Oak Ridge National Laboratory
REVIEW
• MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY •

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Science in Sync

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on the cover

Carbon fiber being produced at ORNL's new Carbon Fiber Technology Facility. The CFTF is strengthening industry-government collaborations and accelerating the development and manufacturing of lower-cost carbon fiber that will improve America's competitiveness in automotive, wind energy, infrastructure, and other industrial applications.
Photo: Jason Richards

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INTERDISCIPLINARY RESEARCH

Transformational potential

Interdisciplinary research is a hallmark of national laboratories. From the beginning the laboratories have combined science and engineering disciplines to address complex issues at a scale and technical depth that is difficult—and sometimes impossible—to reproduce elsewhere. Early examples at ORNL included integrating nuclear engineering, chemical engineering, materials science, and instruments and controls to advance reactor technology and integrating chemical separations, radiochemical engineering, and nuclear physics and chemistry to develop isotope production technologies.

Solutions to major technological challenges rarely fit within a single discipline, and interdisciplinary research combined with the unique facilities and mission focus of the laboratories provide an ideal platform for addressing these challenges. This sort of extended collaboration is the model Energy Secretary Ernest Moniz has put forward for finding solutions to our most pressing energy problems.

The articles in this *ORNL Review* demonstrate that interdisciplinary research continues to flourish at ORNL. From recently formed interdisciplinary centers including the Consortium for Advanced Simulation of Light Water Reactors, BioEnergy Science Center, Critical Materials Institute and Climate Change Science Institute to the assembly of interdisciplinary teams around emerging opportunities in carbon fiber, additive manufacturing, and membrane science, ORNL is tackling a new generation of interdisciplinary challenges.

All of these initiatives have transformational potential. CASL is delivering on its mission to provide a highly accurate and usable virtual reactor that harnesses the power of advanced computing to simulate operational and safety aspects of light water reactors. BESC is advancing the science and technology of bioenergy by specifically addressing recalcitrance (the resistance of plant cell walls to being broken down by microbes and enzymes), which is the central challenge of deriving ethanol from biomass.

CMI is applying interdisciplinary strategies to the difficult problem of ensuring an adequate and affordable supply of critical materials, such as rare earth elements for clean energy technologies. The CCSI is combining climate modeling, ecosystem science and data science to improve and extend the reach of climate predictions. Multi-disciplinary initiatives in carbon fiber and additive manufacturing offer the potential to revolutionize the transportation and manufacturing sectors, and combining the power of neutron science with biology and supercomputing is presenting opportunities to solve biomedical problems once considered intractable.

Interdisciplinary research is in our DNA. The frontiers of science and technology often reside at the boundaries between disciplines—and it is this interdisciplinary space that ORNL is uniquely positioned to develop and exploit.

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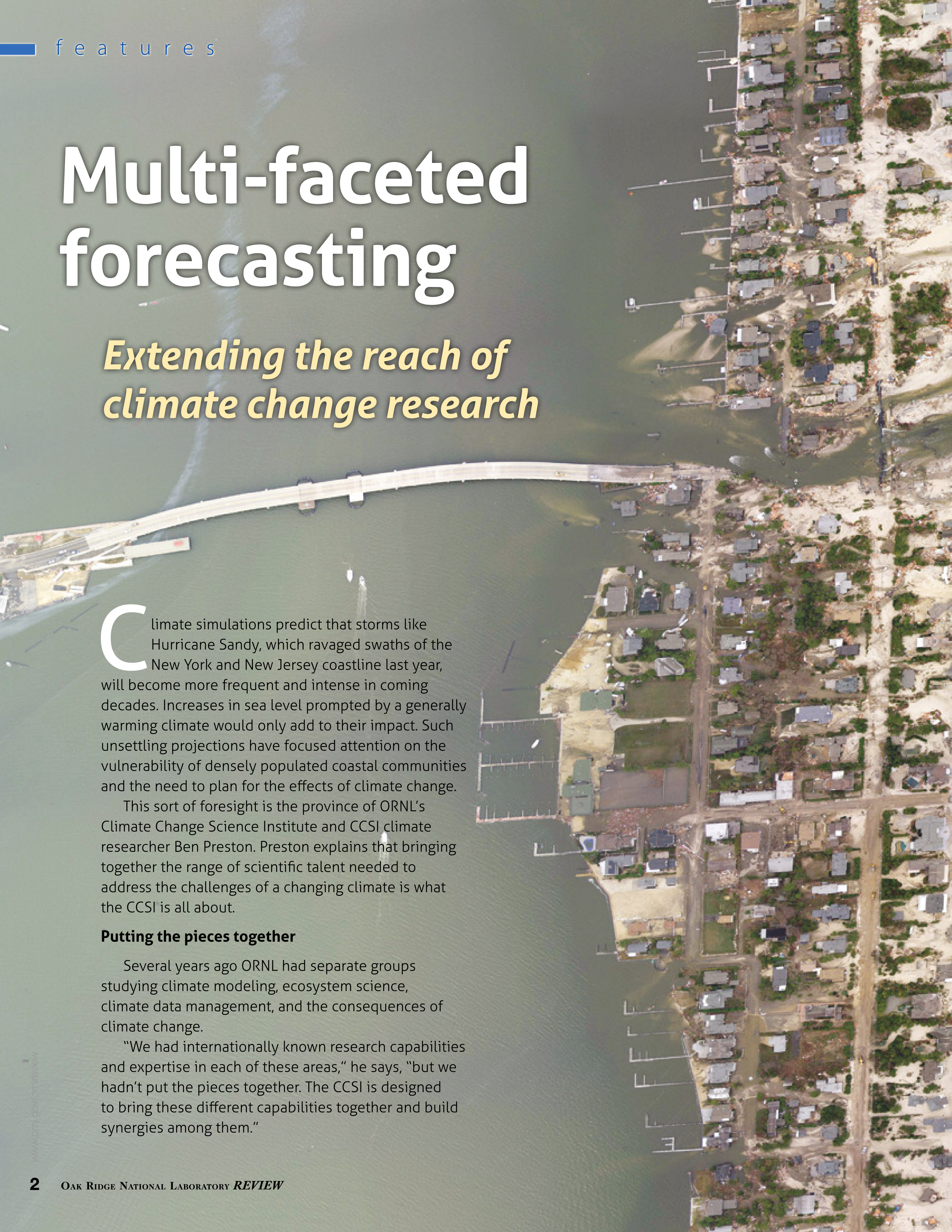


Multi-faceted forecasting

Extending the reach of climate change research

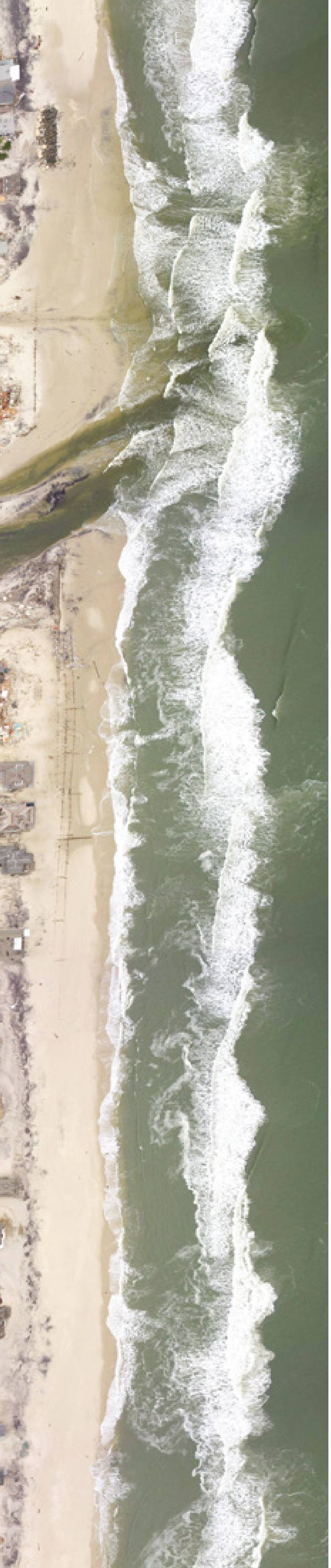
Climate simulations predict that storms like Hurricane Sandy, which ravaged swaths of the New York and New Jersey coastline last year, will become more frequent and intense in coming decades. Increases in sea level prompted by a generally warming climate would only add to their impact. Such unsettling projections have focused attention on the vulnerability of densely populated coastal communities and the need to plan for the effects of climate change.

This sort of foresight is the province of ORNL's Climate Change Science Institute and CCSI climate researcher Ben Preston. Preston explains that bringing together the range of scientific talent needed to address the challenges of a changing climate is what the CCSI is all about.

Putting the pieces together

Several years ago ORNL had separate groups studying climate modeling, ecosystem science, climate data management, and the consequences of climate change.

"We had internationally known research capabilities and expertise in each of these areas," he says, "but we hadn't put the pieces together. The CCSI is designed to bring these different capabilities together and build synergies among them."



Preston, who also serves as the institute's deputy director, said collaboration has already produced results through the CCSI's Next-Generation Ecosystem Experiments.

"This study of the effects of warming on Alaska's terrestrial ecosystems relies on both ecosystem scientists and climate modelers to understand how the ecosystems of the high Arctic are affected by climate change," he says.

The effort, involving dozens of researchers from several national labs and universities, is generating a lot of data—in the form of observations of surface and subsurface ecosystem processes as well as modeling data. As a result the CCSI is also calling on data management specialists to organize and manage the data to make it available to the rest of the research community.

"The NGEE project illustrates the kind of interdisciplinary research the institute is doing," Preston says. "Anyone interested in the consequences of climate change—whether he or she is working on a global scale or regional scale—would benefit from having access to climate modelers who can tell them something about how the climate is going to change, what's going to happen with extreme weather, and on what timescales. This broad-based expertise enables our studies to say something about what the consequences of a changing climate could be for areas as diverse as energy production, agricultural yields or the risks to coastal communities."

Energy impacts and more

Since the CCSI's primary sponsor is the US Department of Energy, its research on the societal consequences of climate change naturally focuses on the US energy sector.

To understand how climate affects the nation's energy infrastructure, scientists need to know how it affects basic environmental factors such as water availability—because producing energy often involves using a lot of water—or how changes in the climate might affect the productivity of different types of bioenergy crops.

Some of the effects of Hurricane Sandy on Mantoloking, New Jersey. Photo: National Oceanic and Atmospheric Administration, Remote Sensing Division

"Our major focus is on energy," Preston explains, "but in order to do that we really have to consider a range of energy systems, which means we have to look at many different types of impacts."

The institute also studies how changes in the global climate could affect homeland security (as a result of disruptions such as crop failures or food shortages) or critical infrastructure (through the impact of drought on hydroelectric power generation, for example) and the possible impact of storms and rising sea levels on coastal communities.

"Hurricane Sandy brought the vulnerability of certain areas of the coast into sharp focus," Preston says. "These storms may not happen frequently, but when they do, densely developed areas have a huge amount of exposure."

He explains that places such as New York and New Jersey are growing quite rapidly, particularly along the coast. So if a storm like Sandy hits the same area 50 years from now, the damage is going to be that much greater.

"A lot of my work focuses less on what's happening with the climate or with physical systems like buildings and infrastructure, and more on understanding what's happening with society—how it changes over time in terms of demographics, economics, and risk management," he says. "We want to know how those factors interact with the effects of a changing climate."

The CCSI uses a number of computational tools to better understand this relationship. These include many computer-based climate models mixed with scenarios that CCSI scientists develop by analyzing trends in population growth and economic development.

"To consider the possible future social and economic impacts of changes in the climate, we need to know where people and resources will be located," Preston says.

In harm's way

A recent study by Preston published in *Global Environmental Change* makes the point that climate change and changes in society can't be viewed as unrelated.

"Everyone wants to know how the climate is going to change," Preston says. "Can we predict future climate change? Can we predict changes in the frequency or intensity of extreme weather events like heat waves or hurricanes or flooding? If we only think about the climate, we see that a lot of our understanding of future consequences is dominated by what we know or don't know about these climate variables. However if you look back at the last century, you'll see that economic losses related to extreme weather events have been rising—not necessarily because of climate change, but because we have been developing hazardous landscapes and putting more and more people in harm's way."

To illustrate this point, he notes that before the proliferation of air-conditioning, Florida was not a place where too many people wanted to live. However, since the 1960s the population of Florida, as well as the rest of the US Southeast, has been booming—despite the fact that it's particularly prone to hurricanes and flooding.

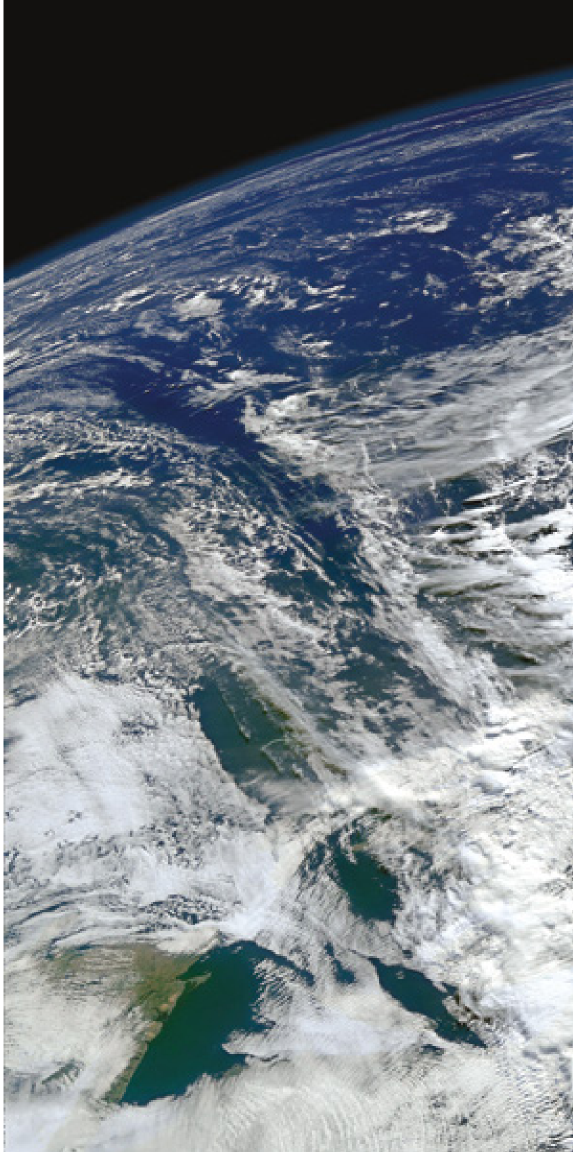
The study considered how changes in population and wealth across the US will influence exposure to leading causes of climate-related damage such as hurricanes, wildfires, tornadoes and flooding.

"We know losses related to these events have a particular geographic pattern," Preston says. "Losses related to hurricanes, for example, are related to coastal areas, particularly in the Southeast. Wildfire damage is specific to the Southwest. Tornadoes and floods mainly strike the Midwest."

Turning this general information into detailed maps required plowing through a great deal of historical loss information, mostly federal government records. Once Preston had national maps of the distribution of losses, he projected future patterns of "societal exposure"—that is, how many people will be living in these areas in coming decades and how well-off they will be.

"To do that we developed a demographic model based on historical information," he explains. "We generally know what the population size is for every US county at present, and we know the birth rates and death rates for various age groups and ethnicities. Using this information we built a model of the future population for every county. We also made the assumption that the economies of the counties will continue to grow over the next few decades as they have in recent decades. This assumption is open to question, but at least it allows us to project the implications if we continue on our current path."

Multiplying the average wealth of an individual in each of these counties by the number of people gave researchers a measure of the economic exposure for each county. Then they predicted the change in population of each county over time. The model predicts, for example, that the population of the Great Plains is expected to decrease over coming decades, while the urban and coastal areas of the South are likely to continue to experience increases in population that are higher than the national average.



By integrating climate and demographic information in this way, researchers came to a number of conclusions about what areas of the country were most at risk for climate-related damage. For example, Florida's losses resulting from extreme weather events are expected to grow up to a factor of 5 by 2050 due to increasing population and wealth.

"This kind of information allows us to place the discussion about climate change in some kind of context," Preston says. "Yes, we're concerned about climate change.

Polygonal patterns in Arctic soil provide researchers with a unique natural laboratory in which to study the Arctic and, by extension, the Earth's climate. Photo: NGEE-Arctic project

A NASA satellite image of Hurricane Sandy and associated weather systems. Photo: NASA Earth Observatory image by Robert Simmon with data courtesy of the NASA/NOAA GOES Project Science team

Yes, we're concerned about how it might influence hurricanes and other extreme events, but a lot of the big changes in such events are projected to arise in the latter half of the century. If you're talking about the next few decades, losses in these rapidly developing areas might increase by a factor of 2 or 5 or even more, simply because we're putting more people in harm's way."

Pressure for predictions

Preston acknowledges increasing pressure to move from understanding how climate systems work to making predictions—whether it's projecting how the climate will change over the next several decades or predicting agricultural yields next year.

"That expectation is putting new demands on our science and modeling capabilities, and it might send us back to the drawing board to develop the next generation of computational tools," Preston says. "Of course, that's understandable; it's the iterative nature of science. We want to continually bring our best tools to bear on any question."

Newly acquired data may be able to provide some of the information needed to predict changes in the climate.

"Our Next-Generation Ecosystem Experiments are a good example of that," Preston says. "We actually don't know a whole lot about the dynamics of Arctic ecosystems, how carbon dioxide is released from permafrost, or how these things might influence the global climate system. Large-scale experiments like NGEE allow us to gain a better understanding of what's going on at the process level. We can use that knowledge to improve our models."

He also notes that there's a growing recognition within the climate science community that some simulation tools may not be up to the challenge of providing long-term predictions of climate change impacts. For example, agricultural crop models that are used to simulate the effects of climate change on agricultural productivity often do not capture the range of crop responses to climate, particularly climate extremes, observed in the real world.

"There is a move in the crop modeling community to start from scratch and build new models that are designed from the ground up to simulate, capture and represent the long-term climate change processes we are interested in," Preston says.

"Scientists have been studying the climate for a long time—centuries. We've made a lot of progress, and we've got a lot of knowledge. Now that our research is having a broader impact and is of interest to a broader audience, the pressure to extend the reach and utility of climate predictions is particularly intense. I think you see this across the climate change arena. The CCSI will play a key role in meeting that challenge." —*Jim Pearce*

3D printing rises to the occasion

ORNL group shows how it's done, one layer at a time

Things have come a long way since the mid-1980s when 3D Systems cofounder Chuck Hull worked out the technology to print objects in three dimensions, one very thin layer at a time.

Hull called his new technology "stereolithography." In it, a guided beam of ultraviolet light is focused on a vat of liquid polymer, solidifying areas where it hits. When one layer is complete, the platform holding the object lowers a bit, and the process is repeated.

The technology was impressive but limited, with the printed objects serving as prototypes but not much else. In the intervening decades, and especially in the last few years, 3D printing has made it to the big time, taking off both in capability and application.

Consider the following:

- Electron beam melting systems create intricate, high-quality components by sweeping a precise layer of metal powder over an object and selectively melting it to the object. Swedish manufacturer Arcam AB has used this process to produce more than 30,000 acetabular cups, the components in a hip replacement that attach to the hip socket and hold the ball joint. These printed components are literally walking all over Europe.
- Boeing uses 3D printing—also called additive manufacturing—to produce more than 20,000 military aircraft parts, and GE Aviation has announced it will produce more than 100,000 additive-manufactured components for its LEAP and GE9X jet engines by 2020.

3D printing at ORNL

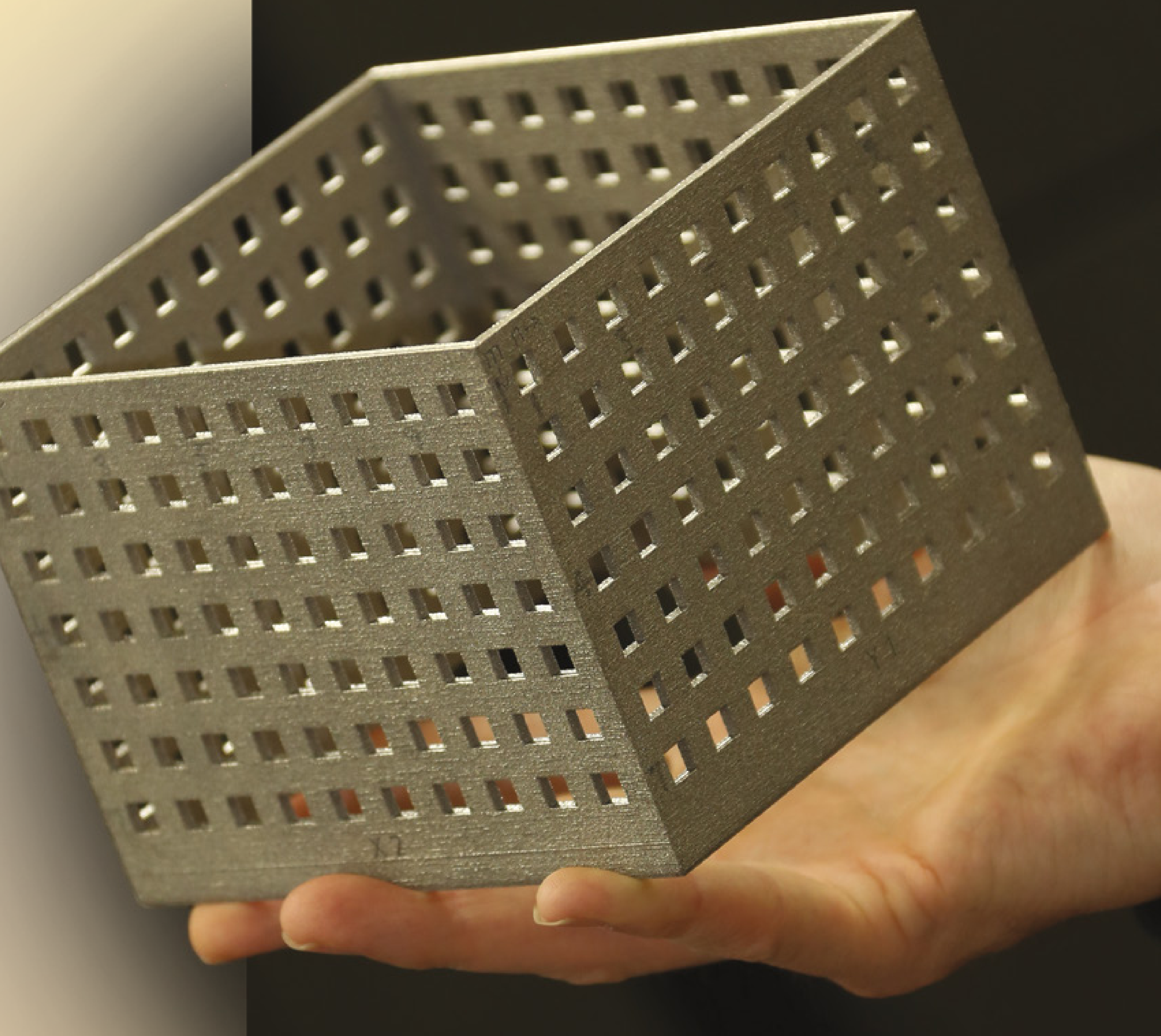
ORNL's focus on printing is led by the the Deposition Science & Technology Group within the Manufacturing Demonstration Facility. The DST is young, created just this year. According to group leader Chad Duty, it works with a variety of advanced manufacturing technologies such as carbon fiber, magnetic field processing and printed electronics.

And, of course, the group works on additive manufacturing. In this realm its role is a combination of research and education. On the research side the group is making use of ORNL's unique strengths, including materials science, neutron imaging and supercomputing.

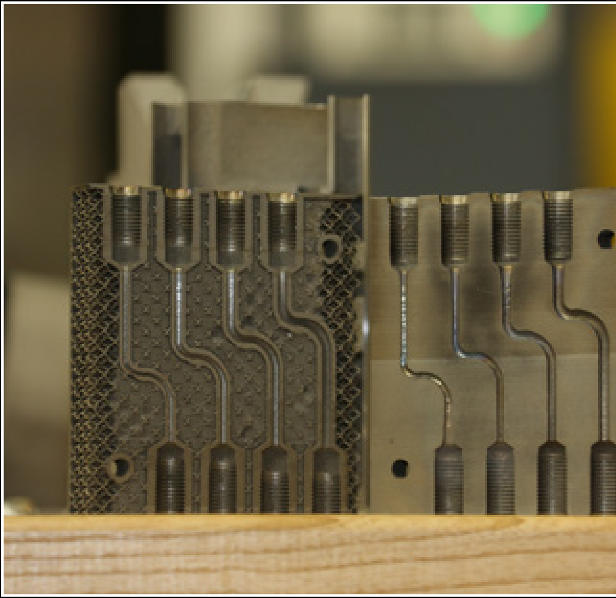
"There are several areas where it makes sense for a national lab to be doing this," Duty says. "One is that we can leverage all the historical strengths of a national lab and bring it to bear on this new technology front."

For instance, warping is a big issue for systems that build parts one layer at a time. The component gets very hot at the point of melting, but surrounding areas may stay cool, depending on the technology. Electron beam systems keep the whole assembly at about 700 degrees Celsius (roughly 1,300 degrees Fahrenheit), which helps to minimize warping. Laser beam systems, on the other hand, don't heat the surrounding material, so warping is a greater issue.

Duty's group is working with Ralph Dinwiddie of ORNL's Scattering and Thermophysics Group to measure temperatures across the printing surface as the component is being produced. The thermal imaging techniques pioneered by this collaboration will allow for a better understanding of temperature differences and, ultimately, the development of ways to reduce warping.



A perforated metal box produced by an Arcam 3D printer. This detailed "calibration" part illustrates some of the versatility of 3D printing. Photo: Jason Richards



3D and neutrons

Quality control is also an issue, one that is especially important in areas such as medical implants or aerospace manufacturing. In response, Duty's group is working with ORNL neutron scientists at both the Spallation Neutron Source and the High Flux Isotope Reactor, using the unique ability of neutrons to look inside materials without damaging them.

"The neutron source can bring a new way of inspecting these materials, optimizing them and reducing residual stress in these components," Duty says. "There's no other way to nondestructively evaluate those kinds of systems."

Supercomputing is also helpful when Duty and his colleagues look at structural issues associated with additive manufacturing. He has been working in this area with Sreekanth Pannala of ORNL's Computer Science and Mathematics Division.

"When you're trying to model a weld beam or weld line, it's very complex," Duty says. "You've got thermal issues. You've got microstructural issues. You've got a moving interface. You've got the phase change of materials from liquid to solid.

"It's a pretty complicated system, and that's just for one weld beam line across a material. In a cubic inch in the Arcam electron beam technology, we've got five miles of weld line," Duty says.

Bigger. Faster. Cheaper.

Duty and his colleagues are also working in a wide range of other areas designed to push forward both the technology and its application in American manufacturing. They are working to improve the materials being used, contributing to the development of high-performance metal alloys and stronger polymers that incorporate carbon fibers. They are working to improve the manufacturing process in an initiative Duty identifies with the slogan "Bigger. Faster. Cheaper."

And they're working to educate manufacturers about what the technology can and can't do. This involves helping manufacturers learn new things and unlearn old ones.

"We're in a kind of second birth for additive manufacturing," Duty explains. "It went through a phase [in the 1980s] called 'rapid prototyping,' and some people were saying, 'It can do everything; we'll do away with all other types of manufacturing.' And then it cooled off.

"A lot of folks went through that cool-off period. They tried it, it didn't work, and they've written it off. And they think this is the second verse of the same song. We help them take another look at it."

One challenge that requires both the technical expertise found across the lab and Duty's personal role as a technology evangelist is something he refers to as "the valley of death"—the collection of practical limitations that prevents a wonderful idea in the laboratory from making it into production.

"That's kind of why my group exists: to help companies transition things that are really cool to things that are commercially relevant," Duty says. "One of the things we do in a manufacturing demonstration facility is demonstrate the technology, show people what can be done with that technology, start their wheels turning, and help them work through problems in their industry where it can be useful."

In fact, Duty says, additive manufacturing is not appropriate in every situation. If you're producing 10,000 simple, inexpensive brackets a day for the automotive industry, chances are pretty good that making that bracket on a 3D printer is not a good idea. On the other hand, if you're making a low-volume component that is expensive, complex and specialized, Duty and his colleagues would like to talk with you.

"The areas where it's really getting initial traction are where you would expect," Duty says. "It will be in those areas that have really high margins, like biomedical, aerospace, defense and nuclear. In general, these are areas where the parts are really complex, highly customized and produced in low volumes."

Complexity is not a bad thing in additive manufacturing; it's not even that much of a challenge. Because these systems build a structure one layer at a time, they don't care

how complex it is. In fact, a complex mesh is an easier job for additive manufacturing than a chunk of metal. The Arcam system, for instance, can lay down about 5 cubic inches of material in an hour, whether that material is spread out over a fine mesh or plopped down as a cube.

This new reality takes some getting used to.

"It's completely non-intuitive," Duty noted, "which is why it's so paradigm-shifting. People think, 'I can really make this into something useful, but it would really complicate the design.' And we say, 'That's good; we can make it faster and cheaper for you if you do that.'"

For example, his group was working with a company that produced impeller blades, rotors within a pipe that have the job of increasing or decreasing fluid pressure. The company asked them to duplicate the part exactly.

The problem—or more accurately, the opportunity—was that the piece had been designed for casting, with the angles, thicknesses and other compromises that are necessary when you pour molten metal into a mold.

Duty and his colleagues certainly could make an exact duplicate of the impeller, but they were convinced they could do better. So they asked the company to redesign the piece for additive manufacturing.

"They took two days to do the redesign," he says, "and we made the other version. We tested it out; it met all the performance metrics, and it was 56 percent lighter because they got the wall thicknesses down. For a rotating piece of machinery, weight reduction is huge."

The story illustrates both the potential of additive manufacturing and the challenge it presents to existing ideas of what manufacturing involves.

"If you're trying to use additive manufacturing to make the exact same thing that you're already making, you're using it wrong," Duty explains. "You're not thinking about it right. The real potential and opportunity here is to do things that you can't do today." —Leo Williams

(Above) ORNL scientist Chad Duty removes a finished part from a production-grade 3D printer.
Photo: Jason Richards

(Left) 3D printing can build products from a variety of materials for products ranging from heavy equipment to biomedical implants.
Photo: Jason Richards

Tag-team R&D

Closing in on a carbon fiber solution

Stronger than steel and a third its weight, carbon fiber is a hot commodity—not so much for what it does, but for what it could do. Today carbon fiber is found in fast cars, jetliners and specialty sporting goods from bicycles to bass boats. Because it's a lot more expensive than steel, however, it hasn't been able to make the jump to the broader consumer market for inexpensive cars and other everyday items.

What would cheaper carbon fiber mean? One quick example: The US Department of Energy estimates that competitively priced carbon fiber could reduce the weight of key vehicle components by more than 60 percent—dramatically increasing gas mileage. The appeal of more economical transportation is undeniable, so it's not surprising that DOE is working with auto companies and other manufacturers to make cheaper carbon fiber a reality.

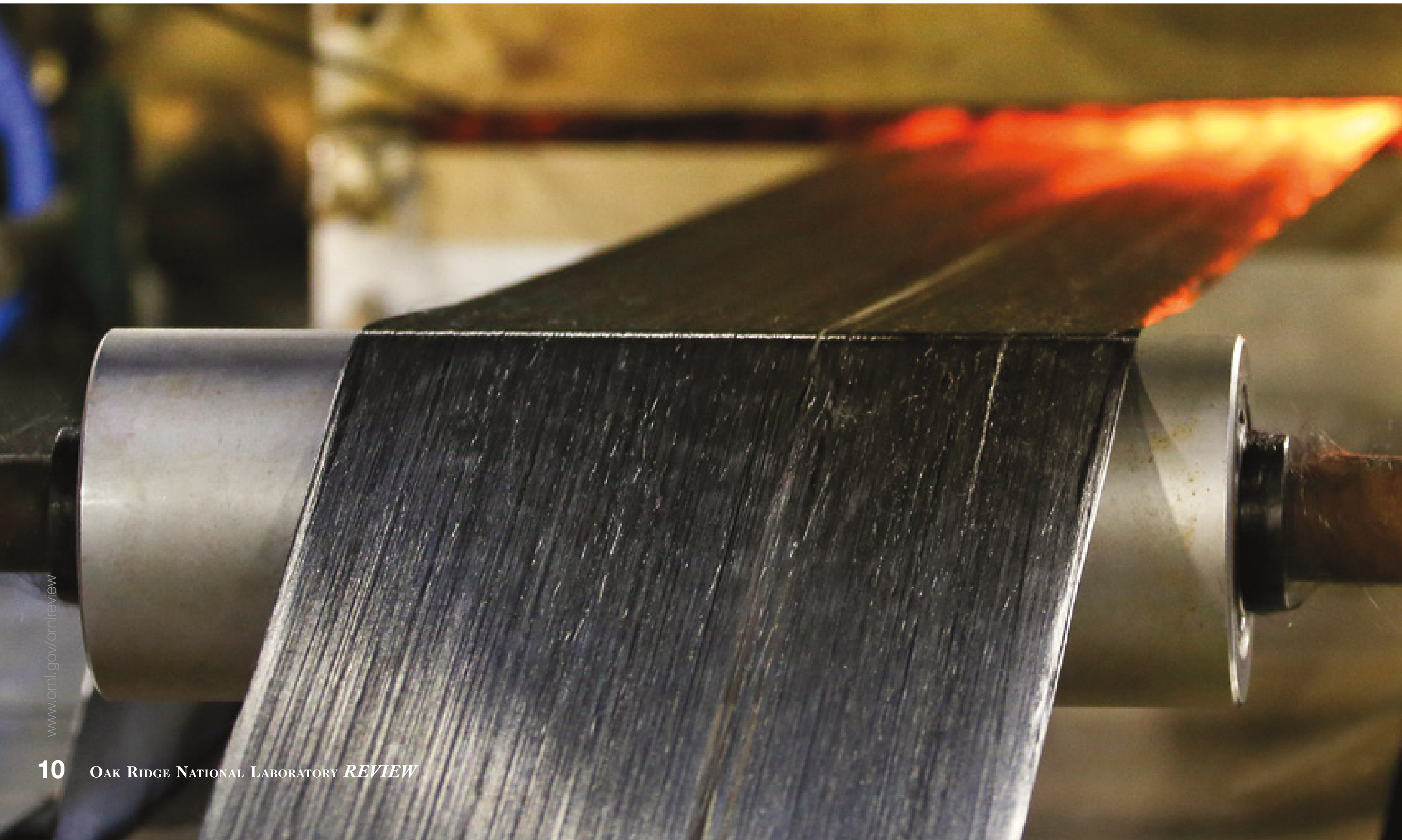
That's where ORNL comes in. The laboratory has been investigating various methods of reducing the cost and increasing the strength of carbon fiber for years. One of these efforts uses lignin, a common manufacturing byproduct, as the raw material or "precursor." Lignin is a rigid, woody material that allows trees and other plants to stand upright. It's also churned out in huge quantities by paper mills and biofuel refineries.

"We're investigating lignin because 50 percent of the cost of manufacturing conventional carbon fiber is the cost of the precursor, and lignin is relatively inexpensive," ORNL materials scientist Amit Naskar explains. "Today 90 percent of carbon fiber is manufactured from polyacrylonitrile, or PAN—a material that is chemically similar to the synthetic acrylic fabric used in clothes. Although versatile, PAN is relatively expensive, and it's petroleum-based."

Interdisciplinary advantage

Part of the mission for Naskar and his colleagues from the laboratory, the University of Tennessee, and the Georgia Institute of Technology and industrial partners from the Carbon Fiber Composite Consortium has been to find a lower-cost, renewable alternative to PAN.

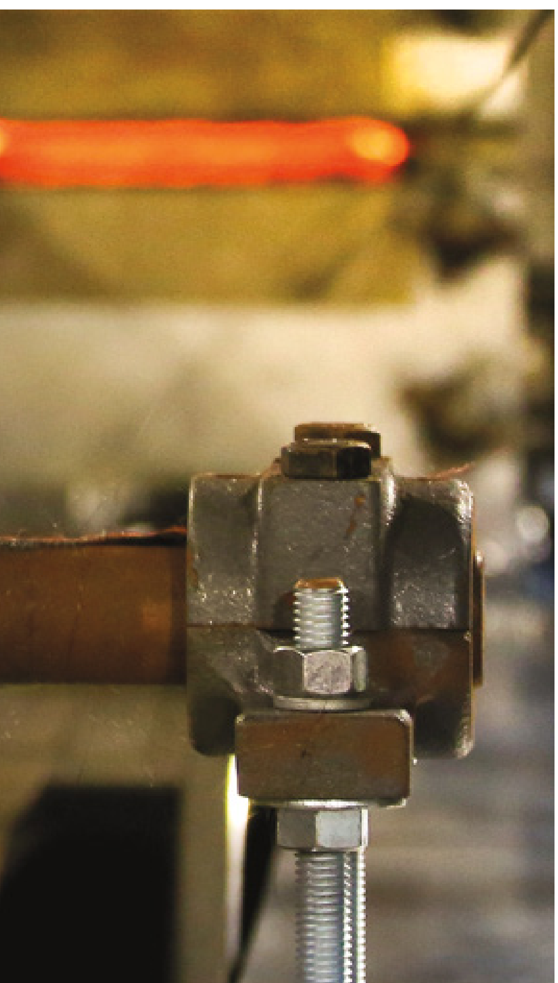
Naskar describes the project as an "integrated interdisciplinary program" that includes researchers from ORNL's BioEnergy Science Center, who are investigating what genetic characteristics yield the best lignin for creating carbon fiber; polymer chemists, who are developing ways of chemically modifying the lignin to provide better carbon fiber; and composite researchers, who are developing protocols for conventional composite fabrication and printing compos-



ites at ORNL's newly built manufacturing demonstration facility.

"An interdisciplinary team provides a means of attacking a problem from a number of different sides," Naskar explains. "Creating cheaper, stronger carbon fiber is our goal, so anyone who has a new idea for improving the process or the product is welcome to work on that. Each research group has its own goals, but we share information and developments with one another."

"For instance," he says, "bioscience colleagues recently told us that they had isolated a different type of lignin and an associated gene that was behaving differently from others in a particular species of tree. We suggested extracting the lignin and chemically analyzing it to examine the interconnections among molecules to see if it might have applications in carbon fiber production. If we weren't working together, I would never have known about this development. My polymer science colleagues found a composition that provides a higher carbon yield after modification of the lignin, and we are working on producing fiber from such compositions."



Understanding structure

Quite a few of the lab's interdisciplinary resources have also been focused on the problem of revealing and refining lignin's molecular structure to make it a better fit for the carbon fiber production process.

Naskar describes lignin as "a very difficult molecule." Lignin has an irregular, three-dimensional nature that is problematic because the raw material for carbon fiber must first be extruded into spaghetti-like filaments called "fiber tow" or spun into mats of interconnected thread-like fibers that are eventually converted to almost pure carbon through a sequential heating process.

"It's not easy to process lignins into a common form that can be spun into fiber," Naskar explains. "We need to determine how much we can do, in terms of chemistry, to make it more suitable for the spinning process."

Naskar notes that the task of analyzing and understanding lignin's structure is made easier by the lab's extensive resources. He and his colleagues are using two DOE user facilities at ORNL. Both the unique characterization tools at the Center for Nanophase Materials Sciences and the neutron scattering capabilities of the High Flux Isotope Reactor have been vital to understanding the various configurations of lignin molecules.

"Sometimes people ask us why we are trying to understand lignin on the molecular level rather than spending our time developing the carbon fiber, " Naskar says. "I always say these activities are interconnected. The structure of lignin molecules has important implications for the process of creating carbon fiber. Once we demonstrate the feasibility of producing carbon fiber using conventional techniques, then we can investigate the advanced processing methods that are being developed by other ORNL researchers."

ORNL's Carbon Fiber Technology Facility is producing low-cost carbon fiber for composite parts

The team is also working with biofuel refineries and paper mills to modify their processes to create lignin with properties that are better suited to carbon fiber processing. This "high-quality" lignin will theoretically require less filtering and chemical modification.

"We have evaluated 27 lignin samples, both from biorefineries and pulping operations," Naskar says, "and we are continuing to work with those who can provide us with large quantities that might enable us to scale lignin fiber production to a level that it could be used as a commercially viable feedstock for carbon fiber."

A challenging task

Naskar emphasizes that developing low-cost carbon fiber will be a high priority for years to come—not only for the laboratory and DOE, but also for dozens of businesses and industries.

"We have a target of demonstrating a path for improvement in the properties of this material within two or three years," he says. "Then we can work with industry to scale up the process. This would offer an excellent opportunity to extensively use the Carbon Fiber Technology Facility that DOE's Office of Energy Efficiency and Renewable Energy built at ORNL to demonstrate that we can produce industrial quantities of low-cost carbon fiber."

To ensure that interaction with industry and research partners remains at a high level, the laboratory also started the Oak Ridge Carbon Fiber Composites Consortium, which includes more than 50 industrial partners, including carbon fiber manufacturers, automotive companies, paper companies, and other businesses related to biomass and lignin production, all dedicated to promoting innovation in the carbon fiber production process.

"It is a very challenging task," Naskar admits, "but we're an integrated team, and we're working together to solve it." *—Jim Pearce*

Hunting for hydrogen

ORNL neutron and supercomputing facilities illuminate biomedical research

Given that approximately half of the atoms in the human body are hydrogen atoms, you might think that locating this abundant element would be easy. Not so, says ORNL's Paul Langan, director of the Biology and Soft Matter Division.

"Hydrogen is by far the most common element found in biological systems, but it is also the smallest element," Langan says. "It is very difficult to study because it is so light and mobile."

Hydrogen's elusive nature can be attributed partly to it having only a single electron, which helps form critically important hydrogen bonds. This electron is shuffled around with the hydrogen atom in almost all biochemical reactions. As a result hydrogen is practically invisible to techniques such as x-ray and electron scattering that rely on interactions with electrons.

"Most of the other atoms in biology like carbon, oxygen and phosphorus have tons of electrons, so they interact with x-rays easily," Langan says. "X-ray diffraction, an important technique in biology, can provide the skeleton or general shape of a protein, DNA or whatever biological molecule you're looking at. But the skeleton doesn't show you where the hydrogen atoms are. That's a big problem because those hydrogen atoms are involved in the chemistry that underpins the biology."

(Left) The IMAGINE diffractometer is one of several new ORNL neutron instruments that will enable advances in biomedical research. Photo: Jason Richards

Researchers who want to study these biochemical reactions can now turn to neutrons, which, unlike x-rays, can more easily detect the presence of hydrogen. Neutron diffraction—a technique first pioneered at ORNL in the 1940s—is now helping biomedical researchers tackle today's research challenges in areas such as drug design and antibiotic resistance.

Neutrons to the rescue

Neutrons can be found in ample supply at ORNL, where they are produced at the Spallation Neutron Source and the High Flux Isotope Reactor. These two US Department of Energy user facilities welcome scientists from around the world to conduct studies in physics, chemistry, biology, engineering, materials science and other fields. As three new instruments dedicated to the study of crystals of molecules such as proteins come online over the course of the next year, Langan anticipates that ORNL's neutron facilities will become a new resource for the biomedical community, opening up new lines of research.

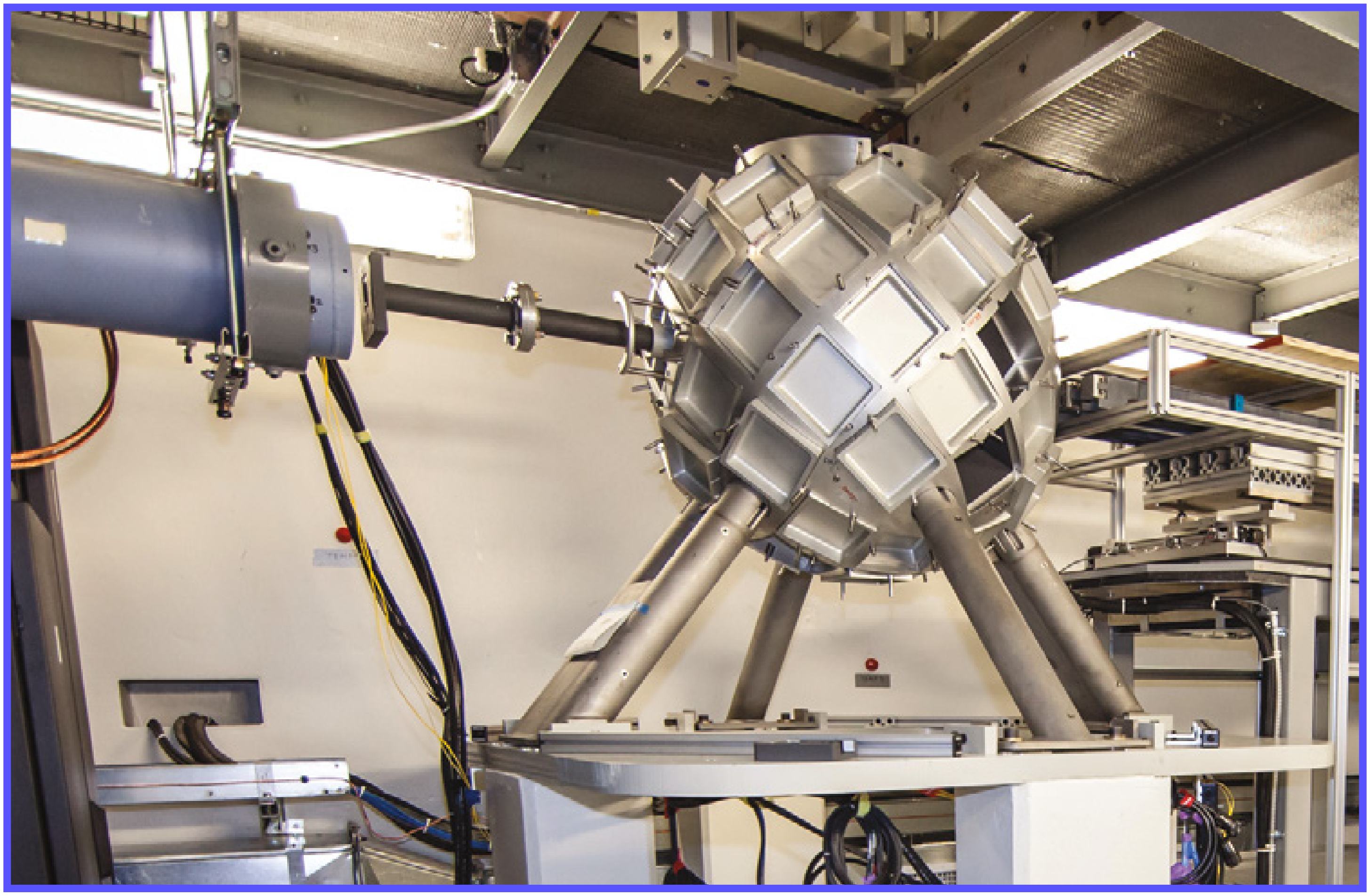
"We only have one beamline in North America that allows us to do this type of biological study," Langan says. "We're going to quadruple the capacity for neutron protein crystallography in the US over the next year."

The term beamline refers to how neutrons are used once they are produced: Beams of neutrons are guided toward different instruments designed to study certain characteristics or properties of a sample. Once neutrons reach the sample, they bounce off in different directions, creating a pattern that researchers analyze to determine the sample's structure and other properties.

The three new instruments—named TOPAZ, IMAGINE and MaNDi—will offer scientists unprecedented tools for studying the structure of molecules, in particular large biological molecules such as proteins. For instance, improvements in instrument design will allow researchers to study very small samples—a major benefit to those who prepare protein crystals for use in neutron studies.

Growing protein crystal samples in the lab is an arduous and time-consuming process, and some proteins simply cannot form large crystals. The ability to analyze smaller crystals with neutrons will open up new avenues of research that were once off-limits.

In addition, the comprehensive suite of instruments at ORNL allows researchers to look at a problem from multiple angles: for example, studying the dynamics of a system in one experiment and then determining its



The MaNDi instrument at ORNL's Spallation Neutron Source will allow for the study of large biological molecules such as proteins. Photo: Genevieve Martin

structure at a different instrument. Neutrons are nondestructive, meaning that a single sample can be used multiple times because its properties are not altered by interactions with neutrons.

"Biological structures are continually moving and can also be incredibly complex," Langan says. "The capabilities we have at ORNL in neutron science create a virtual microscope, which enables researchers to conduct experiments at different length and time scales. Crystallography can provide atomic-level information, whereas beamlines for small angle scattering, reflectometry and imaging can provide information at larger length scales.

"Tying the results together using high-performance computing capabilities at Oak Ridge allows us to focus in and out on a particular structure or system. When we view these biological structures through our virtual microscope, they come to life when they are animated by information from dynamic neutron spectroscopy beamlines and computer modeling."

Although neutron studies can stand on their own merits, they work best in tandem with other techniques, such as x-ray analysis. In a recent study, Langan and his ORNL colleague Andrey Kovalevsky were part of a multi-institutional research team that used neutrons from the Institut Laue-Langevin in France to refine their understanding of an enzyme that had been studied with x-rays for 20 years. The team looked at the interactions between HIV protease, a protein produced by the HIV virus, and an antiviral drug commonly used to block the virus' replication.

"We found that the hydrogen atoms thought to enhance the binding of the drug are not actually responsible for its enhanced binding," Langan says. "When this drug interaction was examined using x-rays, they didn't show where the hydrogen atoms were, so assumptions were made about the presence of hydrogen bonds. We now know these assumptions are wrong. Our neutron structure provides us with extra information that will be used to retune or redesign that drug into being more effective.

"Our cells contain a complex network of biochemical reactions, with different enzymes facilitating different stages of those reactions. X-ray crystallography can show you the shape of those molecules and how they might bind to substrates or small molecules, but to understand the chemistry in biology, to understand how the catalytic mechanism occurs, you need neutrons."

Mysterious membranes

Neutrons are also a necessity for John Katsaras, an ORNL researcher who holds a joint appointment with Canada's National Research Council. Katsaras uses both neutron and x-ray techniques to study cell membranes, the boundary layers around cells that are involved in numerous biological processes. Biologists have studied membranes for decades, but many mysteries remain about their complex structure and function.

"We have experiments that we would like to do to resolve research questions that have been ongoing for 40 years," Katsaras says. "Neutrons are almost uniquely positioned to do this."

One question that Katsaras and collaborators would like to tackle with neutron scattering is the existence of "lipid rafts" in living cells, a topic of much debate in membrane biology. Membranes consist of two layers of fatty molecules called lipids, which are interspersed with other molecules, mainly proteins.

Toward the end of the 1970s, researchers began to suspect that instead of forming an even pattern throughout the membrane, certain areas of the lipid bilayers would clump together and separate from the surrounding material. Scientists also began to understand that these segregated areas, or rafts, could play a role in a range of cellular functions, including drug uptake and interactions with pathogens. But the theorized rafts remained frustratingly invisible.

"We can study these rafts in carefully controlled model systems, but the question of their existence in living cells is like a biological black hole," Katsaras says. "It has been shown through biochemical means that rafts probably exist, but no one has ever seen them or characterized them.

"Why is that so? Is it because they don't exist, or is it the fact they're very small? Or is it the fact they're transient? They could be appearing and disappearing all over the place, but if you're only looking at one spot with optical techniques, you may not see them."

Neutron scattering can be used to probe a relatively large amount of material, allowing scientists to draw conclusions about the bulk material instead of a single location. Katsaras plans on using neutrons to detect lipid rafts in living cells by exploiting the biological contrast in the rafts and the surrounding areas.

"Everything in life is contrast," Katsaras says. "If your clothes and your face were the exact same color, then I couldn't tell where your face was. You need contrast. X-rays are relatively poor in contrast when it comes to biological materials. Neutrons, on the other hand, can be very good, especially when you induce contrast by exchanging hydrogen for deuterium."

Deuterium is an isotope of hydrogen that neutron scientists use as a labeling tool. By substituting deuterium for certain hydrogen atoms, researchers can more easily track the position of the labeled atoms because neutrons "see" the difference between the two isotopes as a black and white contrast.

Making supercomputers sweat

Katsaras is among a fleet of ORNL researchers developing ways to integrate the force of the lab's neutron facilities with its computing clout. ORNL has long held leadership roles in supercomputing and neutron science, but only in recent years have the two fields started to build upon the other's successes.

Powerful supercomputers including ORNL's Titan—ranked the world's second fastest as of June 2013—are capable of running simulations that require mind-boggling amounts of calculations. But real-world data is still needed to keep the complex simulations based in reality, Katsaras says.

"Computational simulations need to be validated by experimental data," he says. "If there is no validation, because these systems are so complicated, it is very difficult to know if you're on the right track."

One of Katsaras's proposed projects would unite complementary powers of neutron scattering and simulation to study an entire vesicle, a molecule that mimics the composition of an asymmetric cell membrane. One such vesicle is about 50 nanometers in diameter, about 2,000 times smaller than the average diameter of a human hair.

"That may seem very small, but it would make Titan sweat," Katsaras says. "It's about 60 million atoms, whereas most people are working with systems that are a hundred thousand atoms. That is enormous."

The fine-grained simulation of a whole vesicle will help researchers better understand how cell membranes are structured and how they interact with other molecules within and outside the cell.

"Membranes' structure may dictate how drug action happens," Katsaras says. "This could lead to an understanding of how a drug interacts with a membrane or how it communicates. You need both experiment and simulation. The simulation, in this case, gives us the finer, atomistic detail—if we could trust it. Experiments give us a broader perspective and validation of the simulation. Basically, it's a system of checks and balances."

Through a National Institutes of Health consortium in partnership with Lawrence Berkeley National Laboratory, work is already under way at ORNL to develop the computational tools needed to understand data from neutron crystallography studies.

Langan also envisions creating a biomedical neutron technology research center at ORNL that would further integrate the lab's supercomputing and neutron capabilities, as well as offer training and assistance to biomedical researchers.

"ORNL's emerging capabilities in neutron science are providing the biomedical research community with unprecedented opportunities to solve problems once considered intractable," Langan says. "It's a truly exciting time." *—Morgan McCorkle*

Diversify, replace, recycle

Energy labs and partners come together to ensure supplies of critical energy materials

Across the US, energy labs are working to turn a widespread shortage of critical energy materials into a boon for domestic mining and clean energy industries.

The US Department of Energy's new Critical Materials Institute, led by Ames Laboratory, brings together experts from ORNL, Idaho National Laboratory, Lawrence Livermore National Laboratory, seven universities, and seven industrial partners.

ORNL chemist Bruce Moyer, who leads CMI's effort to diversify the supply of critical materials, explains that the institute is focused on ensuring the availability of materials that support clean energy technologies—particularly rare earth elements that are critical to producing electric vehicles, wind turbines, solar energy, batteries and energy-efficient lighting. He notes that DOE's 2011 Critical Materials Strategy identified five rare earth metals (dysprosium, terbium, europium, neodymium and yttrium) whose availability could affect clean energy technology deployment in coming years.

Two of these, dysprosium and neodymium, are particularly critical to the production of the strong magnets used in electric motors. Without them, magnets would be weaker, and products such as electric vehicles and wind turbines would be less efficient and too costly to operate.

Beyond the rare earth elements for magnets, CMI is also addressing supply issues related to phosphors—compounds which often depend on the very scarce rare earth metals europium, terbium and yttrium and are used in energy-efficient lighting. Another CMI focus is on potential shortages of two elements DOE describes as "near-critical": lithium, because of its importance to battery manufacturing, and tellurium, for the role it plays in solar panel production.

Working smarter

"There are three main ways to approach the challenge of ensuring that we have the materials we need," Moyer says. "One is to diversify the supply. The second way is to find substitutes, and the third way is to develop technologies for recycling. ORNL is most heavily involved in investigating the first two for CMI, though we do have activities taking place in developing recycling technologies as well as in developing new computational tools to accelerate the molecular design of new separation agents."

An innovative example of diversifying the supply of a key material, in this case lithium, can be found in California's Imperial Valley, where six power plants are using superheated geothermal brines from deep underground to generate steam for the production of electricity. The lithium-rich brine would normally then be pumped back into the ground; however, CMI industrial partner Simbol Materials is working with the utility to re-route the brine through a process that extracts lithium before the liquid is recycled. ORNL's chemical separations expertise is helping Simbol increase the efficiency of its extraction process, which is currently being run on a relatively small "pilot" scale.

"We plan to work with Simbol to develop new separation materials, sorbent materials and membranes that are lithium-selective," Moyer says.

Efforts to improve the supply side of the equation for rare earths aim to find new sources, which then could enhance mineral processing efficiency and encourage the development of new uses for the more abundant rare earth metals.

Moyer explains that when ore containing rare earth minerals comes out of the ground, the rare earths make up a very small fraction of the material. The key challenge becomes separating the 1, 5 or 10 percent of the ore that contains rare earth metals from the rest of the rock. Then the resulting "concentrate" can be economically processed to recover and purify the individual rare earth elements.

"One of our most exciting projects combines ORNL's strengths in the dynamics of mineral interfaces and molecular design with Colorado School of Mines' strength in mineral processing to develop new froth flotation agents to concentrate rare earth minerals from ore," Moyer says.

In froth flotation, crushed and ground ore particles are mixed with water and detergent-like molecules called "collectors," which attach themselves very selectively to the surfaces of the desired mineral particles in the mixture—rare earth minerals, in this case. Air is then bubbled through this mixture to create froth.

"We can adjust the chemistry of the flotation agent so the particles we're interested in stick to the bubbles and the others are washed away," Moyer says. "Despite the apparent simplicity of this technique, advancing the technology will require expanding the limits of interfacial science and molecular design."

Moyer and his colleagues are working with the mining chemical company Cytec and the mining company Molycorp to apply this technique to the task of improving Molycorp's mining operations.

"Our first goal is to develop a new flotation agent and process chemistry that will help our partners increase their recovery of the rare earths from the ore," Moyer says. "This project is being led by Colorado School of Mines."

ORNL's flotation agent design team includes experts on characterizing the structure and dynamics of mineral-water interfaces, as well as chemical scientists who are designing new flotation agents that can selectively bind to the surface of the bubbles as well as to the rare-earth-containing particles. Once new agents have been developed, Moyer's team will send them to the Colorado School of Mines for testing. The most effective ones will be passed along to ORNL's partners at Cytec to enable them to produce and test the agents in larger quantities.

"Our hope is that Molycorp will think this process looks attractive and will want to conduct a large-scale test at its facility," Moyer says.

Exploring alternatives

CMI's program to develop alternatives to rare earth materials includes efforts to devise magnetic materials that use fewer rare earth materials, as well as new phosphors that, ideally, don't use any. Brian Sales, an ORNL materials scientist and deputy head of the program, explains that critical materials aren't just a problem for the future; they're part of everyday life. He notes there are a billion or more fluorescent lights in use, and the phosphors in each of them contain a substantial amount of rare earth material.

The institute's search for alternatives to rare earth materials benefits from its interdisciplinary perspective. Materials theorists often work with computational scientists and materials scientists to develop potential solutions. The result is an ongoing cycle of theory, computation and laboratory research. This may seem redundant, but it moves researchers steadily toward their goals.

"As laboratory scientists we take suggestions from theorists and computational simulations all the time," Sales says. "Generally, they can't point us in a specific direction or at a specific combination of materials. Their guidance is more like a compass than a GPS system. That's why this kind of research has to be an iterative process."

Sales suggests that alternatives to rare-earth-containing phosphors might be found in the next two or three years. "Of course, it will take a while longer than that before they're implemented by industry," he says. "We have been very pleased with General Electric's enthusiasm. They will be testing the materials we've come up with at their Cleveland plant. I think substitute materials for phosphors probably have the best chance of making a real impact in the next few years."

Substitute materials for magnets, he suggests, have real possibilities but will probably take a bit longer. "A lot of research organizations have been working on this," Moyer says. "It's a much harder problem, so we'll have to come up with some novel approaches."

Critical partnerships

CMI is operating on five-year timeline for success. Moyer emphasizes that the institute will measure its success or failure in terms of the impact of its technologies on the supply of critical materials.

"You have to work closely with industrial partners to do this kind of thing," he says. "If industry doesn't use our technology, then it won't have an impact, and it won't do a thing to reduce material criticality. However, if we develop a technology and industry uses it to increase the supply of these materials, then we can say that CMI really made something happen." Ⓡ *—Jim Pearce*

(Above) ORNL materials scientist Orlando Rios works with a high-field processing magnet that uses both radio frequency heating and a strong magnetic field to alter the microstructure of materials to improve their magnetic properties.
Photo: Jason Richards

(Below) ORNL materials scientist Michael McGuire covers the other end of the thermal spectrum with a liquid helium-cooled physical-properties-measuring system that also employs an intense magnetic field to synthesize and measure the properties of alternative magnetic materials.
Photo: Jason Richards

Potent partnerships

CASL simulations add insight into operating nuclear reactor cores

CASL Core Partners

- Electric Power Research Institute
- Idaho National Laboratory
- Los Alamos National Laboratory
- Massachusetts Institute of Technology
- North Carolina State University
- Oak Ridge National Laboratory
- Sandia National Laboratories
- Tennessee Valley Authority
- University of Michigan
- Westinghouse Electric Company

CASL Contributing Partners

- Anatech
- CD-adapco
- City College of New York
- Core Physics, Inc.
- G S Nuclear
- Imperial College London, UK
- Florida State University
- Pacific Northwest National Laboratory
- Pennsylvania State University
- Rensselaer Polytechnic Institute
- Southern States Energy Board
- Texas A&M University
- University of Florida
- University of Notre Dame
- University of Tennessee, Knoxville
- University of Texas, Austin
- University of Wisconsin

Powerful computers and great minds from national laboratories, academia and industry are already notching successes that could help commercial light water nuclear reactors operate more efficiently and reliably for decades.

Through the Consortium for Advanced Simulation of Light Water Reactors, the first Energy Innovation Hub established by the US Department of Energy just three years ago, researchers recently performed their first full-scale simulation of a reactor during startup. While that's a significant milestone, it represents just the beginning for this partnership of 10 core players, says CASL Director Doug Kothe, who noted that leadership computers such as ORNL's Titan—the fastest in the US—are providing unprecedented modeling and simulation capabilities.

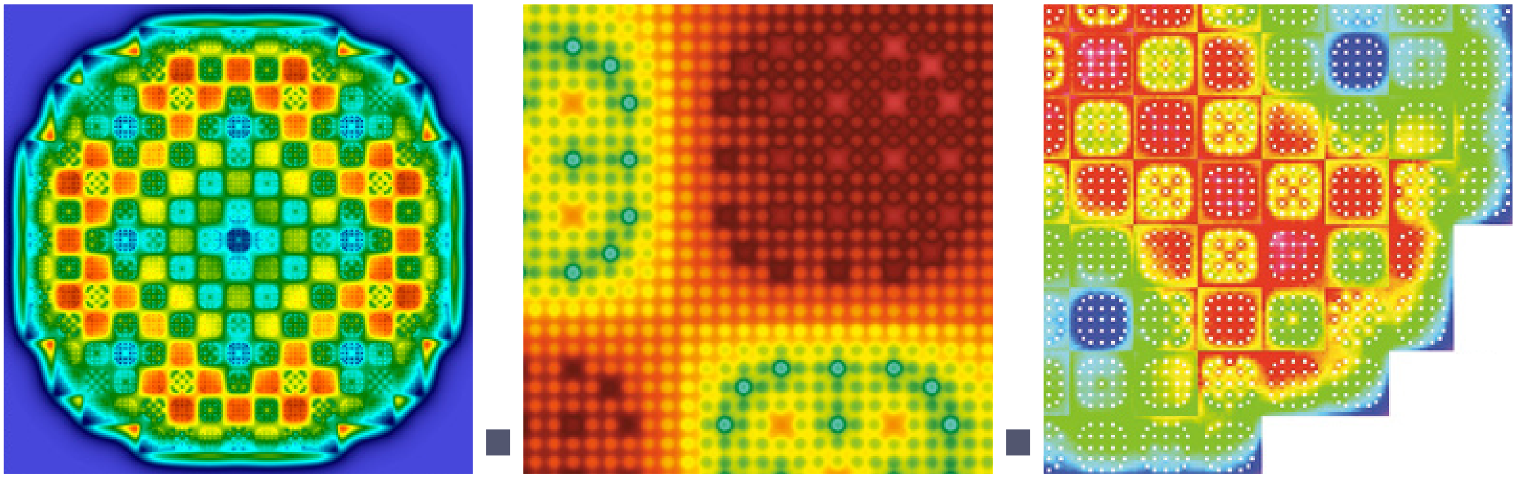
"With CASL tools using Titan, our scientists are seeking to gain a better understanding of what's happening with, for example, tens of thousands of fuel rods in a reactor core," Kothe says. "The amount of information we can see is not only unprecedented, but also revealing." This new window into a reactor core, while initially made possible through CASL modeling and simulation technology that effectively utilizes high-performance computing platforms like Titan, can then be used to increase the capabilities of industrial-class computers in common use today.

The recent simulation used CASL's new Virtual Environment for Reactor Applications. The VERA simulations were directly compared against operational data taken at Tennessee Valley Authority's Watts Bar Nuclear Plant, and the favorable comparisons showed that the software environment is both accurate and useful. Through VERA and simulations to come, researchers will gain a better understanding of reactor performance with much greater fidelity than provided by methods of the past.

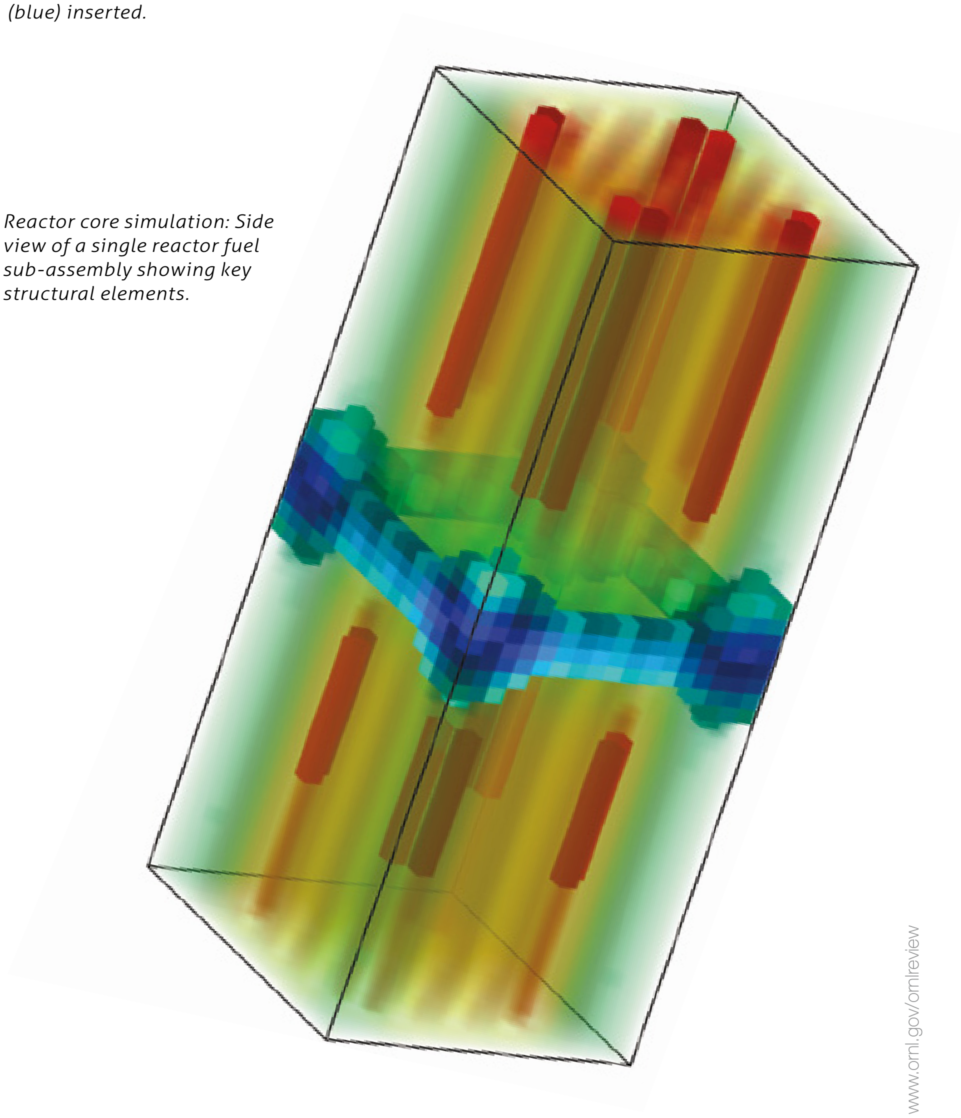
While this initial VERA simulation focused on the startup cycle, future simulations will examine full power operations of the TVA reactor, which will utilize current VERA development that is integrating the thermal hydraulics behavior, fuel performance and surface chemistry. These additional capabilities will allow not only a greater understanding of operating reactors, but also spark insights that Kothe and colleagues are confident can stimulate advances in reactor operations.

"Our vision is to predict with confidence the safe, reliable and economically competitive performance of nuclear reactors through science-based modeling and simulation technologies," Kothe says. "These predictive technologies can then be deployed on common computers used broadly throughout the nuclear energy industry."

CASL is headquartered at ORNL, and its core partners include: the Electric Power Research Institute, Idaho National Laboratory, Los Alamos National Laboratory, Massachusetts Institute of Technology, North Carolina State University, Sandia National Laboratories, TVA, University of Michigan, Westinghouse Electric Company and ORNL.



Reactor core simulations: (Left) a slice through the full core showing power generation (red signifies more power, blue less); (center) a close-up view of several fuel sub-assemblies showing fuel, control pins, and water channels; (right) the lower right corner of a full core view with control rods (blue) inserted.



Reactor core simulation: Side view of a single reactor fuel sub-assembly showing key structural elements.

Industry partners counting on CASL

From the nuclear power plant business' perspective, maximizing the life span and performance of the more than 100 reactors in operation across the nation are of critical importance. With 100,000 megawatts of power generation capacity, today's reactors are supplying nearly 20 percent of US electricity. While a new generation of reactors emerges, many years of useful life remain for these proven sources of power, which represent billions of dollars of investment.

To accomplish their goal of helping industry continue to optimize performance, CASL researchers focus on the in-vessel reactor core phenomena of pressurized water reactors, the most common type of light water reactor in the US. They are studying, for example, the behavior of nuclear fuel during all operating conditions, while looking for potential modifications to enhance safety and efficiency.

Kothe also notes that performance expectations for first-generation nuclear power reactors needed to be conservative in order to guarantee safety with what was then new technology. Fifty years later, modern tools and supercomputers are allowing the CASL team to gain a deeper understanding of underlying processes such as thermal hydraulics, fuel rod performance, neutronics, surface chemistry and corrosion, and structural dynamics.

"For example, our new capabilities will allow us to look closely at reactor core models operating with 193 fuel assemblies, nearly 51,000 fuel rods and about 18 million fuel pellets," Kothe says. "These elements operate in a high-temperature, high-pressure, high-radiation environment for three to five years. Our software is evolving to simulate these conditions and predict performance, providing industry with some of the information it needs to meet its goals."

CASL core partners provide a unique perspective based on decades of working with industry members. Some partners envision CASL research leading to nuclear power plants that are more flexible in operation, using, for example, "gray" control rods, an approach that helps a reactor match power output more closely to demand. Opportunities may also exist for more accident-tolerant fuels, or for improvements to reactor core designs that allow more fuel burnup and consequently less waste to be produced.

For others a state-of-the-art understanding of nuclear power plant phenomena and performance can benefit from advanced modeling and simulation, exactly the role filled by CASL. A rigorous simulation could address scenarios in which power is limited by certain behaviors in the core—with insight potentially leading to reduced fuel costs or increased power ratings.

Meanwhile, other team members are interested in modeling and simulation work that would result in a clearer understanding of reactor safety margins. During the industry's first generation of light water reactor development, safety margins were set very carefully in order to ensure public safety with the new technology. Now, with more than 50 years of operating experience and increased understanding of the science gained through tools such as VERA, there may be some room for margins to be adjusted and performance increased, while still preserving the highest levels of public safety.

VERA in action

Through what the CASL team calls "test stands," scientists are providing early deployment of CASL technologies into active nuclear design and engineering environments.

"Our focus is on enhancing the performance of light water reactors with advanced nuclear reactor modeling and simulation technology," says ORNL's Jess Gehin, a nuclear engineer and member of the CASL team. "Through the test stand effort, we're able to address issues that are important to the nuclear industry. We're also able to receive highly constructive feedback to help us continuously improve CASL's simulation capabilities."

CASL test stands offer flexibility, allowing for siting at a CASL industry partner, council member or collaborator site, and use of ORNL-based computing assets or local computing assets. "In a sense a CASL test stand is similar to a rocket test stand," Kothe says. "We use a test stand to determine performance characteristics of VERA, but I'll add that we also allow and want our industry partners and industry council members to be the ones doing the testing. And we want them to test VERA in the process of trying to do 'real work.'"

Kothe noted that working with Westinghouse, for example, CASL deployed its first test stand at a Cranberry, Penn., site this summer. It is allowing Westinghouse and CASL to apply and test VERA on core physics analysis of the AP1000 Pressurized Water Reactor and its advanced first core design. Simulating the advanced core design provides a challenging scenario to test the VERA tools' prediction capabilities.

In return CASL gets valuable and candid feedback on whether VERA is useful and usable. "This feedback can be in any number of forms—examining feature needs, quality, robustness or computational performance," Kothe says. "The possibilities are endless, but getting this feedback via test stands now is invaluable because it allows our active development to address any problems and issues."

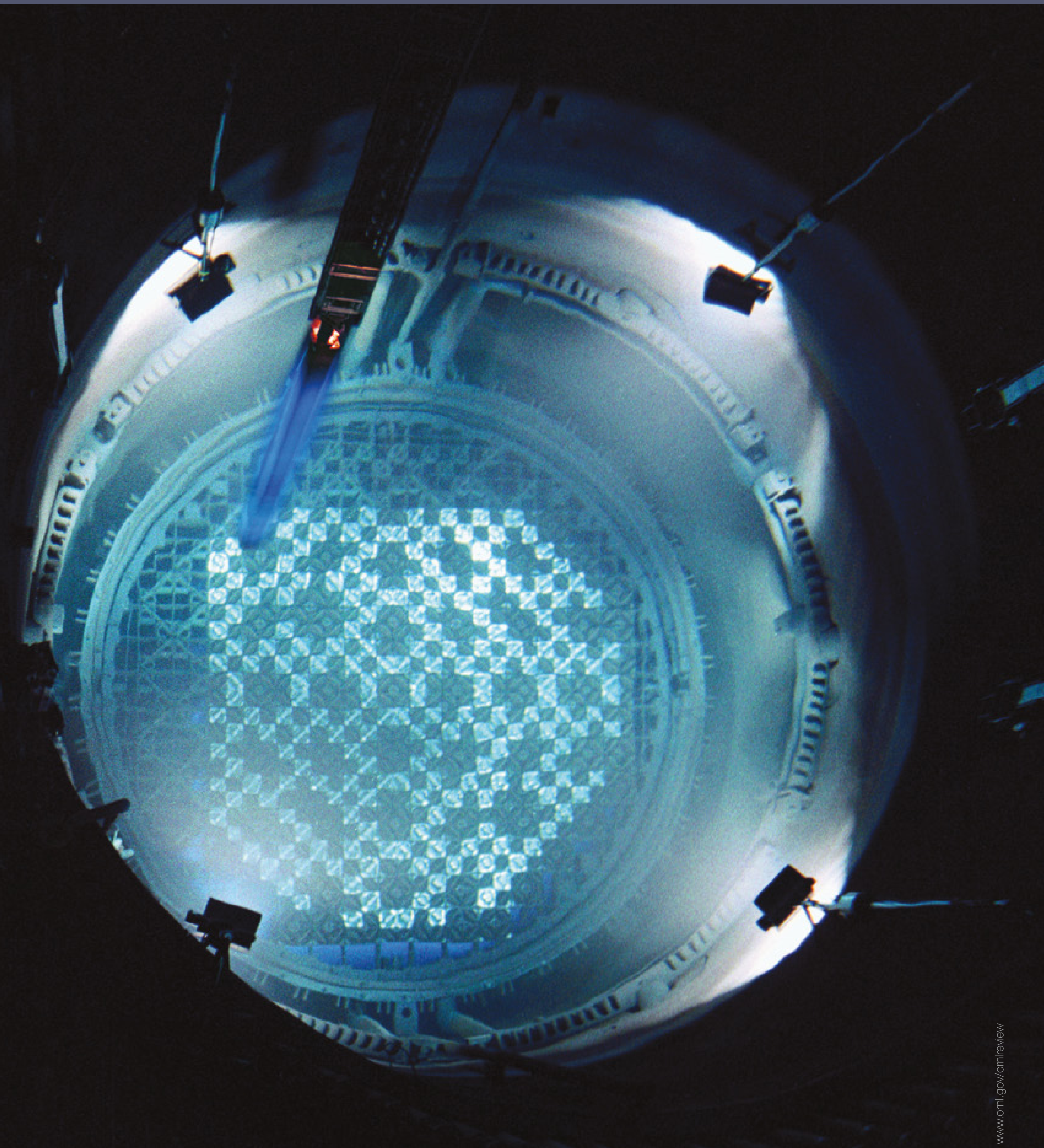
'Challenge problems'

Current industry analysis techniques are effective at helping scientists and engineers understand and predict the performance of materials, components and subsystems of nuclear power plants. Often, however, they are based on a collection of simplifications and calibrations that ultimately limit the applicability and predictability of the technique.

By pressing beyond the techniques of the past and applying contemporary methods, the CASL team is pursuing a deeper understanding of phenomena that are taking place every day in nuclear reactors across the US.

Armed with this collection of capabilities, CASL takes on "challenge problems" that encompass phenomena limiting the performance of some pressurized reactors. These problems are what drive the development of higher-fidelity tools that combine multiple complex physical and chemical processes taking place simultaneously. By demonstrating the application of these tools to existing issues, immediate insights can be delivered to the commercial nuclear power industry. As Gehin sums it up, "With CASL, we are developing the next generation of reactor simulation tools that offer huge potential for improving our abilities to simulate reactor operation and performance." R

View of a reactor core showing the removal of a fuel assembly during a refueling outage. Photo: Tennessee Valley Authority



Better Biofuels

Better biofuels

ORNL researchers are pooling expertise to unlock green energy

Using some of the world's most powerful machines, ORNL scientists are tackling major bioenergy problems by outsmarting nature.

The Energy Independence and Security Act of 2007 calls for the production of 36 billion gallons of renewable fuel by 2022. It's a lofty goal because neither the chemical nor biological process that converts biomass into biofuel is ready to be scaled to that magnitude.

"Biomass has a huge potential to be used for energy, but industrially we need better technology to mass-produce biofuels cost-competitively," says Loukas Petridis, a researcher working in the lab's Biosciences Division. "We know that we can produce ethanol from materials like grass, wood chips and even newspapers, so the question now is: How can we improve the efficiency of the biofuel production process?"

Biological blockage

One of the biggest roadblocks preventing the economically viable production of biofuels is lignin, a glue-like substance found just beneath a plant's surface that serves as a plant cell's first defense against man and beast.

Lignin intertwines with sugars called cellulose and hemicellulose in plant cell walls. Its hardiness protects a plant's inner structures from microbes and fungi, but lignin has been a major frustration for bioenergy researchers.

During biofuel production—a process that converts plant mass into alcohol—lignin blocks enzymes from breaking down cellulose into the sugars necessary for fermentation.

"Our goal is to understand, on a molecular level, exactly why biomass is so resistant, or recalcitrant, to breakdown," Petridis says. "If we can understand this, then we can suggest ways to improve biofuel production."

To solve the problem, scientists are arming themselves with neutrons and supercomputers.

Petridis is collaborating with ORNL's BioEnergy Science Center, a multidisciplinary research group with experts in math, computer science, physics, chemistry and biology who are working together to improve the biofuel conversion process.

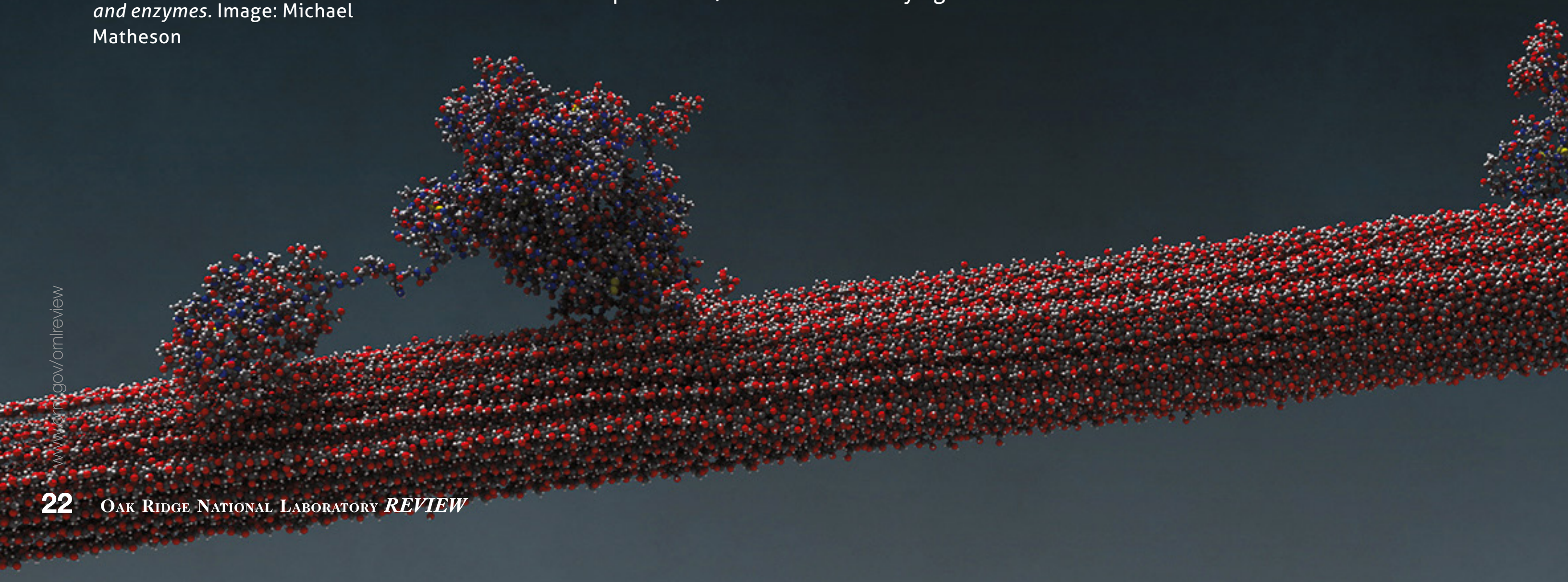
Using simulations from ORNL's Titan supercomputer in conjunction with neutron scattering techniques at the lab's High Flux Isotope Reactor, scientists are studying how individual plant molecules change their shape and structure during biomass pretreatment. Pretreatment is an expensive process that opens cell walls and, in theory, allows enzymes to more easily break down cellulose. But these processes still aren't able to fully degrade the biomass in a timely manner.

"We wanted to understand why biomass remained recalcitrant to enzymatic degradation even after pretreatment," Petridis says. "Our group was one of the first groups to explain this observation on a molecular level."

Simulations and experiments allow researchers to resolve the structure of lignin aggregates down to 1 angstrom, which is about 1 million times smaller than what the naked eye can see. The models reveal how different temperatures can change lignin's structure, causing it to either aggregate or expand. The lignin clumps cause problems in biofuel production because they stick to the enzymes that release sugars from cellulosic biomass.

"Looking at simulations and experiments allows us to form a more holistic picture of this process," says computational biophysicist Jeremy Smith, director of ORNL's Center for Molecular Biophysics and a governor's chair at the University of Tennessee. "Researchers previously believed that lignin only clumped during the cool-down phase, but our models and experiments show us that lignin forms problematic clumps even at the relatively hot temperatures used during pretreatment."

The models also show how and why lignin interacts with cellulose and enzymes. The simulations reveal detailed multiscale



Computer simulations show how and why lignin interacts with cellulose and enzymes. Image: Michael Matheson structures that help people understand biomass recalcitrance and assist engineers who are trying to improve second-generation biofuel yield.

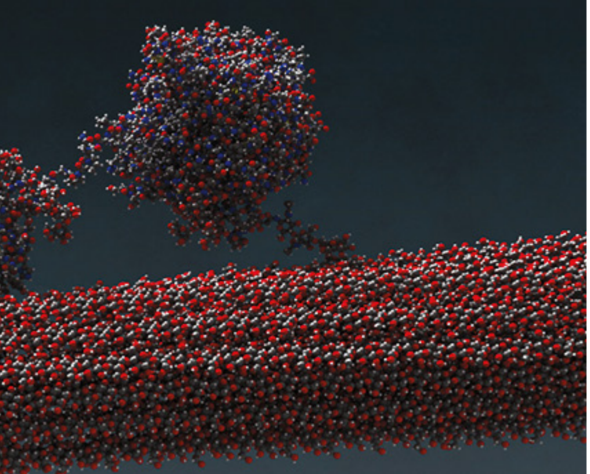
Other ORNL investigators involved in these computer simulations are Roland Schulz, Benjamin Lindner, Xianghong Qi and John Eblen.

Atomic details

As supercomputing power increases over the next 5 to 10 years, researchers will be able to simulate more than just the interaction between lignin and cellulose. They hope to simulate large parts of a living plant cell at atomic detail, including the enzymes and microbes that eat the biomass.

In the meantime ORNL's team has been awarded 78 million hours on Titan through the Innovative and Novel Computational Impact on Theory and Experiment, or INCITE, program. Researchers plan to use these hours to study how lignin behaves in different types of biomass, which will help them identify the plant characteristics best suited for biofuel production.

"The more we learn about biomass, the easier it will be to improve pretreatment and the biofuel production process," Petridis says. "We hope that our studies will help engineers design new pretreatment methods and engineer different types of biomass and enzymes that can harvest more energy from plant materials. In this way we can help the United States begin running on renewables." ® — *Jennifer Brouner*



Little critters, big energy

ORNL team receives $2 million to study use of microbial electrolysis in biorefineries

Scientists are using one of Earth's smallest creatures to solve some of the government's biggest bioenergy problems.

For the next three years, a $2.1 million grant will allow ORNL researchers to use a process called microbial electrolysis to transform plant biomass into hydrogen to produce energy-rich biofuel for use in combustion engines.

With conventional technology, industries convert biomass into bio-oil—a corrosive substance that turns into biofuel after it's treated with natural gas. This treatment provides hydrogen atoms that can deoxygenate bio-oils, but the process also emits a significant amount of carbon dioxide.

The US Department of Energy has given the laboratory the three-year grant to address this environmental issue and boost the hydrogen and carbon efficiency of biofuel production.

"We think we can solve the problem by using live microbes instead of natural gas and chemical catalysts to create biofuels," says project leader Abhijeet Borole of ORNL's Biosciences Division. "We know that microbes can convert organic compounds into hydrogen gas, but the process doesn't yet run at a high enough rate or with enough efficiency to work in a huge reactor where thousands of gallons of the bio-oil aqueous phase need to be treated every day."

Microbial electrolysis cells act like batteries in reverse. Instead of consuming fuel, they actually help create it.

The process requires a small energy input, but the majority of energy is produced by electrogenic microbes—a type of bacteria that generates electricity while dining on organic compounds. These microbes eat the bio-oil's organic acids and produce an electrical current capable of converting the corrosive compounds in bio-oil and water into hydrogen.

"These microbes can reduce the energy normally needed to hydrolyze water by up to 70 percent while consuming the corrosive organic compounds," Borole says.

It's a healthy exchange. Scientists provide the microbes with food, and the microbes, in turn, produce hydrogen to make biofuels that can be used for transportation.

Borole envisions thousands of microbial electrolysis cells configured as stacks alongside other biorefinery unit operations. Each cell will contain electrodes coated with 50 to 100 layers of electricity-generating microbes.

For this process to work efficiently, ORNL's team must build a microbial community that can digest the organic compounds found in the aqueous phase of bio-oils and create a system that can harness the electrical currents produced.

ORNL's team is collaborating with researchers at Georgia Tech and the University of Tennessee to solve these problems and improve other aspects of the biofuel production process. They are also working together to develop membrane separators that can recycle water in biorefineries, improve the process that separates water and oil emulsions, optimize microbial electrolysis and identify the organic compounds in bio-oils available for microbial breakdown. The team includes scientists from a wide range of disciplines—chemistry, biology, microbiology, environmental science and engineering.

"We are working together to develop the microbial electrolysis process and other supporting processes so that eventually microbes can help mass-produce hydrogen to produce biofuel," Borole says. "There is a difference between scientific and technological progress. We want to see if we can bridge that gap." ® — *Jennifer Brouner*

Ben Preston

is the Deputy Director of ORNL's Climate Change Science Institute, which is dedicated to developing a better understanding of the causes and consequences of climate change and informing policymakers about what society can do to respond and adapt to these changes.

Preston's early interest in making science relevant to decision-makers attracted him to the Pew Center on Global Change in Washington, D.C., where he worked as a senior research fellow. He came to ORNL in 2010 after five years at Australia's Commonwealth Scientific and Industrial Research Organization, where he was a research scientist with the Division of Marine and Atmospheric Research.

We asked Preston to share some of his thoughts about the importance of climate science and how policymakers and local and national governments can take advantage of climate change research.

How did you first get involved in climate change research?

I first got involved in climate change research from the policy side. I had been working as a research scientist in environmental biology, but I was always interested in environmental policy—particularly in how environmental science is used to support public policy. To get into policy research, I hunted around for well-respected organizations that were doing policy work. I eventually found a group called the Pew Center on Global Climate Change. I told them that I had a background in science, I hadn't worked on climate specifically, and I was really interested in seeing how science influences policy and how I as a scientist could contribute to that effort. That sold them on me, so I spent four years there, working at the interface between climate science and public policy. This allowed me to bring my scientific training to bear and also to see how scientific information is both used and abused in a policy environment.

As a scientist and spokesperson for climate change research, what's the main message you want people to hear?

The public hears a lot about the uncertainty associated with climate change research and the controversy over what's going to happen in the future. I don't think this does justice to the decades, if not centuries, of research in this area. There is a wealth of knowledge out there that's continually being expanded. We know quite a bit about how the climate works and how it is influenced by human activity. We have a good handle on these things. I think that's a message that doesn't come across in the politicized landscape of climate change.

Climate research encompasses a number of scientific disciplines. How does this broad approach affect the science that is produced?

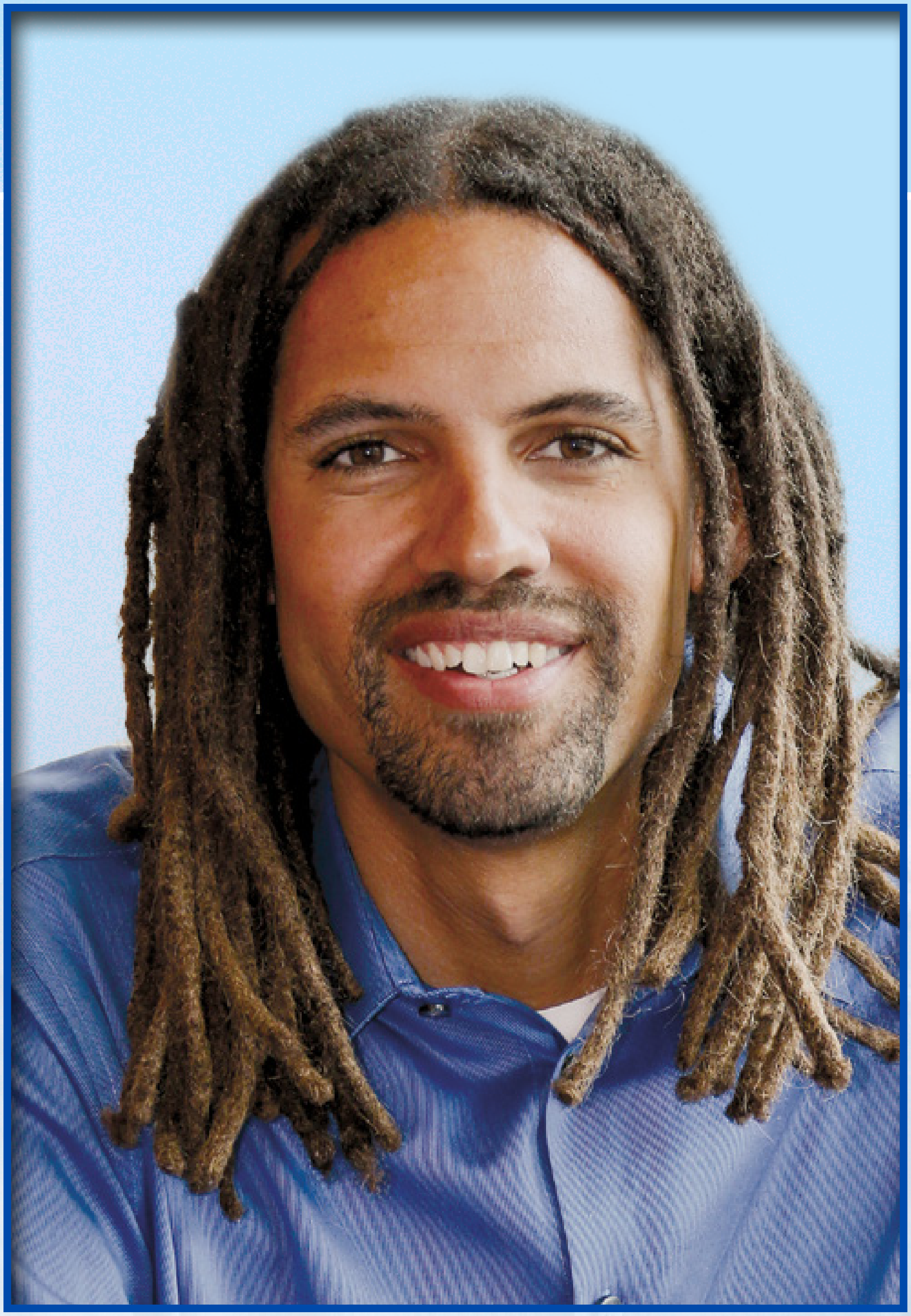
It creates a lot of challenges because each discipline has one piece of the puzzle. It's a challenge to integrate these disciplines, to tell a coherent story about cause and effect, and then to develop a policy response. However, if you're successful, you can create a rich body of knowledge. Bringing all these pieces together allows you to tell a more involved, more complex, and more nuanced story. This level of detail enables us to influence real-world decision-making in both public and private institutions.

You interact with policymakers from time to time. Are you optimistic that public policy will adapt quickly enough to soften the socio-economic impacts of a changing climate?

When I look at the prospects for significant policy intervention at a global scale—for instance, national governments collaborating to reduce greenhouse gas emissions—I am somewhat pessimistic. Over the last decade or more, we have seen that achieving those kinds of international agreements and collaborations is extremely difficult. However, we can also look at what's happening at the local level, the municipal level or the individual level. At those levels I think there are a lot more positive and optimistic stories. States, cities and communities have individually and collaboratively made significant gains in reducing greenhouse gas emissions and have improved their ability to adapt to the current effects of climate change and plan for the future.

What are some of the practical things that national and local governments can do to adapt to climate change?

I think the role of national government is to create an enabling environment in which greenhouse gas mitigation or adaptation



can occur. Governments can also educate stakeholders across the public and private sectors about climate change, as well as alert them to opportunities for reducing risk and creating incentives for behavior in that direction. A lot of my research is focused more on the local level, particularly the role of spatial planning in influencing the exposure of human populations and communities to these kinds of risks. I concentrate on how our decisions about where we place people, development and economic investment ultimately influence what's at risk when extreme events occur. We have recently seen plenty of examples—particularly with regard to extreme weather—of where it would be beneficial to think more critically about how we make those decisions.

What's your definition of success in your work at the Climate Change Science Institute?

One of my definitions of success is having a scientific impact. We can measure this to some extent by looking at our research funding, at how many publications we produce and things like that. For the institute as a whole, these have been increasing.

We would also like to see the institute being recognized by other folks in the research community as a place where interesting, groundbreaking things are happening—a place where high-quality researchers look for opportunities to engage and collaborate.

We want the institute to have an impact in the broader society. We would like to have a greater media presence—to be able to communicate our science to the media in a way that allows the importance of the science to be appreciated in a broader context.

We also want to engage with the private sector. We do this well at ORNL in general, and we're trying to replicate this success in the climate arena. We're always asking ourselves, "How can the science we're doing here be used to benefit the private sector?"

Finally, we want to be able to inform the policy discourse by creating relationships and linkages in the policy arena—with organizations like think tanks and local, state and federal agencies. We want them to believe that Oak Ridge is a place they can turn to for quality science and straight answers on climate change. Ⓡ

ORNL research reveals new challenges for mercury cleanup

More forms of mercury can be converted to deadly methylmercury than previously thought, according to a study published recently in *Nature Geoscience*. The discovery provides scientists with another piece of the mercury puzzle, bringing them one step closer to understanding the challenges associated with mercury cleanup.

Earlier this year a multidisciplinary team of ORNL researchers discovered two essential genes for microbes to convert oxidized mercury to methylmercury, a neurotoxin that can penetrate skin and at high doses affect brain and muscle tissue, causing paralysis and brain damage.

The discovery of how methylmercury is formed answered a question that had stumped scientists for decades, and the recently published findings build on that breakthrough.

Most mercury researchers have believed that microbes could not convert elemental mercury—which is volatile and relatively inert—into methylmercury. Instead of becoming more toxic, they reasoned that elemental mercury would bubble out of water and dissipate. That offered a solution for oxidized mercury, which dissolves in water. By converting oxidized mercury into elemental mercury, they hoped to eliminate the threat of methylmercury contamination in water systems.

ORNL's study and a parallel study reported by Rutgers University, however, suggest that elemental mercury is also susceptible to bacterial manipulation, a finding that makes environmental cleanup more challenging.

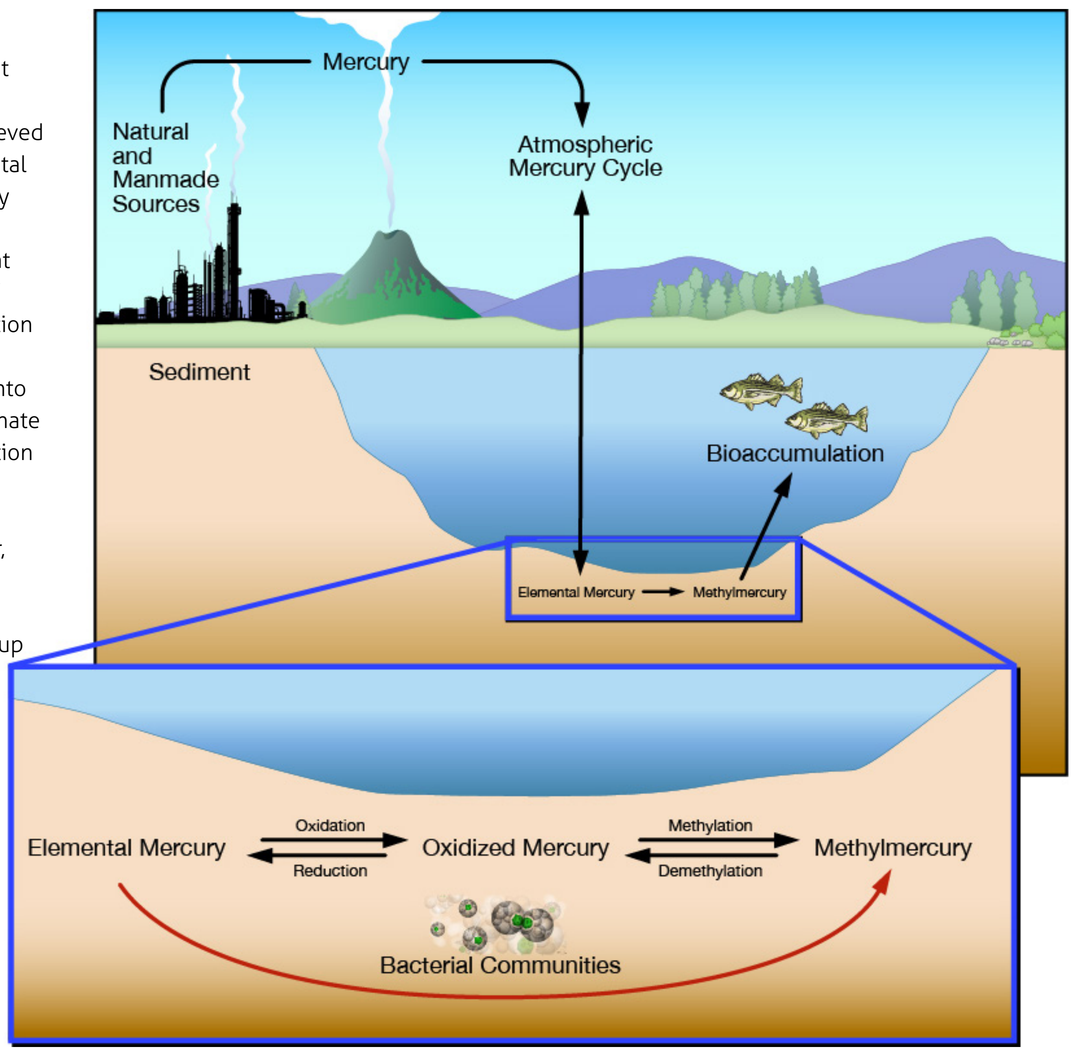
"Communities of microorganisms can work together in environments that lack oxygen to convert elemental mercury to methylmercury," study leader Baohua Gu says. "Some bacteria remove electrons from elemental mercury to create oxidized mercury, while others add a methyl group to produce methylmercury."

Mercury is a toxin that spreads around the globe mainly through the burning of coal, other industrial uses, and natural processes such as volcanic eruptions; various forms of mercury are widely found in sediments and water. Methylmercury bioaccumulates in aquatic food chains, especially in large fish.

The fight against mercury pollution involves scientists with expertise in chemistry, computational biology, microbiology, neutron science, biochemistry and bacterial genetics. Other ORNL efforts are focusing on when, where and why bacteria are producing methylmercury.

"Our research allows us to understand generally where and how bacteria might produce methylmercury so we can target those areas in the future," says ORNL's Liyuan Liang, a co-author and director of the DOE-funded mercury research program. "We are trying to understand the process of microbial mercury methylation. Once we understand the process, we can begin to form solutions to combat mercury pollution." Ⓡ

—Jennifer Brouner



ORNL researchers are learning more about the microbial processes that convert elemental mercury into methylmercury.
Image: Dami Rich

ORNL finding goes beyond surface of oxide films

Better batteries, catalysts, electronic information storage and processing devices are among potential benefits of an unexpected discovery made by ORNL scientists using samples isolated from the atmosphere.

Researchers at the laboratory learned that key surface properties of complex oxide films are unaffected by reduced levels of oxygen during fabrication—an unanticipated finding with possible implications for the design of functional complex oxides used in a variety of consumer products, says Zheng Gai, a member of US Department of Energy's Center for Nanoscale Materials Sciences at ORNL.

The findings are detailed in a paper published in *Nanoscale*.

While the properties of the manganite material below the surface change as expected with the removal of oxygen, becoming an insulator rather than a metal, or conductor, researchers found that the sample showed remarkably stable electronic properties at the surface. Gai emphasizes that the robustness of a surface matters because it is precisely the surface properties that determine, influence and affect the functionality of complex oxides in catalysis and batteries.

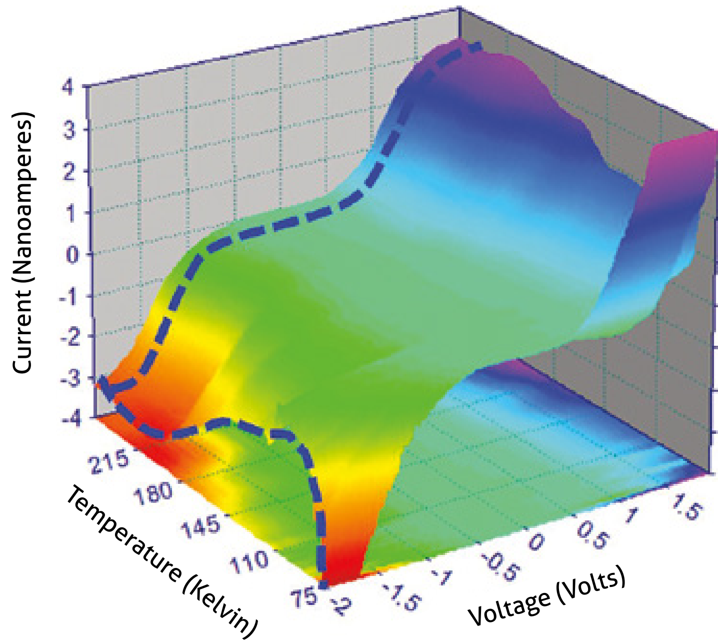
"With these materials being a promising alternative to silicon or graphene in electronic devices, the ever-decreasing size of such components makes their surface properties increasingly important to understand and control," Gai says.

While this work provides a fundamental understanding of a material used and researched for catalysts, oxide electronics and batteries, Gai and lead author Paul Snijders noted that it's difficult to speculate about possible impacts.

"I always say that in basic science we are discovering the alphabet," says Snijders, a member of ORNL's Materials Science and Technology Division. "How these letters will be designed into a useful technological book is hard to predict."

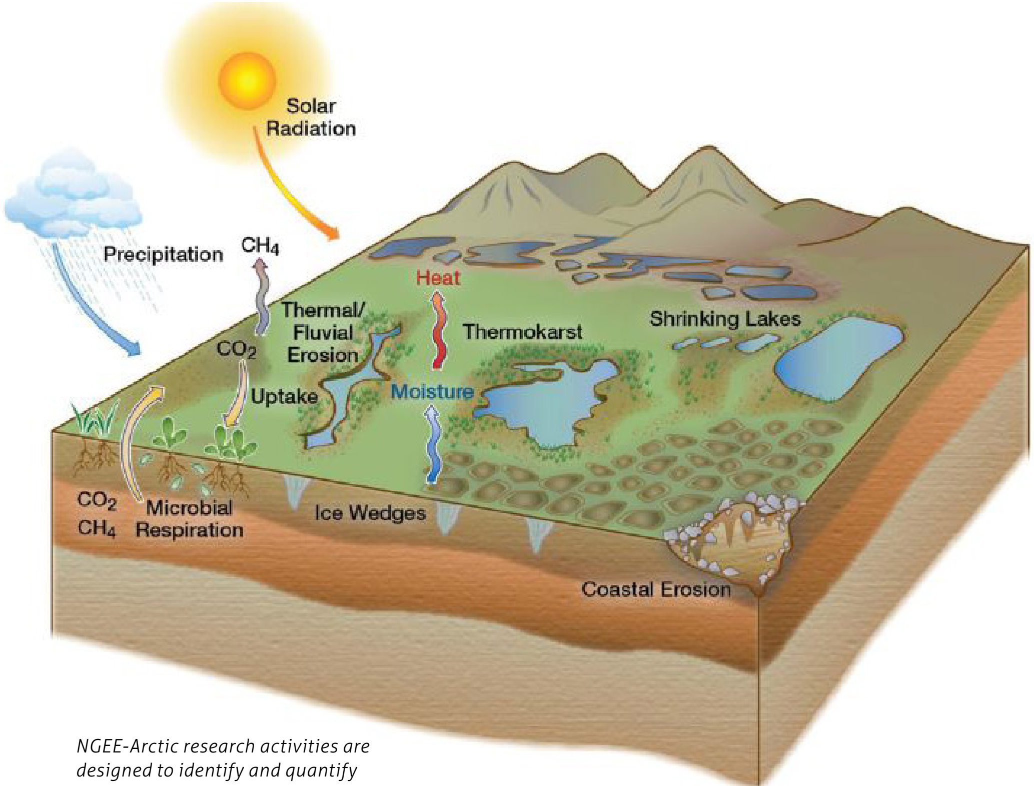
Making this discovery possible was the fact the authors did their experiment using scanning probe microscopy in a vacuum system with no exposure of the samples to the atmosphere. This contrasts with the conventional approach of growing a sample and then installing it in analysis equipment. During such a transfer, scientists expose the material to the water, nitrogen and carbon dioxide in the air.

By studying pristine samples, the ORNL team gained a surprising new understanding of the physics of the material surfaces—an understanding that is necessary to design new functional applications, Snijders says. —*Ron Walli*



This figure shows both the spectroscopic measurement (current as a function of voltage) and the spectroscopic measurement as a function of temperature. Image: Reproduced by permission of The Royal Society of Chemistry

New algorithm enables unprecedented sampling, modeling of Arctic



NGEE-Arctic research activities are designed to identify and quantify mechanisms underlying processes that control carbon and energy transfer in the Arctic biosphere, as well as how those processes play out in a changing Arctic landscape. Image: NGEE-Arctic project

The Arctic is a big, cold and desolate place—not to mention that much of it is fairly inaccessible.

For these reasons, conducting meaningful on-the-ground research there is a tricky business. To characterize the environment, researchers need tools to extend their limited observations to the larger landscape. For example, how different are conditions on one piece of land from those hundreds of miles away? How will those conditions shift in 10, 20 or 30 years?

To answer questions like these, a team of researchers from ORNL and the US Department of Agriculture's Forest Service used a unique algorithm to divide the state of Alaska into "bioclimatic" regions based on the results of climate and permafrost models. The team produced decadal maps of representative regions at multiple levels of division. Data from 2000 to 2009 and an ensemble of model results from 2090 to 2099 revealed how current ecosystems may shift under a changing climate.

"You want to be sure that you take samples that are representative of the larger ecosystem," says team member Forrest Hoffman of ORNL's Climate Change Science Institute, who presented results from the project Aug. 5 in Minnesota at the 98th annual meeting of the Ecological Society of America. The findings were also published online in June in *Landscape Ecology*. "Resource and logistical constraints limit the frequency and extent of environmental observations, particularly in the Arctic, necessitating the development of a systematic sampling strategy to maximize coverage and objectively represent environmental variability at desired scales."

Team members include Jitendra Kumar and Richard Mills of ORNL and William Hargrove of the US Forest Service. Their effort employed a quantitative methodology for delineating sampling domains and showed how the representativeness of eight possible sampling sites may change in the future. The research is useful for informing site selection for the US Department of Energy's Next-Generation Ecosystem Experiments project, or NGEE–Arctic, and determining if measurement sites and networks accurately represent vast and potentially vulnerable high-latitude ecosystems in which natural responses to human-caused global warming are amplified.

Team members developed software that enables a unique algorithm, based on a cluster algorithm, to work on parallel computing systems, thus allowing the analysis of larger datasets.

Ultimately the team hopes to demonstrate that these techniques can be applied at different temporal and spatial scales to meet the needs of individual research groups and climate modelers.

Soon the team will apply the same methodology at a smaller spatial scale to define domains within the Barrow Environmental Observatory in Alaska, where the NGEE–Arctic project is under way. The researchers will use remote sensing to categorize the region's unique polygonal ground features and create input for models to simulate the behavior of Arctic tundra. R

—*Gregory Scott Jones*

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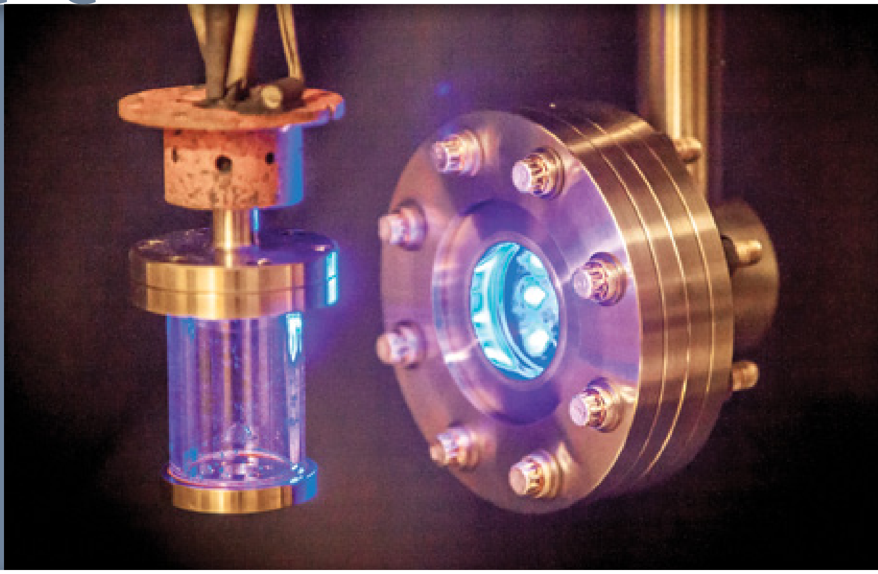
Neutron science:
New insights for revolutionary materials



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