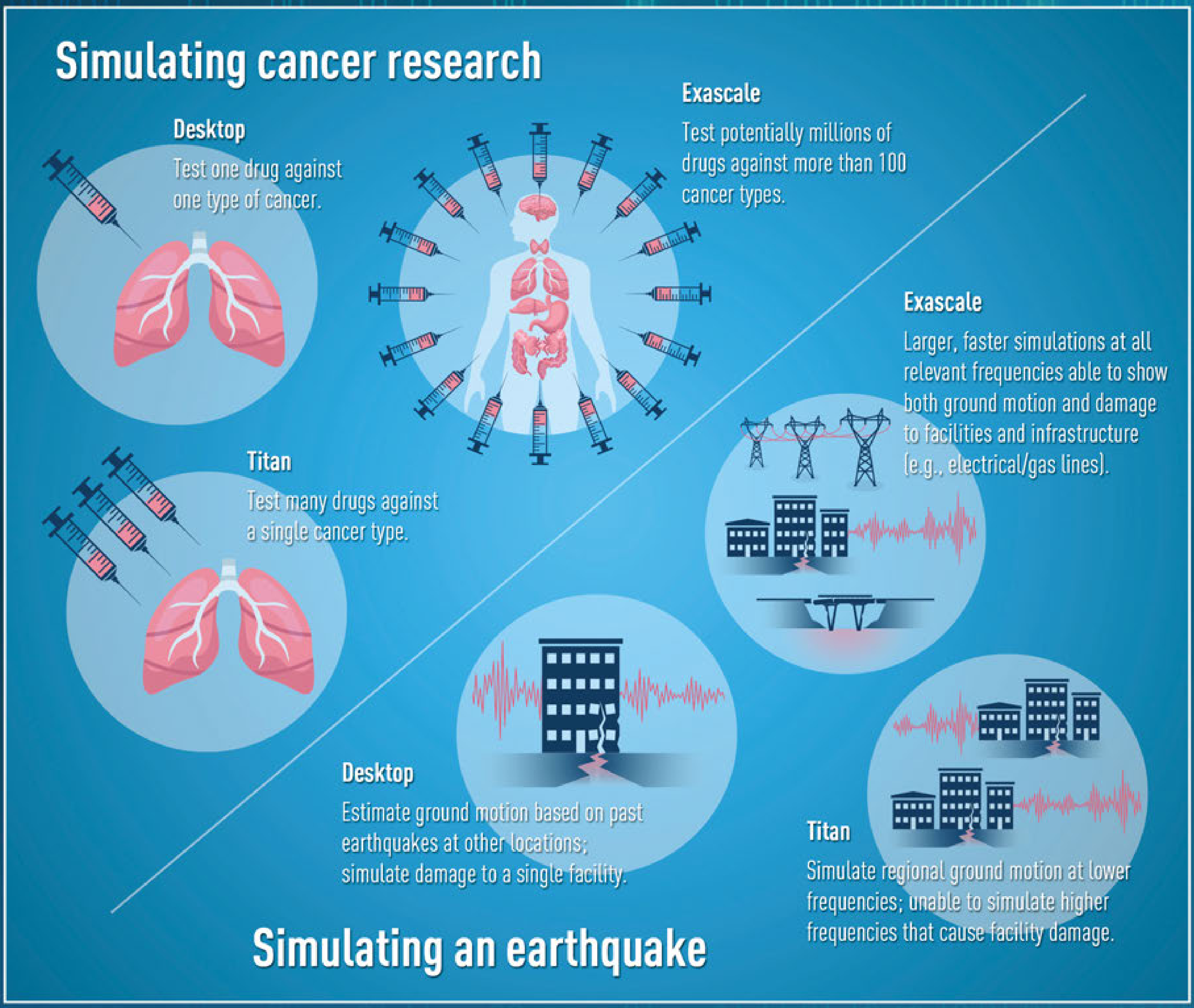
Superheated liquid rapidly decomposes into vapor and liquid droplets. Image credit: ORNL

The promise of exascale computing

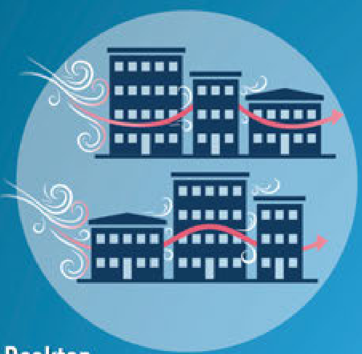
The growing power of supercomputers continues to push the boundaries of our knowledge, whether we're exploring the workings of the universe or looking for better ways to promote clean energy and human health.

Researchers including those at the DOE-supported Exascale Computing Project are preparing for the next computing milestone, which will produce systems performing over a quintillion calculations each second. By contrast a person doing one calculation each second would take more than 30 billion years to reach a quintillion.

Here are just a few ways exascale computers will expand research and development, compared to a single desktop computer and to the nation's most powerful computer today, the Titan system at the Oak Ridge Leadership Computing Facility.



Simulating Earth systems



Desktop

Resolve air flow in an urban area.

Titan

Connect global atmosphere flow to regional weather events such as droughts, heavy precipitation, etc.

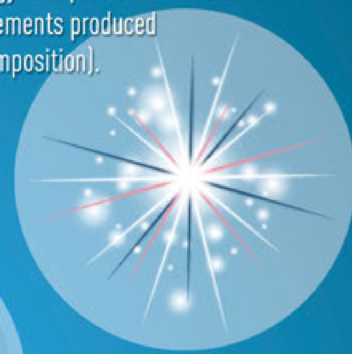
Exascale

Show global climate influencing local weather.

Simulating an exploding star (supernova)

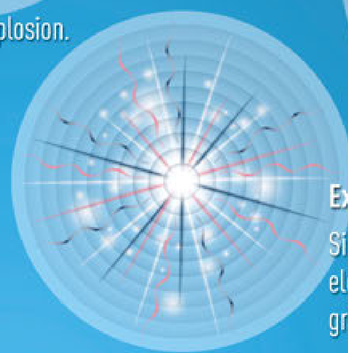
Desktop

Simulate energy of explosion.



Titan

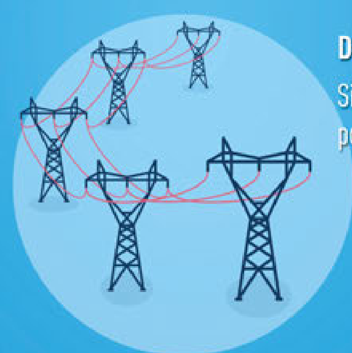
Simulate energy of explosion and amounts of different elements produced (elemental composition).



Exascale

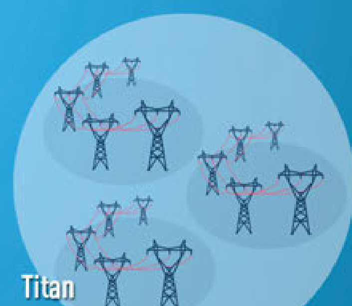
Simulate energy of explosion and elemental composition, plus photons, gravitational waves and neutrinos.

Simulating the power grid



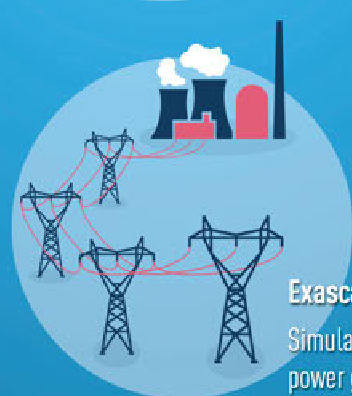
Desktop

Simulate one dynamic scenario of a regional power grid in real time.



Titan

Simulate tens of thousands of dynamic scenarios of the national power grid in real time.



Exascale

Simulate millions of dynamic scenarios of the national power grid with uncertainty in generation and demand in real time.

Image credit: Brett Hopwood, ORNL

Nuclear startup aided by high-performance computing

by Jonathan Hines
hinesjd@ornl.gov

Few jobs are bigger than building a nuclear power plant, a project that takes years and billions of dollars. And once a new plant is finished, how do engineers know it will operate as designed?

That question came up recently for the Tennessee Valley Authority's Watts Bar Unit 2. After six months of testing, the plant went into full commercial operation in October 2016, becoming the United States' first new nuclear reactor in 20 years. It produces about 1,150 megawatts of electricity—enough to power 650,000 East Tennessee homes.

Unlike earlier reactors, however, Watts Bar 2 also had the benefit of advanced computer simulations provided by the ORNL-based Consortium for Advanced Simulation of Light Water Reactors, which models and simulates nuclear reactors to better understand plant behavior.

> *"We're starting to build a case for industry to take the next step in HPC. With our modeling and simulation tools, we are hoping to show industry partners they can solve problems that no one has been able to solve before and make nuclear power a more competitive source of commercial energy."*
>
> — High-performance computing researcher Andrew Godfrey

Both TVA and the reactor's manufacturer, Westinghouse Electric Company, are consortium members. They provided data to CASL, which used high-performance computers at ORNL to carry out the largest time-dependent simulation of a nuclear power plant to date. The simulations confirmed engineers' predictions—including when the reactor would sustain a fission reaction—and provided a detailed picture of the reactor's hour-by-hour behavior during power escalation.

Watts Bar nuclear power plant. Image credit: Tennessee Valley Authority

The project marked the first time CASL had the opportunity to showcase its high-fidelity code suite, the Virtual Environment for Reactor Application—or VERA—as a predictive tool.

"Even though VERA is essentially a research code, the results of our Watts Bar Unit 2 simulations demonstrate that this is a state-of-the-art tool that industry can use to make real decisions," said Andrew Godfrey, senior research and development staff member at ORNL. "In this case CASL's high-fidelity predictions helped cement TVA's and Westinghouse's confidence that the plant would operate as expected. That confidence was later confirmed when measurements made during Unit 2's initial cycle closely matched VERA's simulated results."

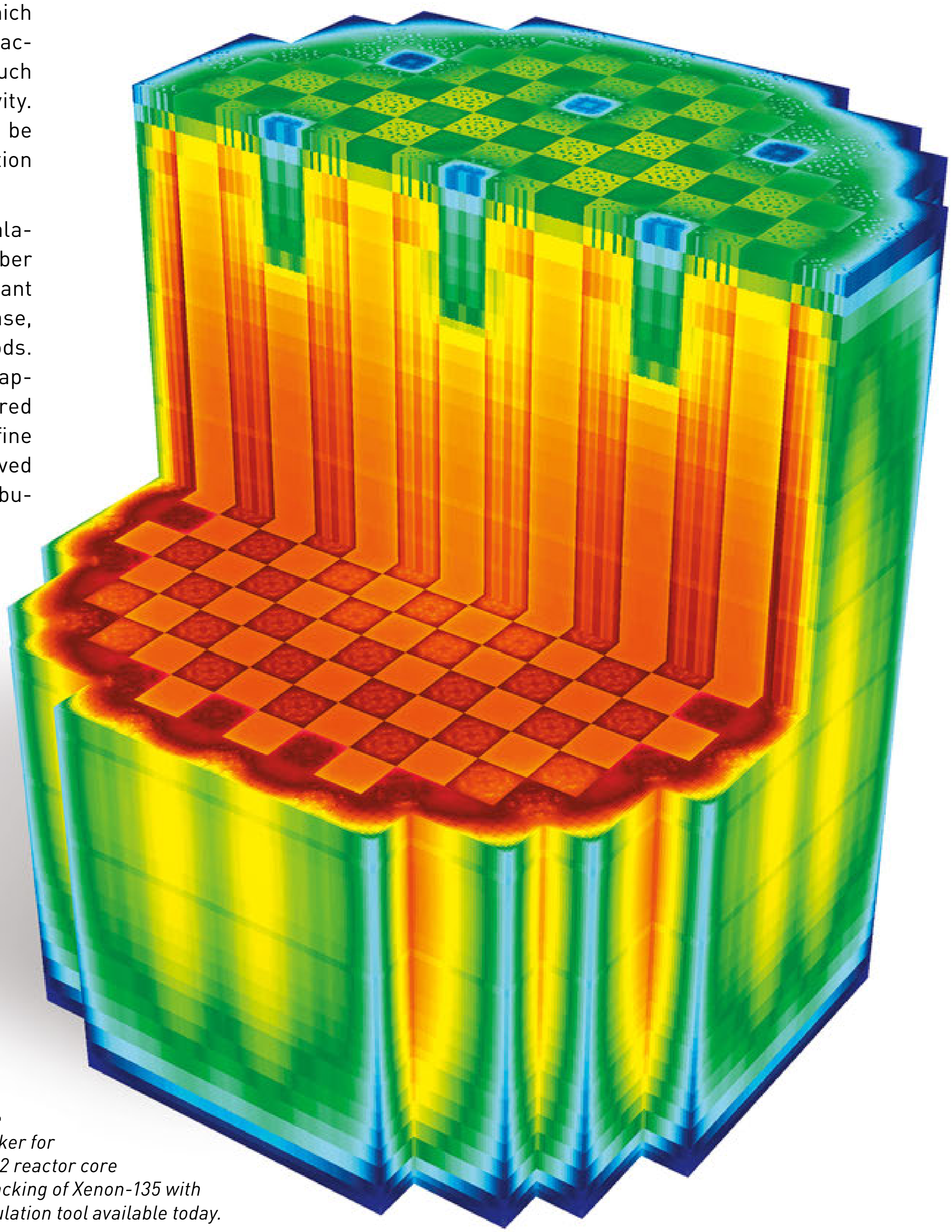
Within light-water reactors, electricity generation starts with controlled nuclear fission sustained by rods of uranium fuel. Knowing when and under what conditions the fuel will sustain a fission reaction is a critical piece of information for plant operators.

Using VERA, the CASL team built a model of the Watts Bar 2 reactor core before the plant's startup. Simulations of the core's initial cycle calculated reactor startup conditions and the underlying physics up to the point of self-sustaining fission. Specifically, the CASL team used VERA to predict boron levels, which control reactivity, and control-rod reactivity worths, which quantify how much control rods affect the rate of reactivity. Both simulated figures were found to be well within acceptable levels, information that proved valuable to TVA at startup.

During Watts Bar 2's power escalation period between June and October 2016, CASL continued to simulate plant power history through the startup phase, which spanned nine shutdown periods. The team produced hour-by-hour snapshots, or state points, that captured significant reactor properties in fine detail, including changes in short-lived fission product isotopes, power distribution, and core reactivity. In total the CASL team calculated 4,128 state points, a task that required more than 2 million core-hours of compute time.

The comprehensive Watts Bar 2 simulations provided CASL with excellent validation of VERA, which has been adapted to run on relatively small high-performance computers (about 1,000 processing units, or well under 1 percent the power of ORNL's Titan supercomputer). This makes VERA accessible to in-house systems used by companies like Westinghouse.

"We're starting to build a case for industry to take the next step in HPC," Godfrey said. "With our modeling and simulation tools, we are hoping to show industry partners they can solve problems that no one has been able to solve before and make nuclear power a more competitive source of commercial energy."



A visualization showing the distribution of the fission product Xenon-135, an important marker for predicting reactor behavior, in the Watts Bar 2 reactor core during startup. VERA enables the detailed tracking of Xenon-135 with greater fidelity than any modern reactor simulation tool available today.
Image credit: Andrew Godfrey, ORNL

Guarding the grid:

Exploring methods to protect critical infrastructure

Stephanie Seay
seaysg@ornl.gov

Modern technology has made it far more efficient, flexible, and environmentally friendly to produce and consume electricity.

We no longer rely on energy from large electromechanical machines alone. Instead, the nimbleness provided by power electronics, computing, sensors, and the internet has opened the door to renewable energy sources such as wind and solar. This technology even allows you to be an energy provider by, for instance, installing rooftop solar panels and selling excess electricity back to your local utility.

There is, however, a downside to the new complexity inherent in the electric grid. Gains in digital controls mean there are more points of access for those who would cause deliberate harm through cyber intrusion.

While cyberattacks have not caused power outages in the United States, intrusions on Ukraine's power grid in 2015 and 2016 are often cited as examples of the weakness inherent in the interconnectedness of our power system. In the attacks, hackers opened dozens of circuit breakers and shut off power to customers.

The challenge for the United States is to come up with solutions to protect communications while continuing to make the grid smarter and better able to recover when problems do arise. It is a task made harder by the grid's complexity. The system must continuously operate in real time, making research and deployment of solutions difficult.

One innovative solution is aimed at getting controls and communications for this critical infrastructure completely off the internet. ORNL is investigating ways to take advantage of literal buried treasure—underutilized fiber optic capacity already accessible to utility systems across the country that can be used to move those functions onto private networks using "dark" or unlit fiber.

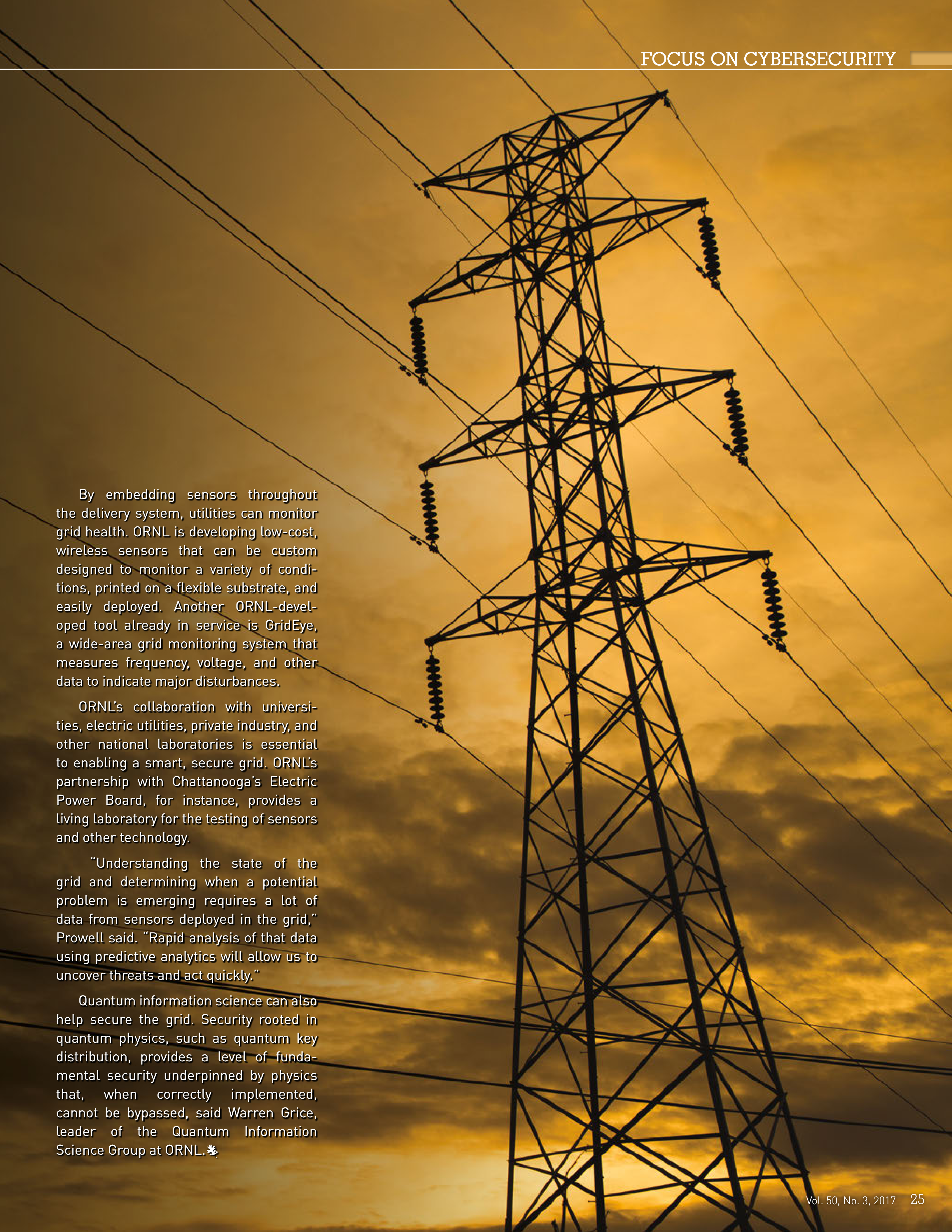
"We are evaluating the overcapacity of fiber that was deployed in the past two decades and determining whether this can be used to create a communications and control architecture where we can apply some of our innovative cyber-physical security concepts," said Tom King, director of ORNL's Sustainable Electricity Program.

Myriad other technologies can also harden the grid. To Mark Buckner, leader of ORNL's Power and Energy Systems Group, one of the fundamentals for grid security is resiliency. "No matter if a problem is natural or manmade, you want the grid to be able to handle it," he said.

One key issue for resiliency is interoperability—ensuring the grid operates smoothly despite the many actors involved. Buckner's group is already working with partners from the public and private sector to develop standards to enhance interoperability.

> *"Understanding the state of the grid and determining when a potential problem is emerging requires a lot of data from sensors deployed in the grid. Rapid analysis of that data using predictive analytics will allow us to uncover threats and act quickly."*
>
> — ORNL cybersecurity researcher **Stacy Prowell**

Stacy Prowell, chief cybersecurity research scientist and manager of ORNL's Cybersecurity for Energy Delivery Systems program, said resiliency and cybersecurity rely on a collection of solutions from better situational awareness to modeling, identifying and resolving threats.



By embedding sensors throughout the delivery system, utilities can monitor grid health. ORNL is developing low-cost, wireless sensors that can be custom designed to monitor a variety of conditions, printed on a flexible substrate, and easily deployed. Another ORNL-developed tool already in service is GridEye, a wide-area grid monitoring system that measures frequency, voltage, and other data to indicate major disturbances.

ORNL's collaboration with universities, electric utilities, private industry, and other national laboratories is essential to enabling a smart, secure grid. ORNL's partnership with Chattanooga's Electric Power Board, for instance, provides a living laboratory for the testing of sensors and other technology.

"Understanding the state of the grid and determining when a potential problem is emerging requires a lot of data from sensors deployed in the grid," Prowell said. "Rapid analysis of that data using predictive analytics will allow us to uncover threats and act quickly."

Quantum information science can also help secure the grid. Security rooted in quantum physics, such as quantum key distribution, provides a level of fundamental security underpinned by physics that, when correctly implemented, cannot be bypassed, said Warren Grice, leader of the Quantum Information Science Group at ORNL.

Start your engines:

Neutrons get a look inside a running engine

by Ashley Huff
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In a first-of-a-kind experiment, researchers used neutrons to investigate the performance of a new aluminum alloy in a gasoline-powered engine—while the engine was running.

A team from ORNL worked with industry partners to perform the test, which looked at whether a high-performance alloy that is promising for automotive applications held up under the heat and stress of an internal combustion engine.

The feat was a first for the Spallation Neutron Source, says Ke An, lead instrument scientist for the facility's VULCAN instrument. "This was the first time an internal combustion engine has been run on our diffractometer, and, as far as we know, on any other," he stated.

The unique properties of neutrons allow them to penetrate materials in a nondestructive fashion, revealing fundamental details about a material's atomic structure. VULCAN uses neutrons to measure strain and stress on large industrial samples, which made it ideal for evaluating a cylinder head cast from an aluminum-cerium alloy developed by ORNL in partnership with Eck Industries.

The experiment was led by ORNL materials scientist Orlando Rios, who has been working through DOE's Critical Materials Institute to explore the use of cerium as a strengthening agent for aluminum alloys.

"Our experiment confirmed that our alloy outperforms other aluminum alloys at elevated temperatures," Rios stated.

"The automotive industry is currently interested in alloys that can hold up to the high-heat demands of new, energy-efficient technologies," he explained. "Our aluminum-cerium composition shows exceptional stability at temperatures above 500 degrees centrigrade [932 degrees Fahrenheit], which is unheard of for aluminum alloys."

"With an aluminum alloy stable at high temperatures, engines could run hotter, and components could be made lighter, boosting efficiency and fuel economy," explained Eric Stromme, a Navy Tours with Industry Fellow who assisted on the project.

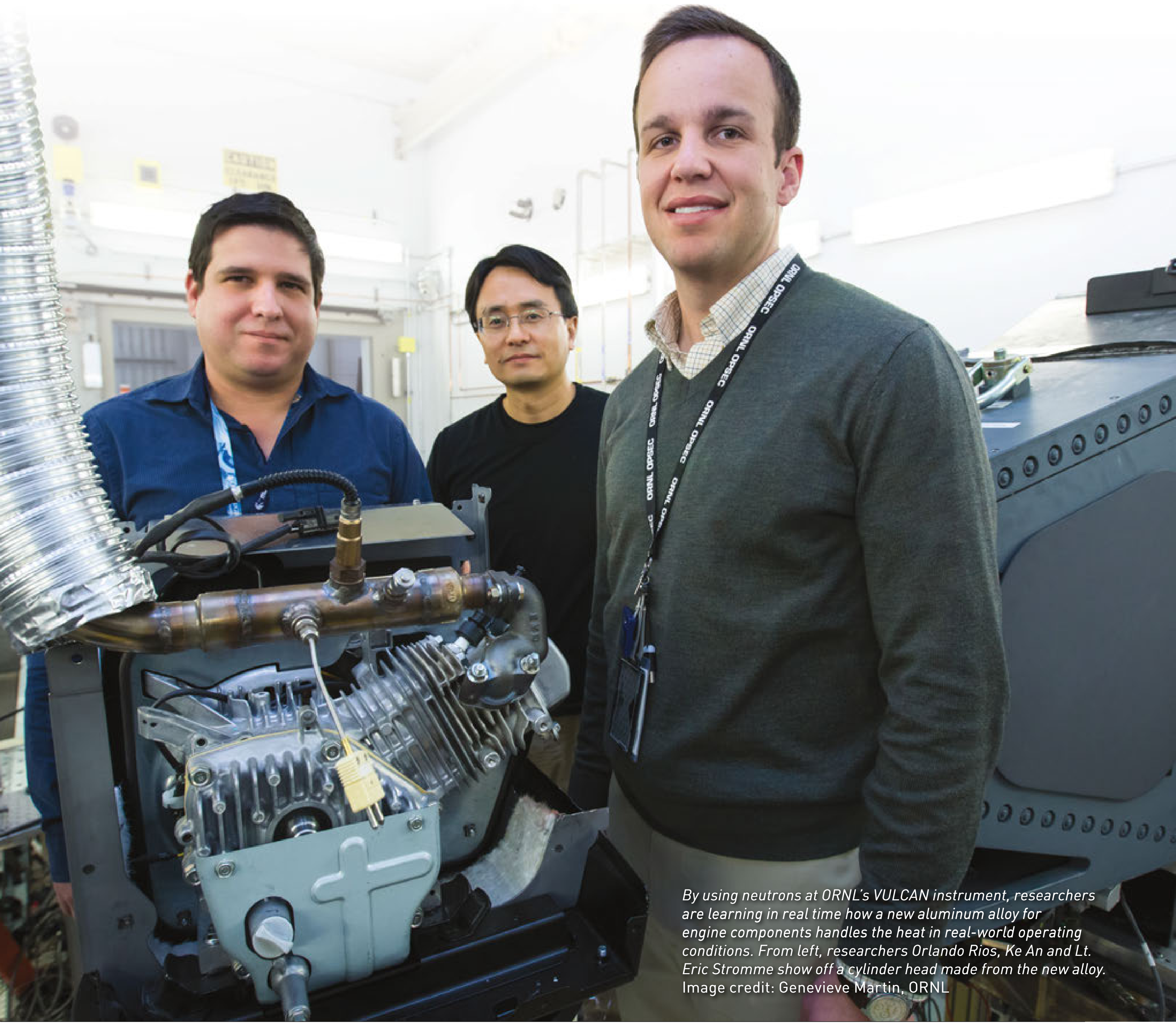
Aided by colleagues at the Manufacturing Demonstration Facility and the National Transportation Research Center, Rios's team cast the Al-Ce cylinder head using 3-D-printed sand molds and retrofitted the component to a prototype engine designed specifically for VULCAN.

Over the three-day experiment—with the engine stopping and restarting via a remote ignition from VULCAN's control room—neutron diffraction allowed the researchers to "see" the high-temperature stability of Al-Ce during the engine's operating regime.

> *"The entire team was impressed by the quality of the data from VULCAN, especially given that the neutrons had to travel through an entire engine structure before being observed by our detectors to supply information on the cylinder head at work. That is truly remarkable."*
>
> — ORNL materials scientist **Orlando Rios**

Materials experience complex forces and extreme temperatures during internal combustion, so the researchers wanted to measure material performance during actual operating conditions.

"We really took the engine through its paces. It was probably the loudest experiment to take place at SNS," joked Rios, who worked on the project with ORNL



By using neutrons at ORNL's VULCAN instrument, researchers are learning in real time how a new aluminum alloy for engine components handles the heat in real-world operating conditions. From left, researchers Orlando Rios, Ke An and Lt. Eric Stromme show off a cylinder head made from the new alloy.
Image credit: Genevieve Martin, ORNL

postdoc Michael Kesler and Bredesen Center Fellow Zachary Sims.

"The entire team was impressed by the quality of the data from VULCAN, especially given that the neutrons had to travel through an entire engine structure before being observed by our detectors to supply information on the cylinder head at work," said Rios. "That is truly remarkable."

"What we have accomplished is a proof of concept to prove the feasibility and value of this kind of experiment," said An.

An noted the effectiveness of collaborating across disciplines between ORNL and industry partners to support the effort. He is currently working to streamline the process for future VULCAN users.

"This was a fundamental experiment not only to better understand this alloy but also to provide some broader analysis that will allow new alloys, not only aluminum compounds, to be processed in this way," Rios said. "We hope what we are learning through this experiment can be applied to many other materials in a wide range of applications."

Neutrons zero in on elusive magnetic Majorana fermion

by Jeremy Rumsey
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Neutron scattering has provided new insights into the exotic magnetic behavior of a material that, with a fuller understanding, could pave the way for advanced quantum computing.

Looking within a two-dimensional graphenelike material called alpha-ruthenium trichloride, an ORNL-led research team confirmed magnetic signatures that are likely related to Majorana fermions—elusive particles that could be the basis for a quantum bit, or qubit. The results, published in the journal *Science*, verify and extend a 2016 *Nature Materials* study in which the team from ORNL, the University of Tennessee, Max Planck Institute and Cambridge University first proposed this unusual behavior in the material.

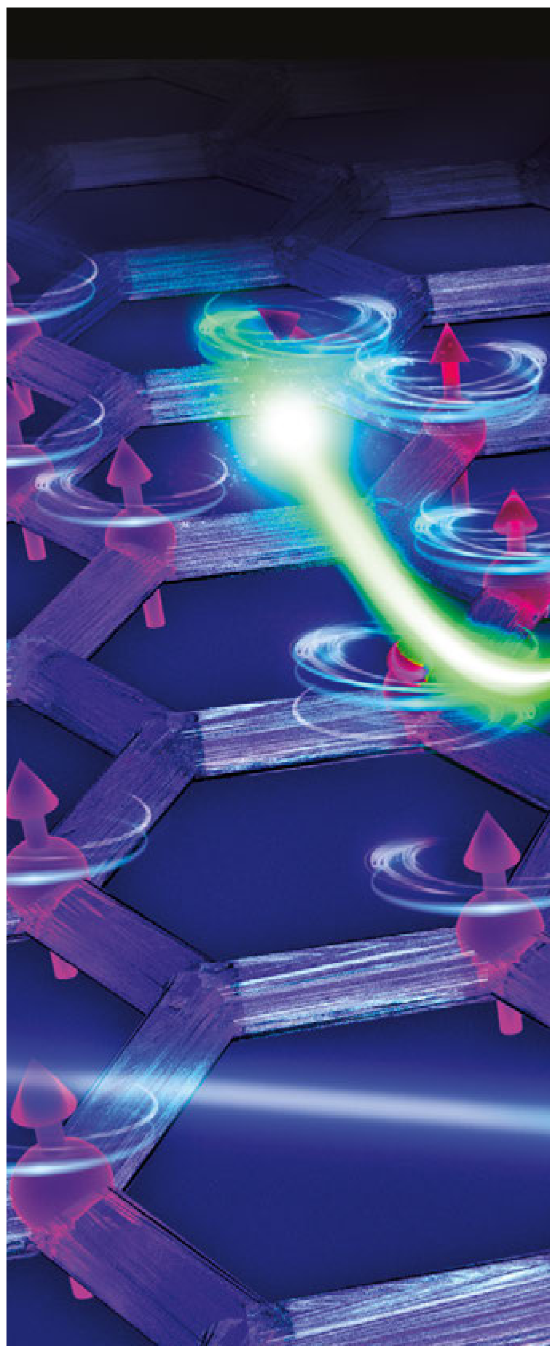
"This research is a promise delivered," said lead author Arnab Banerjee, a postdoctoral researcher at ORNL. "Before, we suggested that this compound, alpha-ruthenium trichloride, showed the physics of Majorana fermions, but the material we used was a powder and obscured many important details. Now, we're looking at a large single crystal that confirms that the unusual magnetic spectrum is consistent with the idea of magnetic Majorana fermions."

Majorana fermions were theorized in 1937 by physicist Ettore Majorana. Unlike electrons and protons, whose antiparticles (the positron and the antiproton) have equal but opposite charges, Majorana fermions are their own antiparticle and have no charge.

In 2006 physicist Alexei Kitaev developed a solvable theoretical model describing how topologically protected quantum computations could be achieved in a material using quantum spin liquids. QSLs are strange states achieved in solid materials where the magnetic moments, or "spins," associated with electrons exhibit a fluidlike behavior.

> *"The improvements in the new measurements are like looking at Saturn through a telescope and discovering the rings for the first time."*
>
> — ORNL Quantum Condensed Matter Division Director **Steve Nagler**

"Our neutron-scattering measurements are showing us clear signatures of magnetic excitations that closely resemble the model of the Kitaev QSL," said corresponding author Steve Nagler, director of the Quantum Condensed Matter Division at ORNL. "The improvements in the new measurements are like looking at Saturn



through a telescope and discovering the rings for the first time."

Because neutrons are microscopic magnets that carry no charge, they can be used to interact with and excite other magnetic particles in the system without compromising the integrity of the material's atomic structure. Neutrons can measure the magnetic spectrum of excitations, revealing how particles behave. The team cooled the material to temperatures near absolute zero (about minus 450 degrees Fahrenheit) to allow direct observation of purely quantum motions.

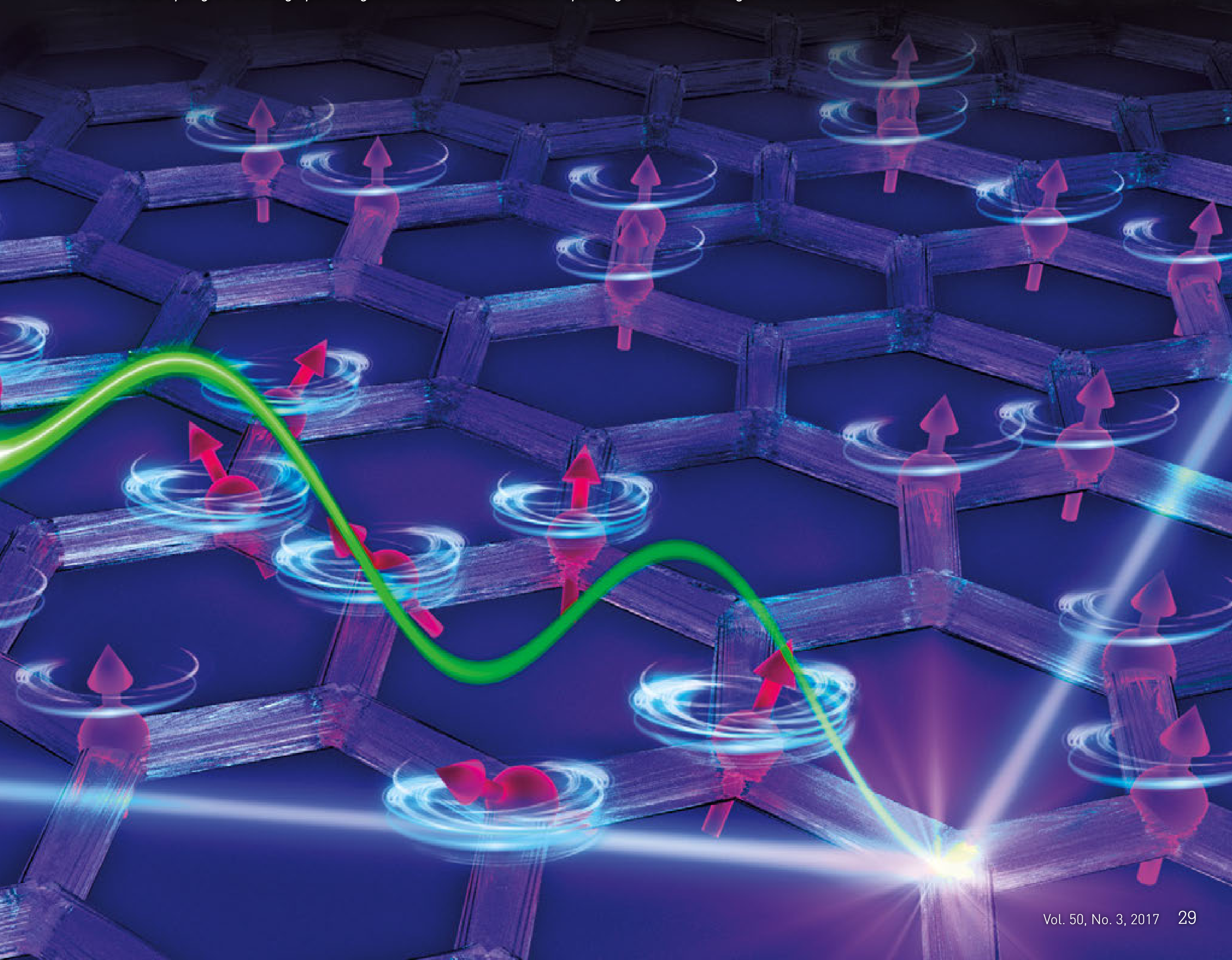
Using the SEQUOIA instrument at ORNL's Spallation Neutron Source allowed the investigators to map out an image of the crystal's magnetic motions in both space and time.

"We can see the magnetic spectrum manifesting itself in the shape of a six-pointed star and how it reflects the underlying honeycomb lattice of the material," said Banerjee. "If we can understand these magnetic excitations in detail, then we will be one step closer to finding a material that would enable us to pursue the ultimate dream of quantum computations."

Banerjee and his colleagues are conducting additional experiments with applied magnetic fields and varying pressures.

"We've applied a very powerful measurement technique to get these exquisite visualizations that are allowing us to directly see the quantum nature of the material," said coauthor Alan Tennant, chief scientist for ORNL's Neutron Sciences Directorate. "Part of the excitement of the experiments is that they're leading the theory. We're seeing these things, and we know they're real."

As neutrons (blue line) scatter off the graphenelike honeycomb material, they produce a magnetic Majorana fermion (green wave) that moves through the material, disrupting or breaking apart magnetic interactions between "spinning" electrons. Image credit: Jill Hemman, ORNL



Neutrons provide the first nanoscale look at a living cell membrane

by Leo Williams
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The membrane of a living cell is central to its well-being. Not only does it protect the cell's contents from its environment, the membrane also decides what gets in and out and participates in a variety of other indispensable processes.

Despite its importance, however, we haven't gotten a good look at the cell's plasma membrane—until now.

An ORNL research team recently performed the first-ever direct nanoscale examination of a living cell membrane. In doing so it resolved a long-standing debate by identifying tiny groupings of lipid molecules that are likely key to the cell's different functions.

The methods developed by the team provide a new experimental platform for biophysical studies of membranes and, potentially, other cell components. It could prove useful for future research on important interactions such as drug-membrane, biofuel-membrane, and even antibiotic-membrane interactions.

The multidisciplinary project—led by biophysicist John Katsaras, chemist Bob Standaert and microbiologist James Elkins—was performed at the lab's High Flux Isotope Reactor and Spallation Neutron Source using the bacterium *Bacillus subtilis*. The team published its findings in the journal *PLoS Biology*.

A cell's membrane is a thin bilayer of lipid molecules that also contains proteins. Researchers have been uncertain about whether membrane lipids are randomly distributed in the membrane or sometimes organize into groups—so-called lipid domains that are thought to enable functions such as signaling between cells.

"It became a debate," Katsaras said. "Some people believed they existed, while others believed they didn't. There was a lot of circumstantial evidence that could support either side."

> *"It became a debate. Some people believed they existed, while others believed they didn't. There was a lot of circumstantial evidence that could support either side."*
>
> — ORNL biophysicist **John Katsaras**, on lipid domains thought to enable cell functions

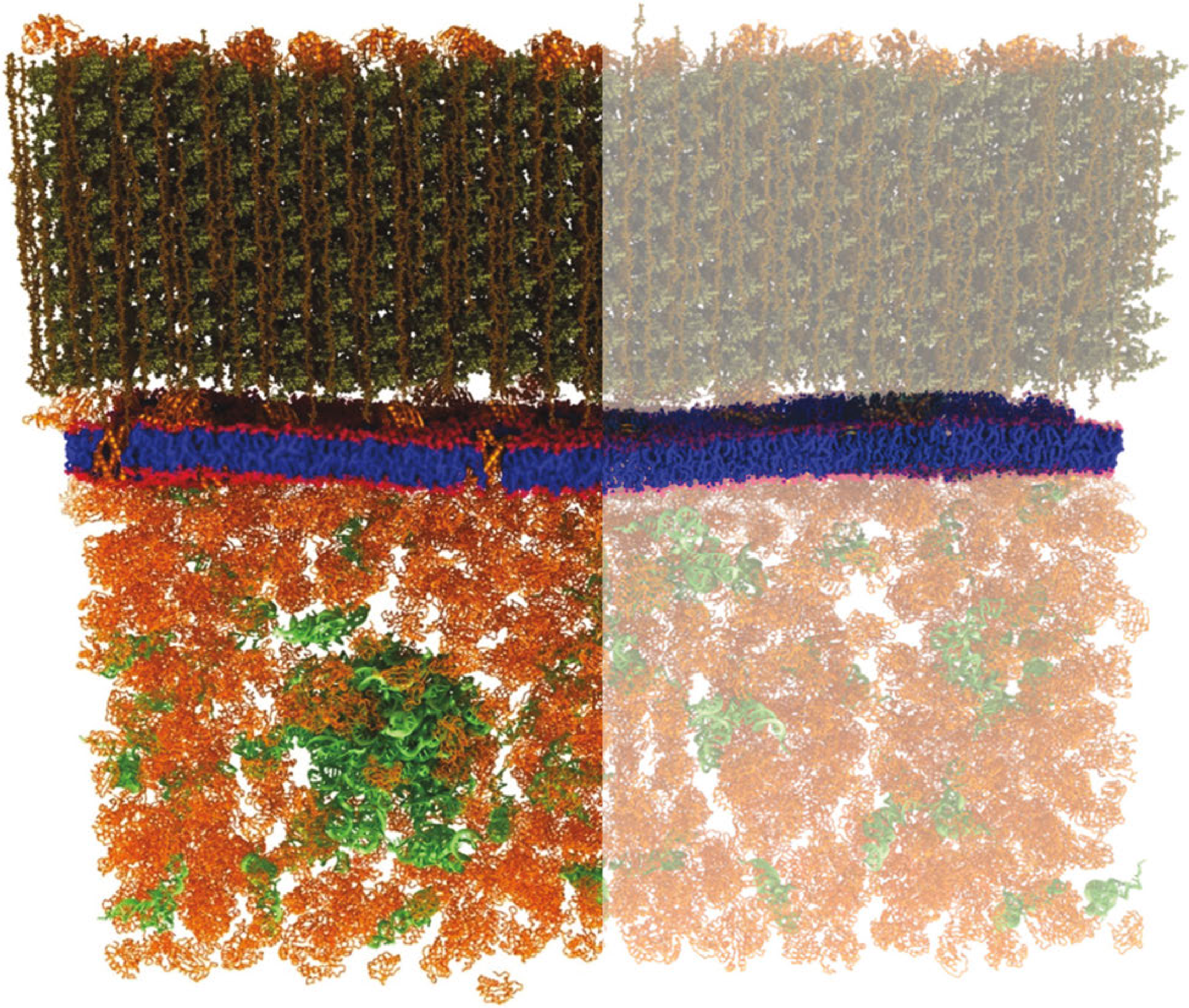
Neutron scattering analysis was key to the project's success. Lipid domains are too small to be seen by optical microscopes. However, neutrons have no such limitation and can provide a nanoscale view of a cell. Moreover, unlike other nanoscale tools, neutrons can be used for examining a live cell without damaging it.

While neutron scattering overcame the limitations of the other technologies, it had its own challenges. The first was to develop an experiment in which neutrons scattered off of lipid molecules in the membrane without interacting with other components of the cell, such as proteins, RNA, DNA and carbohydrates. The next challenge was to distinguish one type of lipid molecule from another.

The solution to both challenges lay in the use of deuterium, an isotope of hydrogen whose nucleus contains a neutron as well as a proton. By contrast, common hydrogen nuclei contain a proton but no neutron. While a biological cell itself perceives little difference between normal hydrogen and deuterium, the two isotopes appear very different to neutrons.

The ORNL team created a strain of the bacterium containing enough deuterium to make the cell structures essentially invisible to neutrons. They then ensured that the lipid molecules within the membrane were made up entirely of two fatty acids containing specific proportions of deuterium and hydrogen.

The membrane was free to create any of dozens of types of lipid molecules with



these two fatty acids, with each lipid type then containing a specific mix of the two isotopes. If the lipids were distributed randomly throughout the membrane, then the membrane would appear uniform when exposed to neutrons, akin to an optical background that was medium gray.

If, however, the lipids gathered with others of their type, the background would cease to be uniform and would show the equivalent of lighter and darker gray areas. This is in fact what the team found, with the grey patches measuring less than 40 nanometers across.

The ORNL researchers stressed that these techniques hold promise for other research as well.

"For example, you could use the modified bacteria as a platform for investigating antibiotics," Katsaras noted, "because a lot of antibiotics are really talking to the membrane."

Neutron scattering is a valuable technique for studying cell membranes, but signals from the cell's other components can get in the way (left). An ORNL team made these other components practically invisible to neutrons by combining specific levels of heavy hydrogen (deuterium) with normal hydrogen within the cell. Image credit: Xiaolin Cheng and Mike Matheson, ORNL

More efficient

turbine engines trace roots back a quarter century

During DOE programs to advance industrial ceramic matrix composites, ORNL materials scientist Karren More (foreground, with former ORNL colleague Larry Walker) used transmission electron microscopy and other techniques to pinpoint causes of failure in stress- or field-tested materials made by companies. Image credit: ORNL

by Dawn Levy
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Ceramic matrix composite materials are made of coated ceramic fibers surrounded by a ceramic matrix.

They are tough, lightweight and capable of withstanding temperatures 300 to 400 degrees Fahrenheit hotter than metal alloys can endure. Among other applications, they would allow the turbine engines of aircraft and power plants to operate more efficiently at higher temperatures, burning fuel more completely and emitting fewer pollutants.

A quarter-century after the launch of an ORNL-led DOE program to support CMC development in the United States, the first widely deployed CMC-containing product has now hit the market.

The LEAP aircraft engine has one CMC component, a turbine shroud lining its hottest zone. The shroud lets the engine operate at up to 2,400 degrees Fahrenheit, meaning it needs less air cooling than nickel-based super-alloys. The component is among a suite of technologies that contribute to 15 percent fuel savings for LEAP over its predecessor.

The LEAP engine is manufactured by CFM International, a 50/50 joint venture of Safran Aircraft Engines and GE. Presales to airlines eager to lower their fuel costs

Advanced materials take flight in the LEAP engine, featuring ceramic matrix composites developed over a quarter century by GE with help from DOE and ORNL. Image credit: GE

are staggering—$140 billion at list price for more than 11,000 engines.

In August 2016 the first LEAP engine—on an Airbus A320neo—started flying commercially. Other LEAP engines will fly on the Boeing 737 MAX in 2017.

On the surface, CMCs seem unlikely candidates to revolutionize the technology of air travel.

"A CMC is different than almost all other composites because the matrix is ceramic and the fiber is ceramic," ORNL's Rick Lowden noted.

Combining two brittle materials would typically yield another brittle material. But altering the bond between the fiber and the matrix allows a CMC to act more like a piece of wood. Cracks don't propagate into the fibers from the matrix around them. The fibers hold the material together and carry the load while slowly pulling from the matrix, adding toughness.

DOE's CMC-development program ran from 1992 to 2002, with the agency funding companies to make composites and national labs and universities to characterize the properties of the materials. The cost was about $10 million a year, and industry shared the expense. Companies took materials they'd made to Argonne National Laboratory for nondestructive evaluation and ORNL for microstructural characterization as well as stress and oxidation tests.

"This partnership highlights the value of the national labs," ORNL's Karren More said. "We do work that is fundamental and broad to understand materials' behaviors. We provide necessary information to help the community make decisions about where to go, how to proceed."

ORNL's early findings encouraged industry to abandon carbon as a fiber coating. Carbon oxidized, evaporating as carbon monoxide and carbon dioxide, which rapidly degraded the coating. ORNL engineers recommended oxidation-resistant boron nitride instead.

A follow-on DOE program ran through 2005 and funded companies with promising results to further develop materials and components and, if possible, test them in applications. Total funding was approximately $15 million, with industry's share approaching 50 percent. All told, GE invested $1.5 billion after that to commercialize the technology.

Today success is evident in new CMC factories and jobs. In 2002 GE acquired a CMC facility in Newark, Delaware, which has since grown substantially. A new GE facility for making shroud components opened in Asheville, North Carolina, in 2014. In addition, GE is building two adjacent factories in Huntsville, Alabama—the first to ramp up fiber production and the second to coat fibers and make tape for processing into components. At full scale the Asheville and Huntsville sites are expected to bring 640 high-tech jobs to the areas.

Looking forward, GE will produce an engine in 2019 that has *five* CMC parts—two combustor liners, two nozzles, and one shroud. Presales of this engine—GE9X—are approximately $29 billion at list prices for 700 engines.

For more information: go.usa.gov/xNEkj

Small nanoparticles

have surprisingly big effects on polymer nanocomposites

by Dawn Levy
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Polymer nanocomposites mix particles billionths of a meter wide with polymers, which are long molecular chains. Often used to make injection-molded products, these nanocomposites are common in such disparate products as automobiles, fire retardants, drug-delivery systems and medical devices.

Conventional wisdom held that shrinking nanoparticles beyond an optimal size would make the polymer nanocomposites less effective, yet when an ORNL-led team tried to verify that wisdom, they got a big surprise.

"We found an unexpectedly large effect of small nanoparticles," said ORNL materials scientist Shiwang Cheng.

Blending nanoparticles and polymers enables dramatic improvements in the properties of polymer materials. The behavior of composites depends on the size of the nanoparticles as well as their spacing and interactions with polymer chains. Understanding these effects will allow for the improved design of new composite polymers.

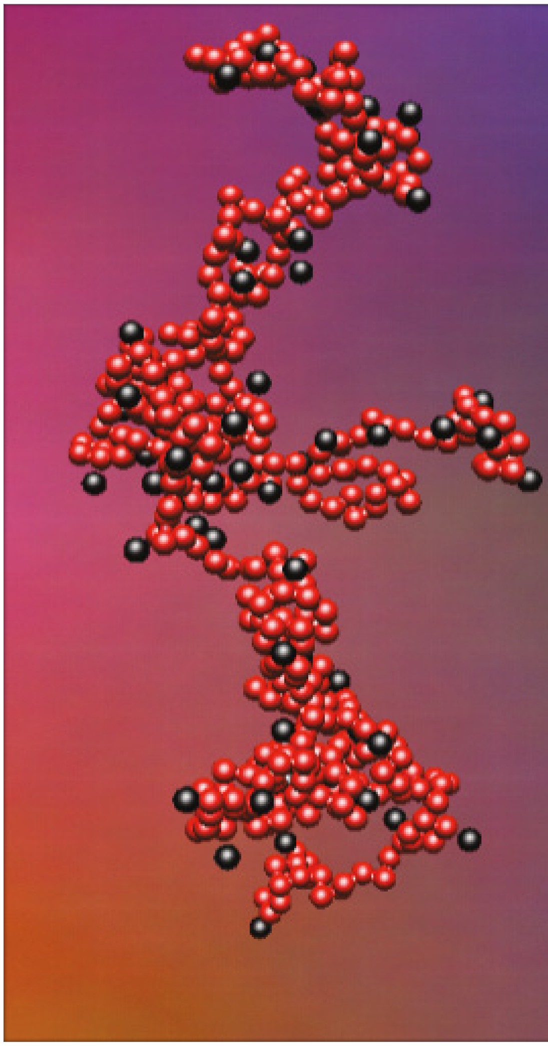
Most conventional polymer nanocomposites contain particles 10 to 50 nanometers wide. In contrast, the ORNL-led study compared polymer nanocomposites containing particles 1.8 nanometers wide and those with particles 25 nanometers wide.

In particular, well-dispersed, small "sticky" nanoparticles improved properties of composites by significantly increasing the temperature above which material starts to flow, known as the glass transition temperature.

One of these properties even broke records: Specifically, raising the material's temperature less than 10 degrees Celsius caused a fast, millionfold drop in viscosity. A pure polymer (without nanoparticles) or a composite with large nanoparticles would need a temperature increase of at least 30 degrees Celsius for a comparable effect.

"We see a shift in paradigm where going to really small nanoparticles enables accessing totally new properties," said physicist Alexei Sokolov of ORNL and the University of Tennessee.

The new properties appear because small particles move faster than large ones and interact with fewer polymer segments on the same chain. Many



more polymer segments stick to a large nanoparticle, making it difficult for a chain to separate from that nanoparticle.

"Now we realize that we can tune the mobility of the particles, how fast they can move, by changing particle size, and how strongly they will interact with the polymer by changing their surface," Sokolov said. "We can tune properties of composite materials over a much larger range than we could ever achieve with larger nanoparticles."

The study, carried out with colleagues from UT and the University of Illinois, required expertise in materials science, chemistry, physics, computational science and theory. "The main advantage of Oak Ridge National Laboratory is that we can form a big, collaborative team," Sokolov said.

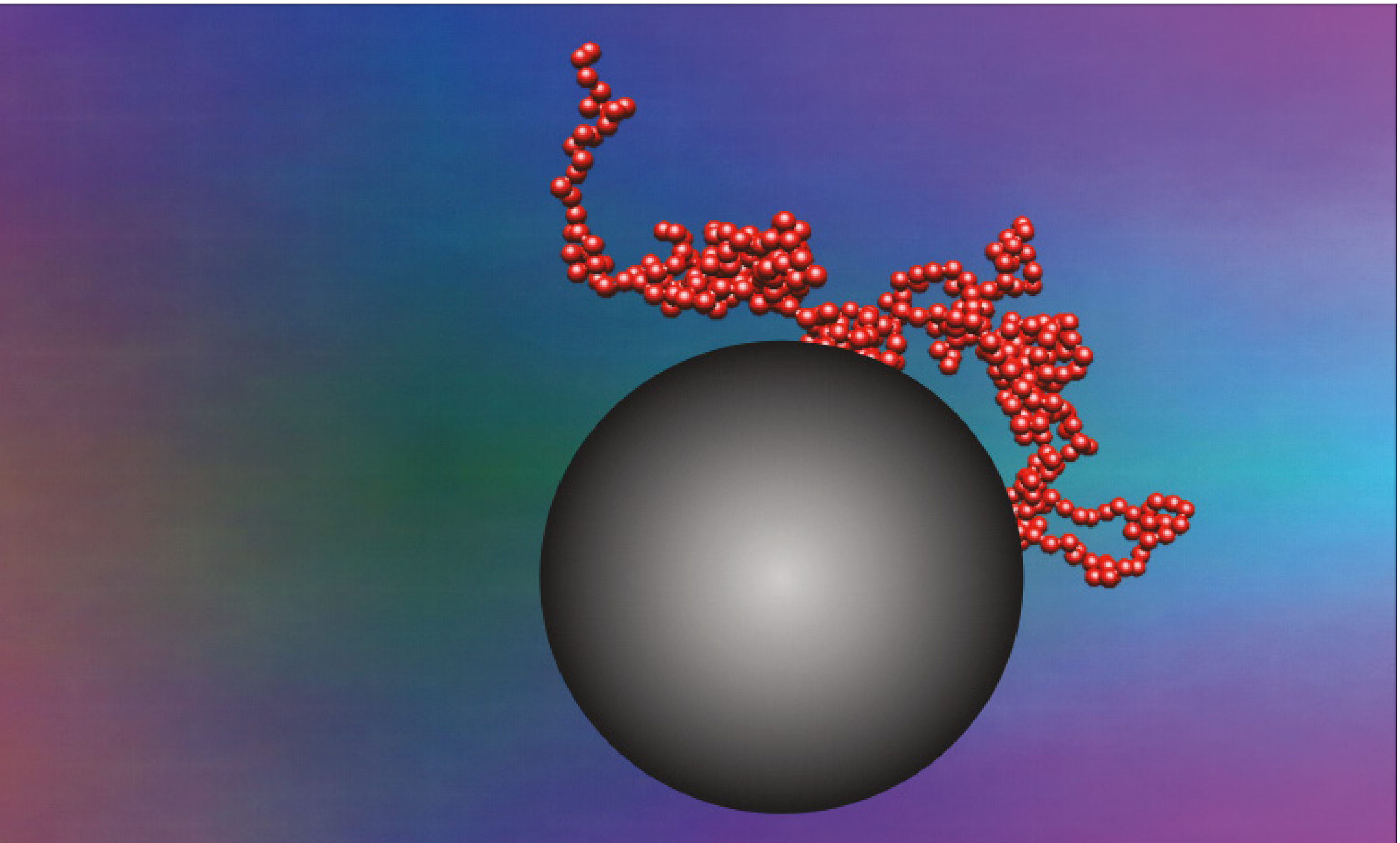
Cheng and UT's Bobby Carroll carried out experiments. Broadband dielectric spectroscopy tracked the movement of polymer segments associated with nanoparticles. Calorimetry revealed the temperature at which solid composites transitioned to liquids. Using small-angle X-ray scattering, Halie Martin of UT and Mark Dadmun of UT and ORNL characterized nanoparticle dispersion in the polymer.

The team also turned to large-scale computer modeling and simulation, carried out by ORNL physical chemist Bobby Sumpter and UT materials scientist Jan-Michael Carrillo.

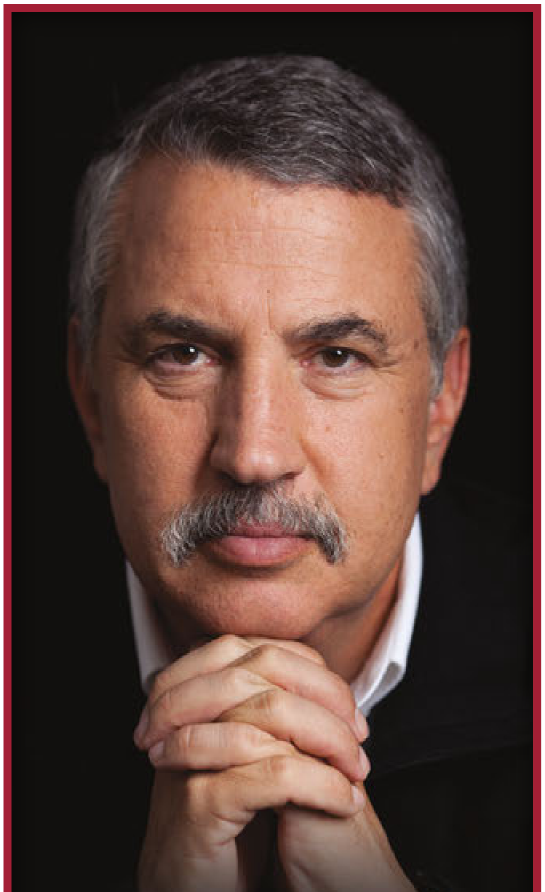
Shi-Jie Xie and Kenneth Schweizer, both from Illinois, created a new fundamental theoretical description of the collective activated dynamics in such nanocomposites and quantitatively applied it to understand novel experimental phenomena such as the changes in viscosity and glass transition temperature. The theory enables predictions of physical behavior that can be used to formulate design rules for optimizing material properties.

Carrillo and Sumpter developed and ran simulations on ORNL's Titan supercomputer and wrote codes to analyze the data on the lab's Rhea cluster. The simulations visualized how nanoparticles moved relative to a polymer chain.

For more information:
go.usa.gov/xN85k



Small nanoparticles (left) stick to polymer chain segments that are about their own size, producing a polymer nanocomposite in which nanoparticles move quickly, making the material less viscous. At right, many segments of a polymer chain stick to a larger nanoparticle, making it more viscous.
Image credit: Jan-Michael Carrillo, ORNL



Thomas Friedman is an award-winning journalist and author. In nearly four decades with the *New York Times*, he has won three Pulitzer Prizes, the first in 1983 for coverage of the war in Lebanon, the second in 1988 for coverage of Israel, and the third in 2002 for commentary on the impact of terrorism.

Friedman graduated summa cum laude from Brandeis University in 1975 and earned a master of philosophy in Middle Eastern studies from the University of Oxford in 1978. He currently writes a weekly column for the *New York Times* and has published seven books, including 2016's *Thank You for Being Late: An Optimist's Guide to Thriving in the Age of Accelerations*.

Friedman delivered the Eugene P. Wigner Distinguished Lecture May 10, 2017, on the topic "Thank You for Being Late: A Discussion of the Social, Political, Ethical, and Economic Implications of the Age of Accelerations."

This is an edited transcript from his question-and-answer session with lab staff.

Distinguished

Thomas Friedman

1. The acceleration of new technology has created a lot of anxiety across the economy. Where will jobs be in the coming decades?

If horses could have voted, there never would have been cars, so we have been here before, but not at the scale and scope of both white-collar and blue-collar work.

There's definitely a much bigger challenge going on now, but I would say a couple of things. One is, I'm always impressed at the creativity of human beings to find and spawn work of value. I was at a conference last September, and a woman there said her job was tagging sharks for Twitter. I thought to myself, "Who in the world knew there was a job tagging sharks for Twitter?" It's probably a good middle-class job.

Number two, what was one of the fastest growing restaurant chains in 2015? According to *Entrepreneur* magazine it was a restaurant called Paint Nite. What is Paint Nite? It's paint-by-numbers for adults in bars. Adults like to get together in bars where an artist draws up a sketch and leads them in painting while they have a few drinks together. Who knew? By the way, those artists make about $50,000 a year for three hours of work, five nights a week.

This falls into a category I wrote about a couple of months ago with my friend Dov Seidman. The column was called, "From Hands to Heads to Hearts." His argument is basically that in the age of acceleration we'll work with our hearts—the one thing machines do not and cannot ever have—and connect hearts to hearts.

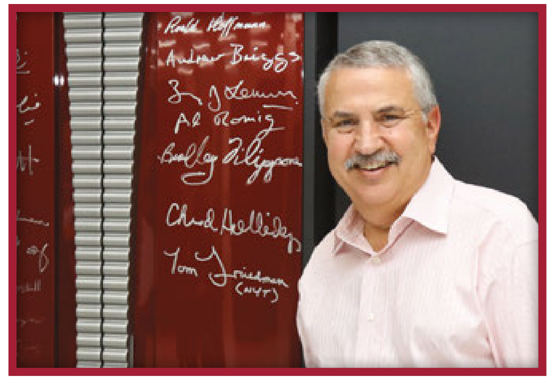
I coined a term in the book called "STEMpathy," because I think the best jobs going forward—and there's data on this now—are those that combine science, technology, engineering and math, and human empathy. It's the STEMpathy jobs that are, I think, going to be the great jobs of the 21st century.

2. How can people prepare for these new opportunities?

Every problem I describe requires more skill. It requires more computational skill, because every job is becoming a data job, and it requires more critical thinking.

At the same time, it requires more lifelong learning. What's new today is that to get a job and hold a job requires more learning up front and more learning across your lifetime. A lot of very good people aren't built that way; they like to come to work, do an honest day's work, and go home, and actually be told what to do.

Lecturer



3. Technology now guides many areas of our lives, whether through Google Maps or dating websites. What will be the role of people in an age of algorithms?

The book is not called *Thank You for Being Late* for nothing; it's a celebration of everything old and slow. And the subtext of the book is that I believe all the things that are important today are things you cannot download. You have to upload them the old-fashioned way, from good parent to good child, good teacher to good student, good mayor to good community, good leader to good institution. The faster the world gets, the more all that old stuff matters.

Look at fake news. We have fake news because the internet is an open sewer of untreated, unfiltered information. It's full of diamonds and gold nuggets and silver, we all know that, but it's also full of rusty nails, broken glass, tin cans and fake news. If we don't build the internal filters into our citizens and our students and our kids the old-fashioned way, under the olive tree, we're going to have a real problem.

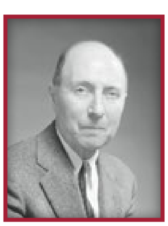
Look at opioid addiction. It's not a law-enforcement problem; it's a community problem. You're only going to fix that when people are embedded in a healthy community.

I want to understand technology, I want to get the most out of it, but I've come back to the thing that really matters, and that's community. For every problem I come up against, community is the answer. In the age of acceleration, national governments are too slow and the single family is too weak, especially since too many are led by single parents. It's going to be the healthy community that's going to be the ideal government unit for the age of acceleration.

4. What do you see as the role for national laboratories such as ORNL?

Our national labs are one of the great pillars of our society, but they're so underbranded in terms of the technologies and breakthroughs they've spun off, from medicine to the auto industry. But they're what make us unique.

In an age of acceleration, you have to accelerate learning too. That's why what you're doing is so important. Finding a way to communicate that to people is a real challenge, but I think it's doubly important now, when small errors in navigation can have such huge negative consequences.



The Eugene P. Wigner Distinguished Lecture Series in Science, Technology, and Policy gives scientists, business leaders and policy makers an opportunity to address the ORNL community and exchange ideas with lab researchers. The series is named after Eugene Wigner, ORNL's first research director and recipient of the 1963 Nobel Prize in Physics.

ORNL is proud of its role in fostering the next generation of scientists and engineers. We bring in talented young researchers, team them with accomplished staff members, and put them to work at the lab's one-of-a-kind facilities. The result is research that makes us proud and prepares them for distinguished careers.

We asked some of these young researchers why they chose a career in science, what they are working on at ORNL, and where they would like to go with their careers.

Vidya Kishore

Graduate student, Manufacturing Demonstration Facility
Ph.D. student, Energy Science and Engineering, University of Tennessee (Bredesen Center)
Hometown: Chennai, India

What are you working on at ORNL?

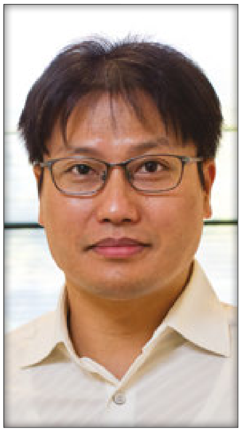
I currently work on characterizing material properties of high-performance thermoplastic composites for large-scale 3-D printing on the Big Area Additive Manufacturing system. My research will contribute to answering the big question in 3-D printing—"What makes a material printable?"—and also involve methods to enhance properties of printed parts.

What would you like to do in your career?

I would like to continue working in the field of polymer additive manufacturing, further exploring its capabilities and contributing to the development of new printable materials.

Why did you choose a career in science?

From childhood my interactions with my father, a chemical engineer, kindled a strong desire in me to understand how things work and solve real-world problems that could have a broad impact. With a career in science, it is exciting to work with people who share a common goal. There is something new to learn every day.



Seong Jin An

Graduate student, Energy and Transportation Science Division
Ph.D. student, Energy Science and Engineering, University of Tennessee (Bredesen Center)
Hometown: Busan, South Korea

What are you working on at ORNL?

My research currently focuses on correlating long-term lithium-ion battery performance with protective film properties. The protective film forms on electrodes during the first few cycles of charge/discharge and makes a battery rechargeable reversibly. This research is necessary to improve the cycle life and safety of batteries.

What would you like to do in your career?

I have been working on analyzing and improving electrochemical energy cells such as batteries and fuel cells. I would like to stay in the electrochemical field and expand my work to develop a new electrochemical cell that is affordable and superior to existing cells.

Why did you choose a career in science?

I chose a career in science because science gives me new insights into challenging problems. Solving problems to help people has always been fascinating to me.

Verity Salmon

Postdoc, Environmental Sciences Division and Climate Change Science Institute
Ph.D., Biology, University of Florida
Hometown: Lafayette, California

What are you working on at ORNL?

I work as part of an interdisciplinary team of scientists whose goal is to improve the representation of arctic ecosystems in Earth system models. My research focuses on understanding the influence arctic plant roots exert on flows of carbon, water and nutrients in these rapidly warming ecosystems.

What would you like to do in your career?

My goal is to pursue research that enhances our understanding of how interactions between plants, soil and microbes impact nutrient cycling in natural ecosystems. I enjoy not only collecting this data but also communicating my approach and findings to other scientists and the broader public.

Why did you choose a career in science?

I decided to pursue a career in science because I love tackling interesting and relevant problems alongside passionate and critical people.

Ahmed Arabi Hassen

Postdoc, Manufacturing Demonstration Facility
Ph.D., Materials Science and Engineering, University of Alabama–Birmingham
Hometown: Cairo, Egypt

What are you working on at ORNL?

As a member of the advanced polymers and composites team at the MDF, my research focuses on the development and characterization of various composite materials for additive manufacturing. These materials, combined with the additive manufacturing process, drastically reduce lead time and cost associated with manufacturing tools.

What would you like to do in your career?

The demand for composite materials is expected to almost double globally by 2020. I am interested in continuing research efforts that deliver transformative scientific solutions to the energy and economic challenges facing the United States. Manufacturing-technologies research is crucial for revitalizing American manufacturing and will lead to job growth.

Why did you choose a career in science?

Science allows us to gain a deeper understanding of our surroundings. I chose a career in engineering, specifically, since it integrates fundamental concepts and theories with applied science to advance technology and improve the lives of people around the globe.

Marissa Wood

Postdoc, Energy and Transportation Science Division
Ph.D., Chemistry, University of Washington
Hometown: Orem, Utah

What are you working on at ORNL?

I work at the Battery Manufacturing Facility developing high-energy-density lithium-ion batteries for cheaper, more versatile electric vehicles. I am currently optimizing electrode processing methods for new high-voltage cathode materials and exploring how electrode microstructure affects electrochemical performance, with the goal of moving toward tunable electrode design and greener battery manufacturing.

What would you like to do in your career?

I would like to continue to work collaboratively with an interdisciplinary team to solve energy problems that will make an actual impact on the world. I want to be in a position where I am continually challenged and always learning.

Why did you choose a career in science?

Science is the foundation of our everyday world, and I love that there is a seemingly endless wealth of knowledge waiting to be discovered. I am amazed by what science has already made possible, and I want to be a part of that meaningful contribution going forward.

Narendran Raghavan

Graduate student, Manufacturing Demonstration Facility
Ph.D. student, Energy Science and Engineering, University of Tennessee (Bredesen Center)
Hometown: Chennai, India

What are you working on at ORNL?

My research focus is on understanding the process-structure (microstructure) relationship in metal additive manufacturing (3-D printing) using a combined computational and experimental framework. Prediction of this relationship *a priori* using numerical modeling of the process reduces the number of cost- and time-intensive trial-and-error experimentations.

What would you like to do in your career?

Additive manufacturing has several key advantages over traditional manufacturing processes. When it comes to industrializing the technology, however, there are challenges. I would like to work on transforming the R&D-level additive technologies to production-scale industrial technology through certification and qualification of parts with the help of computational tools.

Why did you choose a career in science?

I grew up on a farm where my father used to repair/recondition engines and other agricultural equipment himself in the garage. This was the primary reason for my interest in engineering. During the course of my undergraduate engineering years, I understood the significance of the nexus between fundamental science and engineering, which prompted me to take up science as a career.

ORNL, Rickover and the nuclear Navy

by Tim Gawne
gawnetj@ornl.gov

When the second world war ended, the government was left with a new field of science known as nucleonics.

Created in Oak Ridge and at the other Manhattan Project sites as they developed the first nuclear weapons, the field was underrepresented in both published literature and college classrooms. This was no surprise; not only was nucleonics new, it was highly classified.

In an effort to fill the knowledge gaps, ORNL created a training school in 1946 that attracted the attention of the Navy, which was at the time toying with the merits of nuclear power for naval propulsion. The most famous student in this school—who would become arguably the most famous naval officer, period—was Hyman Rickover, then a captain responsible for mothballing ships after the war.

Rickover was senior among the school's eight naval officers, who called themselves the Oak Ridge Naval Group. They initially devoted themselves to the study of radiation shielding and the biological effects of radiation, critical areas if you were going to have your people living with a nuclear reactor for long stretches of time. Rickover himself was known to announce that he was an idiot and that his teachers should treat him accordingly.

Capt. Hyman Rickover (1946)

One of those teachers was Alvin Weinberg, who would eventually become ORNL's longest-serving lab director. It was reportedly Weinberg who suggested that pressurized water reactors—the type also responsible for most of America's nuclear power—would be the best choice for powering the Navy fleet.

That fleet would need well-trained officers. Rickover personally tailored the syllabus that would be used to train hundreds of naval officers, first at the lab and later at the Oak Ridge School of Reactor Technology and the Oak Ridge Institute of Nuclear Studies.

The two men's relationship was personal as well as professional. When Weinberg became the lab's research director in 1948, he received another honor as well: inclusion in a *Washington Post* list of the country's 10 most handsome executives. Rickover clipped the article and sent it to Weinberg with a memo of congratulations.

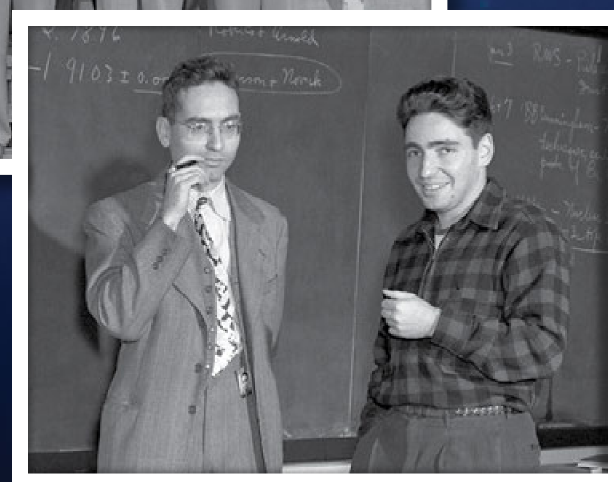
Weinberg got the opportunity to return the gesture when Rickover was promoted to rear admiral in 1953, a controversial move both because Rickover had never had his own command and because he had a habit of alienating his superiors by disregarding their opinions. Weinberg indicated pleasure that those in charge had finally come to their senses.

Rickover invited Weinberg to join President Truman and other VIPs for the June 1952 keel laying of the Nautilus submarine, the Navy's first nuclear-powered vessel. While Weinberg was unable to attend that function, he did join the newly minted rear admiral on the Nautilus for one of its sea trials.

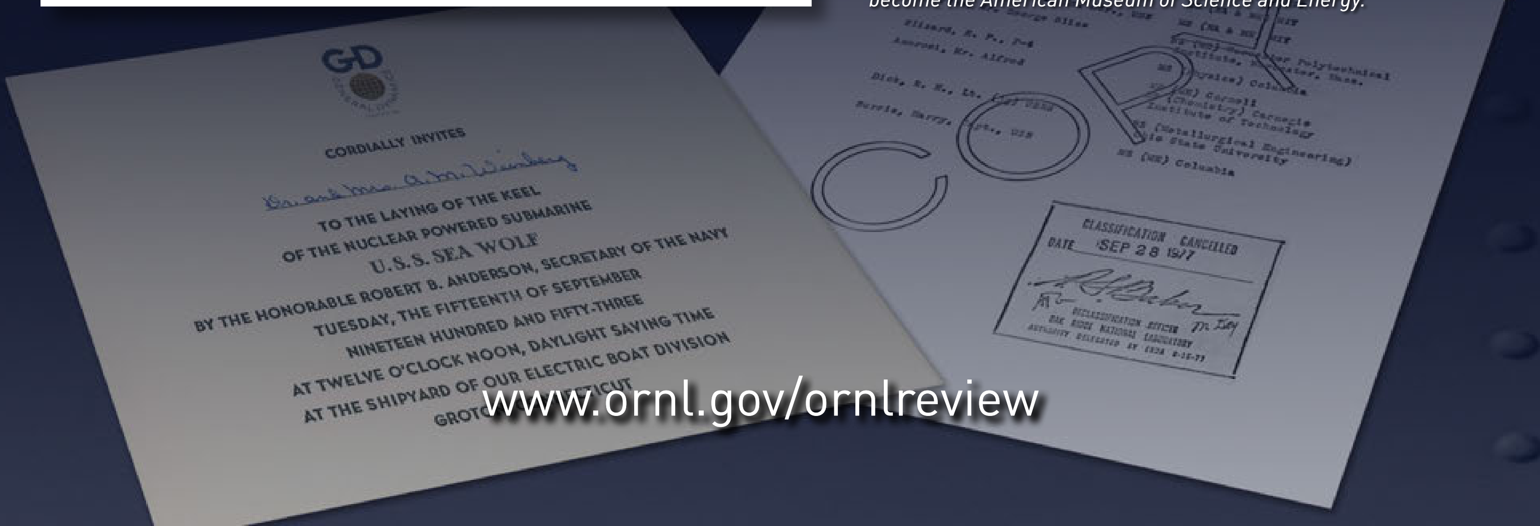
ORNL veteran Ted Rockwell served as Rickover's technical director while the Nautilus was in development and wrote about the naval man in *The Rickover Effect*. According to Rockwell, Rickover had a knack for inspiring or absolutely repelling people.

Indeed, everyone who crossed paths with Rickover seemed to come away with a story. I asked Rockwell during a trip back to Oak Ridge if all the stories were true.

"Rickover was a Grade-A son of a bitch that got things done," Rockwell replied. "We need more people like him—even more so today."



ORNL—known at the time as Clinton Laboratories—launched the first reactor training school in 1946. Students of the school, which was known playfully as the Klinch Kollege of Nuclear Knowledge, included then-Capt. Hyman Rickover and other early members of America's nuclear Navy. At top is a class photo from the school. Below that and to the right is an unidentified student with teacher and physicist Alvin Weinberg (left), who would go on to be ORNL's longest-serving lab director. At left is a later exhibit in Oak Ridge at the American Museum of Atomic Energy, which would eventually become the American Museum of Science and Energy.



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OAK RIDGE NATIONAL LABORATORY REVIEW
PO Box 2008, Oak Ridge, Tennessee 37831-6266

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Oak Ridge National Laboratory is managed by
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DE-AC05-00OR22725

ISSN 0048-1262