OAK RIDGE NATIONAL LABORATORY

Review

Tennessee Together

OAK RIDGE National Laboratory

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OAK RIDGE NATIONAL LABORATORY
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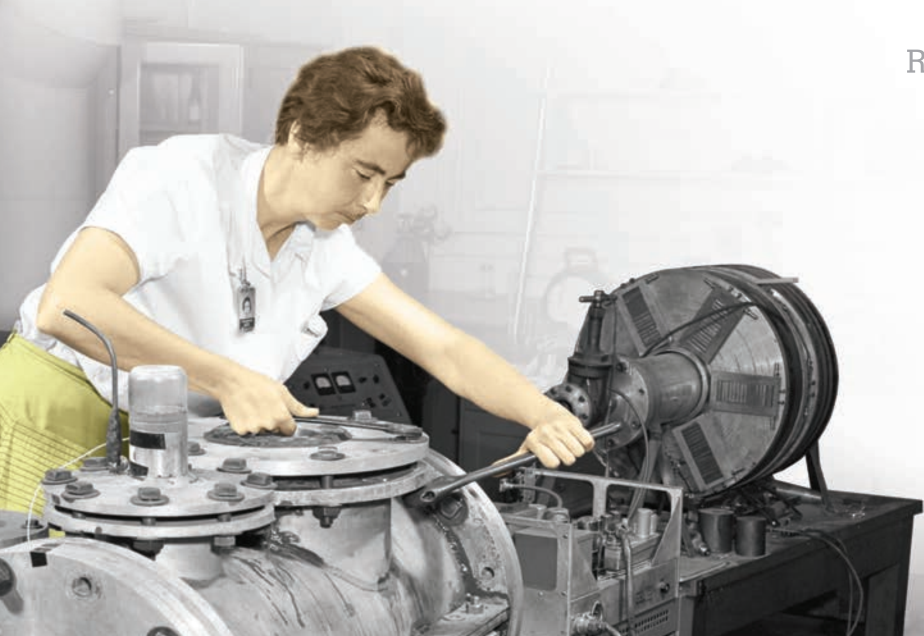
Contents

On the Cover

David Sholl is director of the University of Tennessee-Oak Ridge Innovation Institute. Image credit: Genevieve Martin, ORNL



Former ORNL physicist Frances Pleasonton (see page 40).

UT partnership takes us into the future

ORNL has been collaborating with the University of Tennessee for the better part of eight decades, dating back to 1945.

We have much to show for our partnership. Our institutes and centers have benefitted not only the two institutions, but also — especially — Tennessee students, who have had the opportunity to study under leaders in their fields and take advantage of one-of-a-kind facilities available at a national lab.

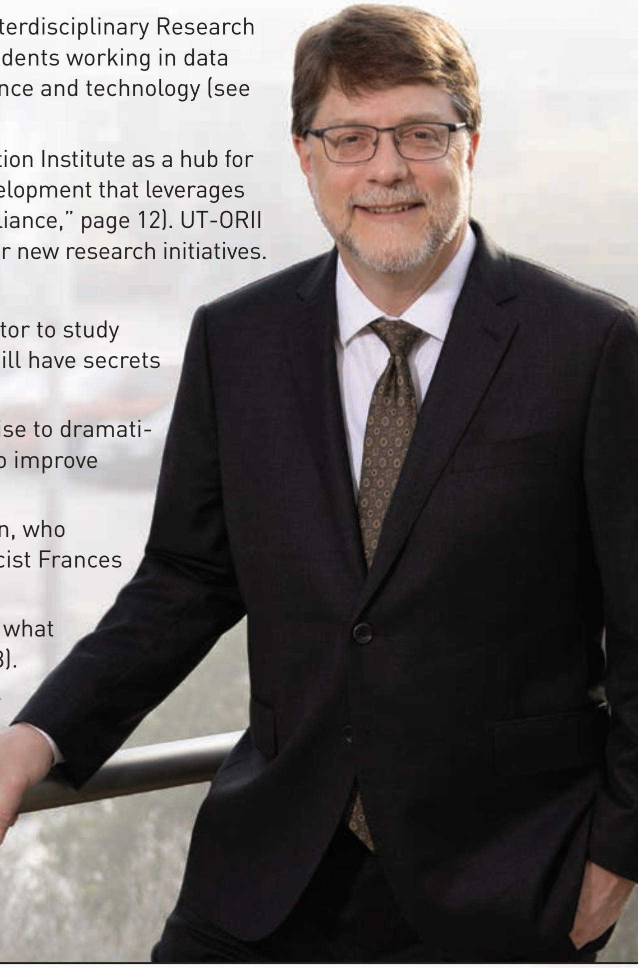
In this issue of *ORNL Review*, we take a look at the lab's relationship with UT, a relationship that continues to make both institutions stronger, more impactful and better able to attract leading researchers and top students (see "Still collaborating after all these years," page 8).

Our collaboration — with key involvement from the state of Tennessee — enriches both our research efforts and our academic responsibilities. It's most visible in UT-Battelle, the collaboration between the university and Battelle Memorial Institute that has managed the lab since April 2000. But it can also be seen in the blending of talented researchers across both institutions.

The Governor's Chairs program was created in 2006 to attract scientists who are leaders in their fields into our labs and classrooms. To date, it includes 13 highly accomplished researchers who strengthen our focuses in areas including nuclear technology, advanced manufacturing and materials sciences (see "Governor's Chairs program attracts scientific luminaries," page 16).

That success was followed in 2010 by creation of the Bredesen Center for Interdisciplinary Research and Graduate Education, which houses about 75 high-achieving doctoral students working in data science and engineering, energy science and engineering, and genome science and technology (see "Doctoral students look beyond academia," page 20).

Finally, in 2021, the state, university and lab created the UT-Oak Ridge Innovation Institute as a hub for discovery and innovation, interdisciplinary graduate education, and talent development that leverages the best of both institutions (see "An institute to supercharge the UT-ORNL alliance," page 12). UT-ORII provides not only a home for existing collaborations but a launch pad for major new research initiatives.



Elsewhere in the *Review*:

- Researchers used neutron scattering at ORNL's High Flux Isotope Reactor to study moon rocks (see "50 years after NASA's Apollo missions, moon rocks still have secrets to reveal," page 28).
- ORNL worked with the Army to produce weld filler materials that promise to dramatically improve high-strength steel repair (see "ORNL teams with Army to improve welds," page 36).
- We take a look back at pioneering ORNL researcher Frances Pleasonton, who explored the properties of the neutron in the postwar years (see "Physicist Frances Pleasonton joined early ORNL studies of the neutron," page 40).
- We talk to postdocs and graduate students working at ORNL to find out what drives their love of science and technology (see "Why Science?" page 38).
- And finally, in Research Insights, our technical staff continues its exploration of additive manufacturing (see "Additive Manufacturing the Future, Part II: Improving the Process," page 42).

On a personal note, this is the first issue of the *Review* that I've had the opportunity to introduce since I became director of ORNL this past October. *ORNL Review* has been communicating important lab research and other news since 1967. I am delighted to be a part of that tradition, and I hope you enjoy reading this issue of *ORNL Review*.

Stephen Streiffer
Laboratory Director

Genome editing tool honed for better renewables

ORNL scientists have used their expertise in quantum biology, artificial intelligence and bioengineering to improve how CRISPR Cas9 genome editing tools work on organisms like microbes that can be modified to produce renewable fuels and chemicals.

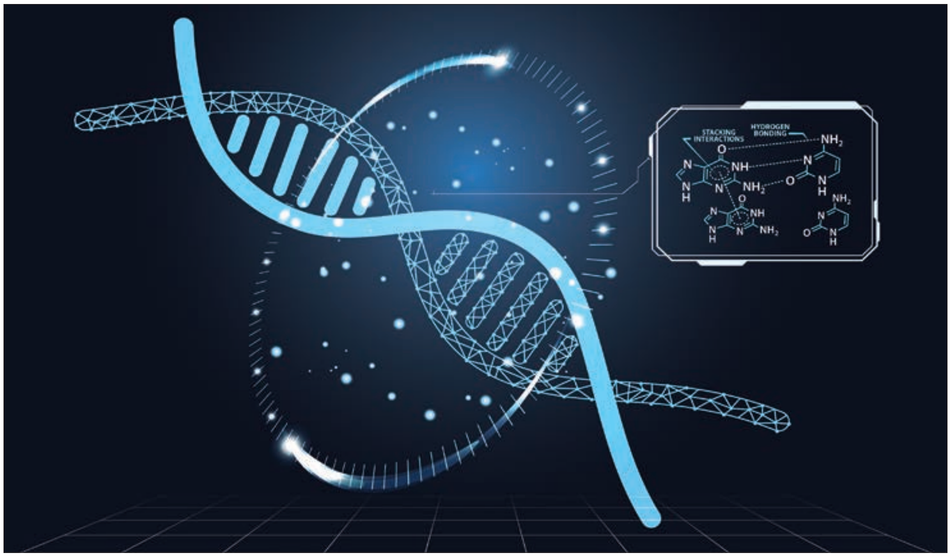
CRISPR is a powerful tool for bioengineering, used to modify genetic code to improve an organism's performance or to correct mutations. The CRISPR Cas9 tool relies on a single, unique guide RNA that directs the Cas9 enzyme to bind with and cleave the corresponding targeted site in the genome. Existing models to computationally predict effective guide RNAs for CRISPR tools were built on data from only a few model species, with weak, inconsistent efficiency when applied to microbes.

"A lot of the CRISPR tools have been developed for mammalian cells, fruit flies or other model species. Few have been geared towards microbes where the chromosomal structures and sizes are very different," said Carrie Eckert, leader of the Synthetic Biology group at ORNL. "We had observed that models for designing the CRISPR Cas9 machinery behave differently when working with microbes, and this research validates what we'd known anecdotally."

To improve the modeling and design of guide RNA, the ORNL scientists sought a better understanding of what's going on at the most basic level in cell nuclei, where genetic material is stored. They turned to quantum biology, a field bridging molecular biology and quantum chemistry that investigates the effects that electronic structure can have on the chemical properties and interactions of nucleotides, the molecules that form the building blocks of DNA and RNA.

The scientists built an explainable artificial intelligence model called iterative random forest. They trained the model on a dataset of around 50,000 guide RNAs targeting the genome of E. coli bacteria while also taking into account quantum chemical properties, in an approach described in the journal Nucleic Acids Research. — *Stephanie Seay*

For more: https://bit.ly/3FRY2Mv



ORNL scientists developed a method that improves the accuracy of the CRISPR Cas9 gene editing tool used to modify microbes for renewable fuels and chemicals production. Image credit: Philip Gray, ORNL

ORNL's Klasky honored as ACM senior member

Hilda Klasky, an R&D staff member in ORNL's Scalable Biomedical Modeling group, has been selected as a senior member of the Association of Computing Machinery, or ACM.

ACM is the world's largest educational and scientific computing society; senior members are those who have worked in a relevant field for at least 10 years, have demonstrated technical leadership and have made significant contributions to the field.

Hilda Klasky

Fewer than 10 percent of ACM's senior members are female, and Klasky said she hopes her new title will motivate female researchers across computing and computational science.

"Being named a senior member is a great honor and a truly humbling experience," she said. "This recognition bestowed upon me by my peers at the ACM is particularly meaningful since ACM is one of the most prestigious organizations in computer science. The designation of 'senior member' holds significant importance as it acknowledges my career-long contributions." — *Scott Jones*

Improving graphite used in molten salt reactors

In response to a renewed international interest in molten salt reactors, ORNL researchers have developed a novel technique to visualize molten salt intrusion in graphite.

During ORNL's revolutionary Molten Salt Reactor Experiment, or MSRE, in the 1960s, scientists first demonstrated the feasibility of nuclear fission reactions with molten fluoride salt used both as a fuel carrier and as a coolant, substituting for the solid fuel and water used in traditional nuclear reactors. Molten salt reactor designs show great promise as a means of carbon-free power generation.

To slow down neutrons so they can easily promote nuclear fission, nuclear reactors use a material called a moderator. To moderate the MSRE, which ORNL ran in the 1960s, scientists used synthetic graphite, which is resistant to thermal shock and dimensionally stable because of its extensive pore system resulting from the manufacturing process. MSRE graphite was custom-made and specially coated to decrease porosity and defend against detrimental effects that may occur when hydraulic and gas pressures cause molten salt to seep into graphite's pores. Moreover, preventing molten salt intrusion avoids additional issues with waste management during reactor decommissioning.

Following the experiment's conclusion in 1969, the potential of molten salt reactors was largely unexplored until the 21st century, and low demand for the specialized graphite led to the material's discontinuation among domestic graphite manufacturers. With an uptick in molten salt reactor research but no MSRE graphite, today's scientists must identify an alternative graphite to successfully moderate nuclear reactions in molten salts. However, ambiguity around the effects of molten salt intrusion poses a barrier to discovery. Scientists have a limited understanding of what microscopic features enable some graphite grades to withstand intrusion better than others and how salt intrusion affects graphite's other properties.

Hoping to resolve these uncertainties, a team of ORNL scientists led by Nidia Gallego and Jisue Moon studied molten salt intrusion across various graphite grades and have validated the first technique to visualize and monitor molten salt penetration depth and distribution in graphite's pores. — *Alexandra DeMarco*

For more: https://bit.ly/3u4z21X

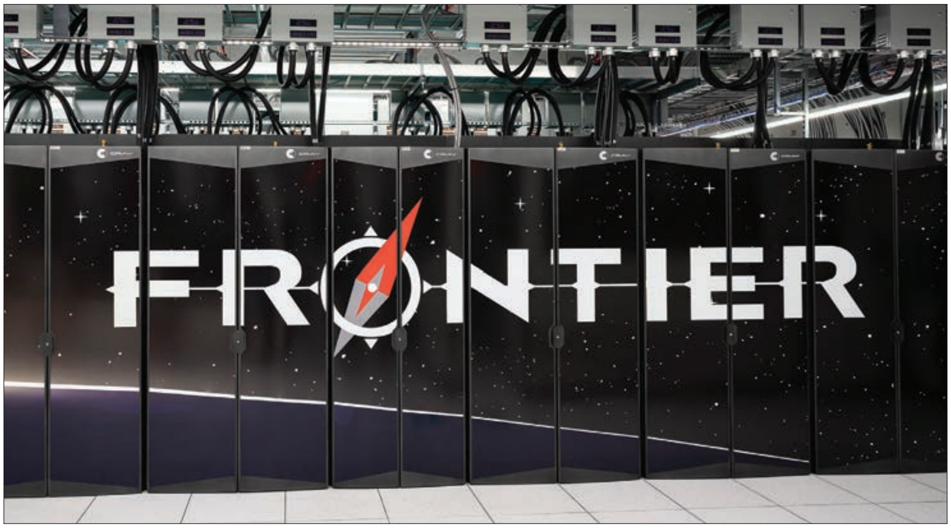
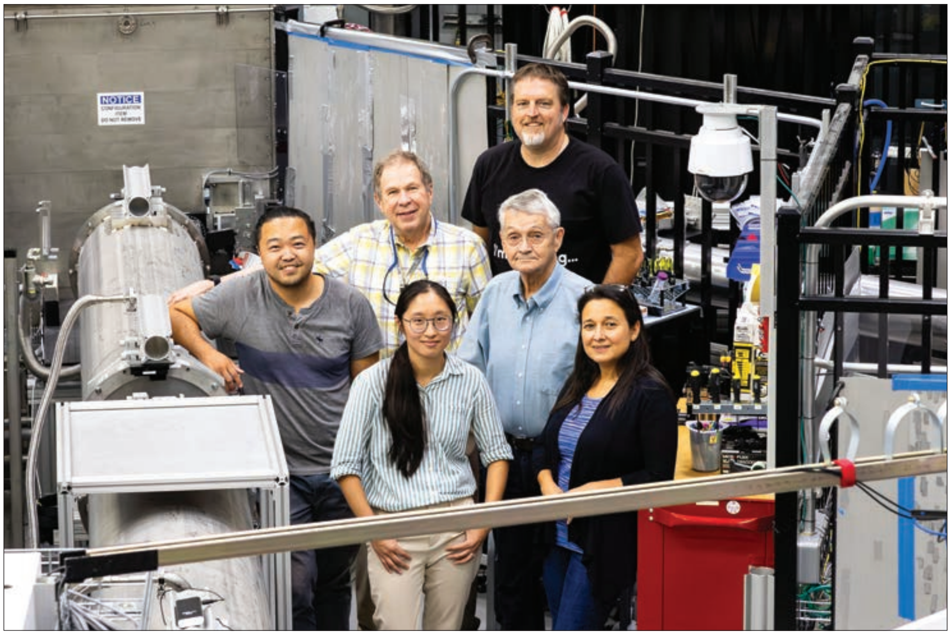


Image credit: Carlos Jones, ORNL



From left, Yuxuan Zhang, James Keiser, Jisue Moon, Cristian Contescu, Erik Stringfellow (back) and Nidia Gallego, with Dino Sulejmanovic (not shown), first visualized molten salt distribution in graphite pores.
Image credit: Carlos Jones, ORNL

Supercomputing program supports 75 projects

The Department of Energy's Office of Science has allocated supercomputer access to a record-breaking 75 computational science projects for 2024 through its Innovative and Novel Computational Impact on Theory and Experiment, or INCITE, program. DOE is awarding 60 percent of the available time on the leadership-class supercomputers at DOE's Argonne and Oak Ridge national laboratories to accelerate discovery and innovation.

The projects will support a wide range of high-impact, computationally intensive research campaigns in a broad array of science, engineering and computer science domains.

Jointly managed by the Argonne Leadership Computing Facility and the Oak Ridge Leadership Computing Facility, the INCITE program is the primary means by which the facilities fulfill their mission to advance open science by providing the scientific community with access to their powerful supercomputing resources. The

ALCF and OLCF are DOE Office of Science user facilities.

This year's awards are the second INCITE allocations on the OLCF's Frontier system, which debuted in May 2022 as the world's fastest supercomputer. Frontier has a High Performance Linpack speed of 1.194 exaflops and a theoretical peak performance of 2 exaflops.

Open to any researcher or research organization in the world with a computationally intensive project, INCITE's application process is highly competitive.

This year, the INCITE awards committee received 108 total proposals with researchers requesting more than 103.5 million node-hours.

For details on all of the 2024 INCITE awardees: https://bit.ly/47h9vRR

Connected, automated cars maximize energy efficiency

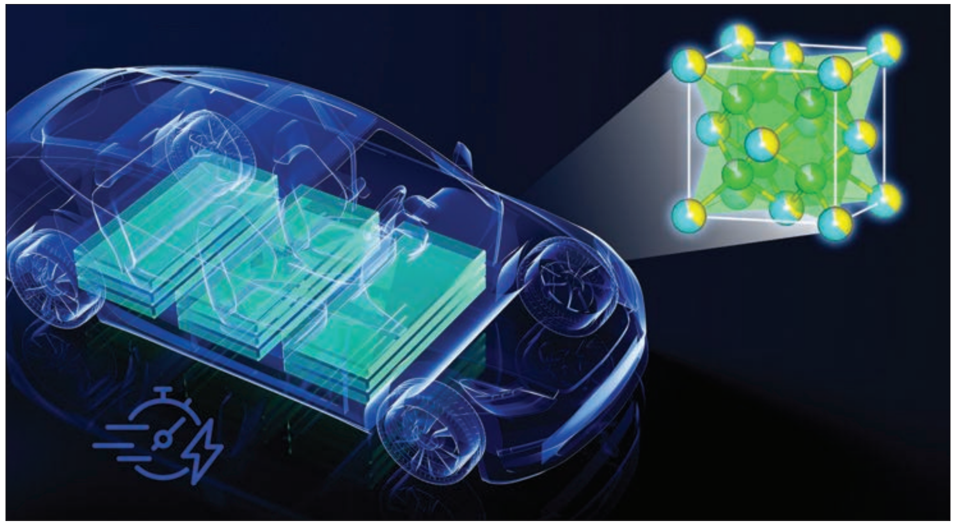
ORNL researchers determined that a connected and automated vehicle, or CAV, traveling on a multilane highway with integrated traffic light timing control can maximize energy efficiency and achieve up to 27 percent savings.

In a demonstration, a plug-in hybrid passenger vehicle in electric mode was driven down a busy corridor in Chattanooga, Tennessee. The test vehicle and the timing of traffic lights along the longitudinal route were controlled by ORNL-developed computer algorithms.

"The energy efficiency of the transportation system and the CAV itself were optimized by avoiding idling, hard braking and accelerating as much as possible," ORNL's Jinghui Yuan said. "With integrated optimization strategies, CAVs can achieve significant energy savings."

Two control strategies were implemented on the traffic signals and the CAV and integrated into a cyber-physical system. They were first tested in a digital twin-based traffic simulation and ORNL's virtual proving ground, the Connected and Automated Vehicle Environment Laboratory. — *Jennifer Burke*

ORNL researchers took a connected and automated vehicle out of the virtual proving ground and onto a public road to determine energy savings when it is operated under predictive control strategies.
Image credit: ORNL



Researchers have shown how an all-solid lithium-based electrolyte material can be used to develop fast charging, long-range batteries for electric vehicles that are also safer than conventional designs.
Image credit: ORNL, U.S. Dept. of Energy

Neutrons offer insights into battery advances

Currently, the biggest hurdle for electric vehicles, or EVs, is the development of advanced battery technology to extend driving range, safety and reliability.

New research has shown how a novel lithium-based electrolyte material (Li9N2Cl3) can be used to develop solid-state batteries that charge faster and store more energy than conventional designs. Experiments revealed the solid-electrolyte was not only stable in normal air environments, but it also inhibited the growth of dendrites — dangerous, branchlike formations that cause batteries to catch fire.

ORNL scientist Jue Liu conducted neutron experiments to observe how lithium moved through the material.

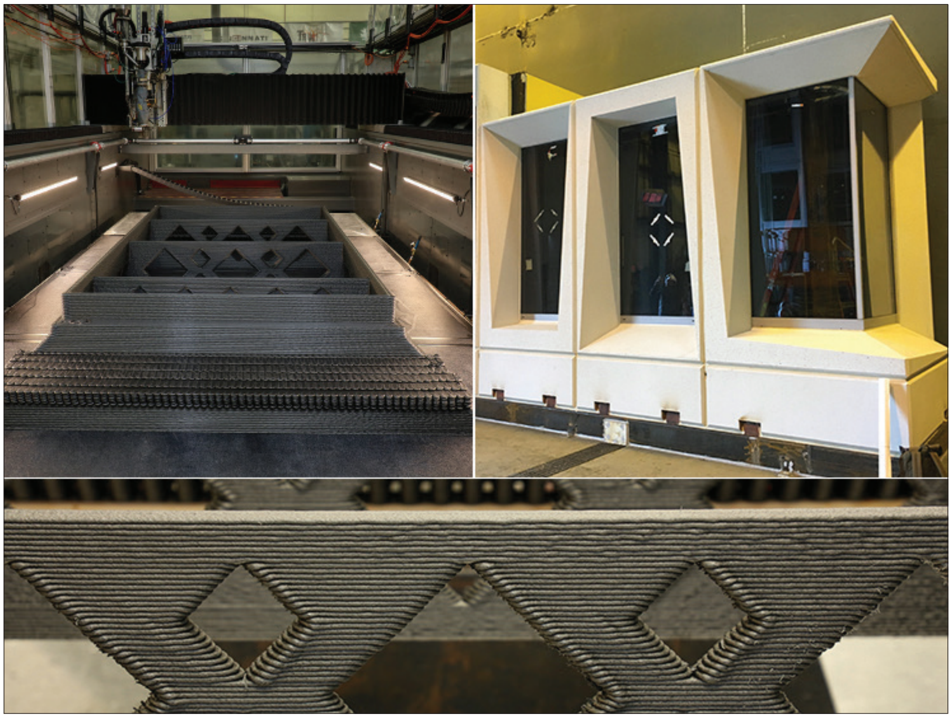
"The material's dry air stability, efficient lithium-ion transport, and high compatibility toward metallic lithium are crucial advances. It's the best of both worlds," he said. "It offers all the performance benefits of liquid-electrolyte batteries that we use every day, but it's safer and more reliable." — *Jeremy Rumsey*

Gene 'hotspot' triggers poplar root growth

ORNL scientists identified a gene "hotspot" in the poplar tree that triggers dramatically increased root growth. The discovery supports development of better bioenergy crops and other plants that can thrive in difficult conditions while storing more carbon belowground.

The team used a vast poplar dataset to identify regulator genes that can trigger hundreds of other gene expressions in the tree. They confirmed the molecular function of one hub gene, PtrXB38, and found that plants with the gene produced prolific and deeper roots. The gene even stimulated the growth of aerial roots on stems and leaves.

"With more roots, these plants absorb more nutrients, grow larger, are more tolerant to drought and can draw more carbon underground for longer-term storage," ORNL's Wellington Muchero said. The aerial roots may also make the plant more tolerant to flooding. "This naturally occurring gene has implications for biomass production, food production and climate change mitigation." — *Stephanie Seay*



ORNL's 3D-printed polymer composite mold was used to produce precast concrete parts for a New York City building. Researchers conducted a techno-economic analysis that highlights the benefits over wood molds. Image credit: ORNL and Gate Precasttin

Printed concrete molds beat out wood molds

ORNL researchers have conducted a comprehensive life cycle, cost and carbon emissions analysis on 3D-printed molds for precast concrete and determined the method is economically superior to conventional wood molds.

Precast concrete is used in building construction and produced by pouring the material into a reusable mold. For decades, these molds have been made from wood — a technique that requires a highly specialized skillset. As an alternative, molds made from fiber-reinforced polymer composites can be 3D printed.

"We developed a techno-economic model that compared costs associated with each method, evaluating materials, equipment, energy and labor," ORNL's Kristina Armstrong said. "3D printing can make complex molds faster, and the composites can be recycled, leading to more economical molds when used many times for precast concrete parts."

Optimizing mold designs also reduces energy demand and carbon emissions. Future studies will further evaluate the recycling impact. — *Jennifer Burke*

Two hybrid poplar plants, middle and right, engineered with the PtrXB38 hub gene exhibited a drastic increase in root and callus formation compared with a wild-type control plant, left. Image credit: Tao Yao, ORNL

New tech recycles mixed plastic waste

Almost 80 percent of plastic in the waste stream ends up in landfills or accumulates in the environment. ORNL scientists have developed a technology that converts a conventionally unrecyclable mixture of plastic waste into useful chemicals, presenting a new strategy in the toolkit to combat global plastic waste.

The technology, invented by ORNL's Tomonori Saito and former postdoctoral researcher Md Arifuzzaman, uses an exceptionally efficient organocatalyst that allows selective deconstruction of various plastics, including a mixture of diverse consumer plastics. Arifuzzaman, now with Re-Du, is a current Innovation Crossroads fellow.

Production of chemicals from plastic waste requires less energy and releases fewer greenhouse gases than conventional petroleum-based production. Such a pathway provides a critical step toward a net-zero society, the scientists said.

"This concept offers highly efficient and low-carbon chemical recycling of plastics and presents a promising strategy toward establishing closed-loop circularity of plastics," said Saito, corresponding author of the study published in Materials Horizons. — *Lawrence Bernard*

Researchers used the open-source Community Earth System Model to simulate the effects that extreme climatic conditions have on processes like land carbon storage. Image credit: Carlos Jones, ORNL

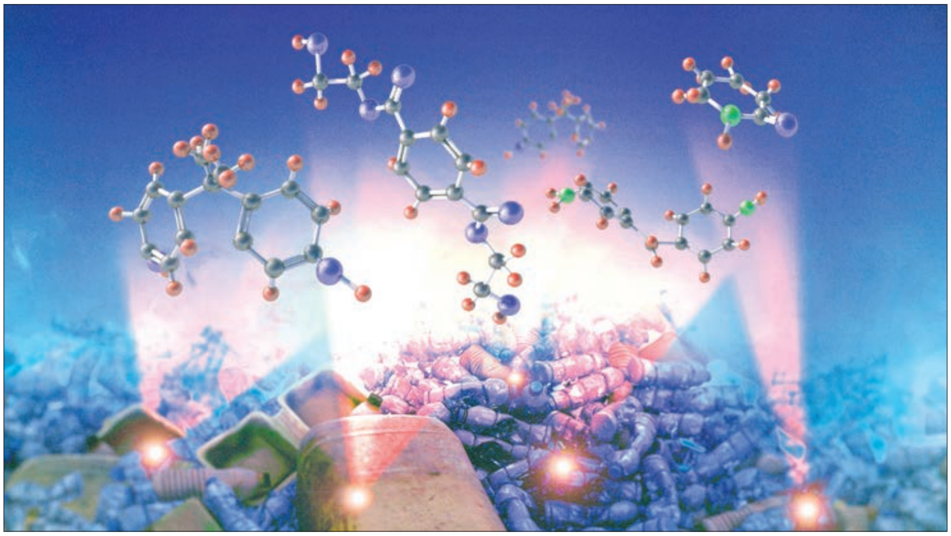
Climate extremes hamper Earth's carbon storage

Researchers from ORNL and Northeastern University modeled how extreme conditions in a changing climate affect the land's ability to absorb atmospheric carbon — a key process for mitigating human-caused emissions. They found that 88 percent of Earth's regions could become carbon emitters by the end of the 21st century.

Climate extremes lasting months or years could reduce plant productivity, which governs Earth's capacity to produce food, fiber and fuel. Plus, events such as wildfires could generate bursts of emissions from carbon stored in forests.

The team used the open-source Community Earth System Model to simulate multiple variables, which enabled a holistic understanding of how climatic conditions interact.

"Our results suggest that meteorological extremes will become more frequent, intense and widespread due to the compound effect of high temperature, drought and fire," ORNL's Bharat Sharma said. "Tropical regions may face these to the most extreme degree." — *Reece Brown*



Valuable chemicals are selectively produced from mixed plastic waste by an ORNL-developed plastic deconstruction process. Image credit: Tomonori Saito, Md Arifuzzaman and Adam Malin, ORNL

Additive manufacturing composite parts production

An ORNL-developed advanced manufacturing technology, AMCM, was recently licensed by Orbital Composites and enables the rapid production of composite-based components, which could accelerate the decarbonization of vehicles, airplanes and drones.

Additive manufacturing compression molding, or AMCM, uses short-fiber-filled polymer and continuous fiber to print directly onto a mold with precise orientation to make parts such as propellor blades or battery boxes.

Compression molding then turns the print into an accurate finished piece. ORNL researchers proved AMCM significantly

ORNL's additive manufacturing compression molding, or AMCM, technology can produce composite-based, lightweight finished parts for airplanes, drones or vehicles in minutes. Image credit: Carlos Jones, ORNL

reduces time and cost by producing 100 parts in five hours with each piece taking less than three minutes to print.

"By combining the fiber control of additive with the low porosity of compression molding, we can enable the high-volume production of next-generation composites," ORNL's Vipin Kumar said. "The mobility and aerospace industries need these lightweight materials to improve the energy efficiency of their applications."

ORNL collaborated with Orbital to develop AMCM on a robotic system. Additional collaborators included IACMI — The Composites Institute.

US, Korean associations honor ORNL's Campbell

ORNL researcher Anne Campbell recently won the Young Leaders Professional Development Award from the Minerals, Metals & Materials Society, or TMS, and has been chosen as the first recipient of the Young Leaders International Scholar Program award from TMS and the Korean Institute of Metals and Materials, or KIM.

The award aims to promote young members' activities and strengthen collaborations. Every year, TMS and KIM will identify one young leader to travel to the other organization's meeting and present a paper.

"I am very honored to be selected as the inaugural recipient of this award," Campbell said. "The collaborations between researchers in the United States and Korea will certainly lead to the deployment of advanced nuclear reactors that will assist with worldwide reduction in carbon emissions. I will use this opportunity to support the continuation of current, and the development of new, collaborations between our country and South Korea for materials needs of future carbon-free energy sources."

Campbell has been an R&D staff member in the Advanced Nuclear Materials group in ORNL's Materials Science and Technology Division since 2016. Her current research involves understanding the effects of irradiation and other extreme environments on material properties.

She will travel to Korea in October 2024 to attend the KIM Fall Conference and present a paper on materials research in support of carbon-free nuclear energy. Her presentation will discuss research at ORNL that supports the rapid deployment of small modular reactors that use graphite to moderate neutrons. The KIM Fall Conference covers a wide range of topics, including metals, high polymers, ceramics, magnetic materials and electronics.

ORNL researcher Anne Campbell will present a paper in Korea next year on materials support of carbon-free nuclear energy. Image credit: Adam Malin, ORNL

Still collaborating

after all these years

by Leo Williams
williamsjl2@ornl.gov

In October 1945, just weeks after World War II ended, the University of Tennessee, Knoxville, offered two graduate physics courses on site at Clinton Laboratories, as Oak Ridge National Laboratory was originally known.

Theoretical Physics 511 and Atomic Physics 411 had just 48 students between them, but they marked the beginning of a symbiosis between the lab and the university that has lasted nearly eight decades and continues to gain strength.

In 1940, Oak Ridge did not exist, and UT had no Ph.D. programs. The reason UT opened its first Ph.D. programs in chemistry and physics was because of Oak Ridge.

— Former ORNL and UT official **Lee Riedinger**

In that time, the two institutions have shared staff, students and research facilities. They have collaborated on institutes and centers designed to strengthen both their research and their ability to attract exceptional researchers and students. They have created prestigious programs that attract leaders in their fields from across the world (see "Governor's Chairs program attracts scientific luminaries," page 16). And in 2000, they deepened their relationship when the UT System partnered with Ohio-based Battelle Memorial Institute to become ORNL's managing contractor.

The long partnership has led to scientific discoveries and impact that could not have been accomplished by either institution alone.

Fast forward to 2021, when UT and ORNL supercharged their relationship with creation of the UT-Oak Ridge Innovation Institute, or UT-ORII (see "An institute to supercharge the UT-ORNL alliance," page 12). According to ORNL Deputy for Science and Technology Susan Hubbard, UT-ORII goes beyond collecting existing collaborations under one umbrella.

"UT-ORII aims to develop a new paradigm for innovation on cutting-edge topics that require multi-disciplinary team-based research paired with world-leading facilities — as well as education and workforce development — through melding select strengths across all the UT System institutions with those at ORNL," she said.

To address these goals, the institute will bump the number of joint faculty by over 100 and the annual number of joint grad students to 500.

"I would say that the global purpose of UT-ORII is to elevate the status and the mission of both institutions," said David Sholl, the institute's director. "And it's to recognize that the university has some very special attributes, ORNL has some unique world-leading attributes. And so it makes sense to look at how we can combine those things together."

Scientists sans degrees

In those early days, though, the relationship was driven by both practical considerations and an existential threat.

On the practical side, Oak Ridge had a Ph.D. problem. The lab had been created just two years before as part of the Manhattan Project's mission to create the world's first nuclear weapons, and many of its researchers lacked graduate degrees. The war had put their educations on hold, and if they couldn't continue those educations locally, they would have to continue them elsewhere. UT, on the other hand, was looking for a partner to help expand its science offerings.

"In 1940, Oak Ridge did not exist, and UT had no Ph.D. programs," said Lee Riedinger, who retired in 2018 after serving in key positions at both institutions. "The reason UT opened its first Ph.D. programs in chemistry and physics was because of Oak

We're at a very exciting phase of this partnership, and we fully expect to realize an amplification in innovation, education and workforce in the coming years.

— ORNL Deputy for Science and Technology **Susan Hubbard**

Ridge. Oak Ridge needed courses taught here so that their valued researchers could work toward Ph.D.s here instead of going back to wherever they came from for the Manhattan Project."

On the existential side, it was unclear whether the Oak Ridge lab would survive the peace. It had accomplished its Manhattan Project mission — to demonstrate a process for enriching the fissionable isotope plutonium-239 — and its fate was in the hands of the federal government.

One of the lab's skeptics was none other than J. Robert Oppenheimer, known as the "father of the atomic bomb." In their book "Atomic Shield: A History of the Atomic Energy Commission," Richard G. Hewlett and Francis Duncan highlight deliberations of the agency's General Advisory Committee concerning the lab in 1947 and share Oppenheimer's communication with the committee:

"The future of the Clinton Laboratories at Oak Ridge was much less clear [than that of other facilities]. The General Advisory Committee had concluded the laboratory was not worth saving. As Oppenheimer had told the Commissioners on March 30, 'Most of us think that the evidence is in that Clinton will not live even if it is built up.'"

Part of the calculus to change their minds and keep the lab open, Riedinger said, was to stress its value to the nearby university. Key voices supporting the lab came from UT, notably William Pollard and Kenneth Hertel from the university's Physics Department. They especially wanted to ensure that the lab's Graphite Reactor — the world's first continuously operating nuclear reactor — and its supporting facilities were around to benefit Southern universities.

"These universities generally lagged far behind top universities in other parts of the country in research and graduate education," Riedinger explained. "Pollard and Hertel's lobbying effort worked, and the U.S. government decided to keep the Oak

Ridge laboratory open and to allow the formation of an official university presence at or near these facilities in Oak Ridge."

He said another boost came from physicist Katharine Way, who in 1945 was the first to suggest a collaboration between the lab and universities across the region. Way left a UT professorship in 1942 to work in the war effort and on the world's first nuclear reactor, a temporary project in Chicago at the Metallurgical Laboratory, which would later become Argonne National Laboratory. At the Met Lab, she collaborated with two giants in ORNL's history: future Nobelist Eugene Wigner, who would become the lab's first director of research and development, and Alvin Weinberg, who would become ORNL's longest-serving laboratory director.

The thing that really attracted me to this position was actually the close relationship that the University of Tennessee and Oak Ridge National Lab had through the UT-Battelle contract. In areas where the Oak Ridge National Lab and University of Tennessee missions overlap, it's really been game changing in terms of recruiting some really stellar faculty that have made significant contributions.

— Governor's Chair for Computational Nuclear Engineering **Brian Wirth**

Way returned to East Tennessee after the war, but she landed in Oak Ridge rather than at UT.

"There was a dinner to welcome her back in Knoxville," Riedinger said, "hosted by a guy in chemical engineering. And Kay Way said 'I've heard of universities around Chicago teaming together to try to leverage the coming Argonne National Lab. You should do something here in the Southeast.'"

That suggestion led the following year to formation of the Oak Ridge Institute of Nuclear Studies, whose charter members included 14 universities from Georgia, Alabama, Louisiana, Virginia, North Carolina, Kentucky, Texas, Tennessee and Washington, D.C. In 1966 ORINS became Oak Ridge Associated Universities, which now counts more than 150 universities among its members.

Managing a national lab

Perhaps the strongest current link between the two institutions can be found in UT-Battelle, ORNL's management and operating contractor since April 2000.

According to Riedinger, UT and state officials saw an opportunity to reinforce the relationship when DOE announced in 1995 that it was separating the ORNL contract from that of DOE's other Oak Ridge facilities — the Y-12 National Security Complex, a nuclear weapons plant, and East Tennessee Technology Park, formerly the K-25 uranium enrichment plant. They had decided against competing for the contract in the early 1980s, but the opportunity seemed much more attractive when it reappeared in 1998.

"We were not ready in '84, but by '98 they had split the contracts," Riedinger said. "And we needed to compete to ensure that we would have a seat at the table and that our joint programs would continue, because the joint programs were so important to us."

Deborah Crawford, UT's vice chancellor for research, innovation and economic development, agrees that UT-Battelle reinforces the bond between UT and ORNL.

"It definitely strengthens the relationship," she said, "and encourages the state to make investments in a partnership that benefits many Tennessee communities, from children in our pre-K-12 schools through high-growth companies that promise economic opportunities for working Tennesseans. It also builds more connectivity at leadership levels."

That connection, she said, helps guarantee the success of ongoing initiatives such as UT-ORII.

"The president of the UT System, Randy Boyd, has a leadership role in UT-Battelle's management of the lab, and that helps solidify the long-term support that is necessary for an initiative like UT-ORII, because it truly is a long-term proposition to achieve the ambitious shared vision that we have for UT-ORII."

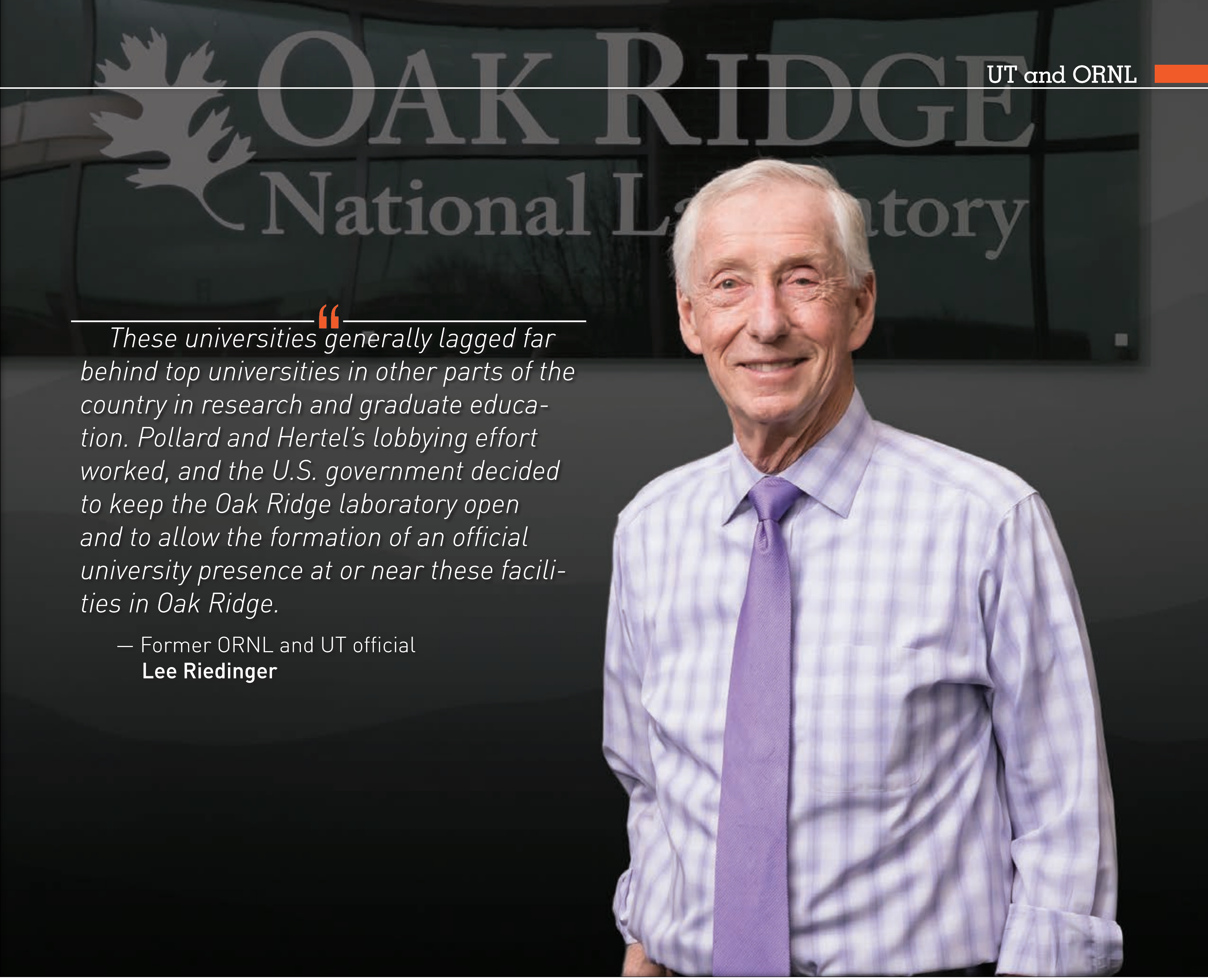
The strength of that connection has also helped in recruiting leading scientists, said Brian Wirth, the Governor's Chair for Computational Nuclear Engineering, who came to Tennessee from the University of California, Berkeley.

"The thing that really attracted me to this position was actually the close relationship that the University of Tennessee and Oak Ridge National Lab had through the UT-Battelle contract," he said. "In areas where the Oak Ridge National Lab and University of Tennessee missions overlap, it's really been game changing in terms of recruiting some really stellar faculty that have made significant contributions."

A good relationship for both the UT System and ORNL

Like any successful relationship, the UT-ORNL collaboration benefits everyone involved. Staff and students across the UT System get access to the lab's talent pool, are exposed to world-leading experimental facilities, and are closer to the DOE mission and programs. ORNL gets access to UT's talented researchers and grad students, as well as economic support from the state. The state finds itself with powerful research infrastructure and expertise that is critical for enhancing economic development. And both institutions become more attractive to incoming staff and students.

"Some UT departments recruit very talented graduate students because of the relationship with Oak Ridge National Laboratory," said UT materials scientist Phillip Rack. Rack is an ORNL alum who served as UT-ORII's interim education director



> *These universities generally lagged far behind top universities in other parts of the country in research and graduate education. Pollard and Hertel's lobbying effort worked, and the U.S. government decided to keep the Oak Ridge laboratory open and to allow the formation of an official university presence at or near these facilities in Oak Ridge.*
>
> — Former ORNL and UT official **Lee Riedinger**

from 2022 through the summer of 2023 (see "Doctoral students look beyond academia," page 20).

"I had a joint appointment at the Center for Nanophase Materials Sciences for 16 years. And you better believe, when I brought a student to campus, we went over to CNMS and they spent an afternoon over there, looking at the equipment, talking with staff, and realizing the opportunity that presented itself."

On the flip side, researchers coming to ORNL have the advantage of teaching and working with students, and in some cases, being joint faculty.

"We consider primary advisor privileges as being a great honor to bestow on a scientist who isn't a tenure-line faculty member," Crawford said. "The Joint Faculty program allows lab scientists to serve as primary advisors for UT graduate students and to be the most significant mentor for them throughout their graduate education programs. Researchers who might otherwise aspire to careers in academia will come to the lab recognizing they can get the best of both worlds through a joint faculty appointment."

Looking to the next 80 years

The last eight decades have shown that UT — Tennessee's flagship university system — and ORNL — the country's largest science and energy laboratory — can accomplish great things when they work together. Starting with those two physics courses in 1945, the two institutions have expanded their collaboration into a range of critical research areas and created a unique learning environment for Tennessee students. Looking to the future, the collaboration — led by UT-ORII with initial support from the Department of Energy and the state of Tennessee — promises to deliver needed scientific and technological breakthroughs while providing unique opportunities for students and workforce development.

"We're at a very exciting phase of this partnership," Hubbard said, "and we fully expect to realize an amplification in innovation, education and workforce in the coming years, which will yield great impacts to the state and the nation."

An institute to supercharge the

UT-ORNL alliance

by Leo Williams
williamsjl2@ornl.gov

The future of the UT-ORNL partnership lies with the UT-Oak Ridge Innovation Institute, or UT-ORII, which named David Sholl as its second director in April and launched two new "convergent research initiatives" this year that exemplify the institute's purpose and promise.

> *UT-ORII represents a culmination of the partnership. UT-ORII was created to serve as an umbrella for the many existing programs, as well as to align great capabilities and expertise across the UT System and ORNL toward accelerating innovation on key challenging topics that are of strategic interest to both organizations.*
>
> — ORNL's Deputy for Science and Technology **Susan Hubbard**

Created in 2021 to consolidate existing lab-university collaborations and launch major new research, the institute streamlines and amplifies research and education collaborations that have grown organically over the 80-year relationship between UT and ORNL. Its efforts are important not only to the two institutions, but also to the state of Tennessee as a whole.

"UT-ORII represents a culmination of the partnership," said Susan Hubbard, ORNL's deputy for science and technology. "UT-ORII was created to serve as an umbrella for the many existing programs, as well as to align great capabilities and expertise across the UT System and ORNL toward accelerating innovation on key challenging topics that are of strategic interest to both organizations."

Focused research

The institute's convergent research initiatives bring together faculty and students through cluster hires that can address critical national challenges requiring multidisciplinary expertise.

The new initiatives announced earlier this year focus on circular bioeconomy systems and radiopharmaceutical therapies. Chosen from among 54 proposals, they join earlier initiatives looking at energy storage and transportation and at clean manufacturing and advanced materials.

The institute will launch a competitive search process for a fifth convergent research initiative later in 2024.

> *Each UT-ORII research initiative represents a huge investment. We're talking about putting 20-plus million dollars of investment into an area and growing it to 20 or more research staff and more than 25 Ph.D. students. It's a very significant effort. And so it's important to make good choices.*
>
> — UT-Oak Ridge Innovation Institute Director **David Sholl**

The circular bioeconomy systems initiative will look at the use of plant-based products in manufacturing.

"I would contrast them with our current economy," Sholl said. "Products — let's say polymers used in manufacturing vehicles — ultimately come from fossil fuel resources. Those carbon atoms go through various chemical transformations and end up as a plastic that's used in a car.

"In the bioeconomy we want to get the same resources by growing plants, either by growing some designated plant or using some waste resource. That's the ultimate difference: We want to use agricultural and forestry resources as the ultimate sources of our chemicals and materials."

UT-ORII's new leader looks forward to groundbreaking research

by Leo Williams
williamsjl2@ornl.gov

The UT-Oak Ridge Innovation Institute has a new leader.

David Sholl, who headed ORNL's Transformational Decarbonization Initiative, took over as the institute's interim director in June 2023, replacing outgoing Director Joan Bienvenue. He became its permanent executive director on May 1.

"It's a great opportunity to really drive some research initiatives in a concerted way," Sholl said. "Often, as a researcher, you keep your head down and work on one thing. This is a chance to take advantage of the strengths of both the lab and the university and bring groups of people together, and that's a very attractive thing."

Sholl came to ORNL in July 2021 from Georgia Tech, where he chaired the Department of Chemical and Biomolecular Engineering.

Sholl holds a bachelor's degree in physics from the Australian National University, as well as a master's degree and Ph.D. in applied mathematics from the University of Colorado.

His research has focused on chemical separations, a process key to a variety of industries, from petrochemical processing to water desalination.

"There's a huge, huge amount of energy that's used at chemical plants to separate chemicals," he said, "separating hydrogen from other molecules, separating ethylene from ethane, and so on. Because there's so much energy used doing that, there's a lot of need to develop new technologies to do it with lower energy pathways. That's what I've worked on."

Sholl is a fellow of the American Association for the Advancement of Science and the American Institute of Chemical Engineers. He has published more than 420 papers and three books and is editor-in-chief of *AIChE Journal*.

Looking forward, he sees great things for UT-ORII as the institute pursues its first two initiatives — focusing on energy storage and transportation and on clean manufacturing — and looks to additional initiatives in the coming years.

"What I'd like us to do is select really critical research thrusts," Sholl said, "things that really matter to the national interest and to the world, and put together interdisciplinary teams that attack those in ways that are very difficult to do if just individual people are bringing their talents.

"And also to bring prominence to our local area. There are already things here at the lab that are really known around the world. But I'd like for us to have research initiatives so that when people ask, who are the best people in the world working on this topic, they think of the University of Tennessee and ORNL."

The initiative includes researchers from UT's Knoxville campus, the UT Institute of Agriculture and ORNL.

Sholl noted that the initiative also emphasizes the recycling of materials, either in their original forms or in different forms for other purposes.

"Usually we want to recycle that polymer to the same polymer," he said. "But there's many other, more intricate ways you can imagine to do this, where something is used first for one purpose, perhaps second for a different purpose, and so on. The 'systems' word in the title is very important here, because you can only contemplate those issues if you have a very integrated interdisciplinary group of people thinking about it."

> *Basically we were created as an umbrella for all of these joint programs that have existed between the lab and the university.*
>
> — Former UT-Oak Ridge Innovation Institute Director **Joan Bienvenue**

The radiopharmaceutical therapies initiative will focus on a new generation of theranostics that combine drugs for therapy and for diagnostic imaging. The research will focus on isotopes that emit radioactive alpha particles, which contain two protons and two neutrons and are identical to helium-4 nuclei.

This initiative includes researchers from ORNL; UT, Knoxville; and the UT Health Science Center, located in Memphis. It will also take advantage of the High Flux Isotope Reactor located at ORNL, which already produces medical isotopes such as actinium-227, produced for the prostate cancer drug Xofigo.

The promise of alpha-emitting isotopes for cancer treatment rests in the fact that they deliver a strong dose of radiation but only within a very short space, thus maximizing their ability to kill cancer cells while minimizing damage to nearby healthy tissue.

"ORNL is an absolutely world-class source of isotopes and expertise around isotopes," Sholl noted. "And there's a huge amount of interest in the medical community about this targeted delivery of radioisotopes.

"The mode of action is that these things work on very short length scales, so if you can selectively deliver it to a tumor, then it will do what you want to that tumor without causing damage elsewhere in the body."

The challenge, he said, is combining the isotopes with chemicals that will find their way to a specific type of tumor and leave other parts of the body alone.

"There's a huge amount of chemistry and medical science that has to happen to make all those things work together," Sholl said. "Expanding this to other treatable forms of cancer is challenging because you have to figure out ways to really connect that isotope atom to that selective chemical that will target the tumor. And so a lot of the fundamental work at ORNL is really about understanding the chemistry that's possible with those isotopes."

A coordinated, statewide effort

The institute is backed by the state of Tennessee, DOE, ORNL and UT. DOE provided an initial $20 million for the institute, and in April 2022 the state provided its full support and another $80 million. The lab is also dedicating resources from its Laboratory Directed Research and Development program.

Joint institute faculty supported by ORNL will be hired through ORNL's scientific directorates. That financial commitment is critically important as UT-ORII considers upcoming research initiatives, Sholl noted.

"Each UT-ORII research initiative represents a huge investment," he said. "We're talking about putting 20-plus million dollars of investment into an area and growing it to 20 or more research staff and more than 25 Ph.D. students. It's a very significant effort. And so it's important to make good choices. But I want us to make forward-looking choices as well."

Boosting students and workers

UT-ORII is also responsible for promoting education at all levels within the state: graduate, undergraduate, K-12 and worker training. These educational programs often predate the institute.

"Basically we were created as an umbrella for all of these joint programs that have existed between the lab and the university," noted Joan Bienvenue, the institute's first director, who's now with the University of Texas System.

The joint programs brought under UT-ORII include the Joint Faculty Program, the Bredesen Center for Interdisciplinary Research and Graduate Education, which places Ph.D. students at both UT and ORNL (see "Doctoral students look beyond academia," page 20), and the Governor's Chairs program, which brings eminent researchers to East Tennessee for joint appointments (see "Governor's Chairs program attracts scientific luminaries," page 16).

By exposing students to team science, world-leading facilities and experts, and both a national laboratory and a university system, UT-ORII programs give students the opportunity to work on bigger, more collaborative projects than they might otherwise encounter.

"Students enrolled at UT have the opportunity to work on the lab reservation, to learn how to work with these large, globally prominent instruments that the lab has, and to tap into the expertise of lab scientists," said Deborah Crawford, vice chancellor for research, innovation and economic development at UT, Knoxville.

"We find that student experiences at a national laboratory are typically eye-opening," Hubbard said. "They get a chance to broaden their knowledge as well as contribute to big team-based challenges that are of national importance."

Students enrolled at UT have the opportunity to work on the lab reservation, to learn how to work with these large, globally prominent instruments that the lab has, and to tap into the expertise of lab scientists.

— UT Knoxville Vice Chancellor for Research, Innovation and Economic Development **Deborah Crawford**

The institute's educational outreach also includes younger students. In pursuing these relationships, it partners with organizations that already have longstanding relationships with Tennessee schools.

"In K-12, there's been a decision made — a good decision in my view — to focus on middle schools, because that's a key point in enabling the trajectories of students," Sholl said. "And we aim to partner with other organizations — for instance UT Extension, which is already working in every county in the state."

A unique environment for innovation

Hubbard came to ORNL in 2022 from Lawrence Berkeley National Laboratory, which has a very close partnership with the University of California, Berkeley. She said ORNL's ties to UT are similarly long and deep.

"The state of Tennessee and the Department of Energy's support of the Institute represents a significant opportunity to align and amplify unique state and federal research assets to great effect.

"UT-ORII focuses on developing a new paradigm for convergent research that will bring the relationship to the next level through strategic alignment and investments in research themes, joint faculty and shared students. The institute will fill a real need, creating a resource-rich and dynamic environment that melds select strengths of ORNL and the UT System in a manner that is expected to have great impact to both the state and nation."

Governor's Chairs program

attracts scientific luminaries

by Leo Williams
williamsjl2@ornl.gov

Of approximately 20,000 employees working at ORNL or in the UT System, 13 stand out most prominently. These are the Governor's Chairs, a group of highly accomplished researchers and academics brought to Tennessee to advance fields that are important to the UT System and to ORNL, such as advanced materials and manufacturing, biology, energy sciences and nuclear technology. Funded by the state of Tennessee and ORNL, the program broadens the unique research partnership that exists between UT, the state's preeminent public university system, and ORNL, the nation's largest multiprogram laboratory.

Now part of the UT-Oak Ridge Innovation Institute (see "An institute to supercharge the UT-ORNL alliance," page 12), the Governor's Chairs program enables the organizations to attract candidates who will leverage the significant benefits and opportunities that come from being associated with both a major university and a national laboratory.

For me, it's environmental remediation. I've done a bunch of different things related to oil spills such as the Deepwater Horizon oil spill.

— Governor's Chair for Environmental Biotechnology **Terry Hazen**

A history of collaborations

The Governor's Chairs program fits into a long history of collaborations between the university and the national lab. Created in 2006 during the administration of Tennessee Governor Phil Bredesen — himself a Harvard graduate with a bachelor's degree in physics — the program is successor to the Distinguished Scientist Program created two decades earlier.

For their part, UT and ORNL bring national and international leaders in their fields to Tennessee, people who have track records of high-impact research and long-standing relationships with funding agencies but who might not otherwise be interested in a career change.

"It's really difficult to grab someone from outside when they're well-rooted," said Yilu Liu, the Governor's Chair for Power Electronics, "but I think the Governor's Chairs program offers a unique benefit for both sides. For UT, it's definitely more resources; I have 30-plus staff — graduate students, postdocs and others. For the Oak Ridge side, you get experienced researchers who already have established reputations. They are able to gain trust and respect from DOE program managers quickly, and that helps in terms of the lab's funding and reputation."

Liu came to UT Knoxville and ORNL after nearly two decades at Virginia Tech, where she was a world leader in research on the electrical grid. Among other accomplishments, she was instrumental in creating North America's Frequency Monitoring Network/GridEye, a network of low-cost, GPS-synchronized monitors that report the frequency, phase angle and voltage of the power grids.

Terry Hazen, Governor's Chair for Environmental Biotechnology, came to his position from Lawrence Berkeley National Laboratory. He noted that the Governor's Chairs program allows the university and the lab to amplify specific areas of research.

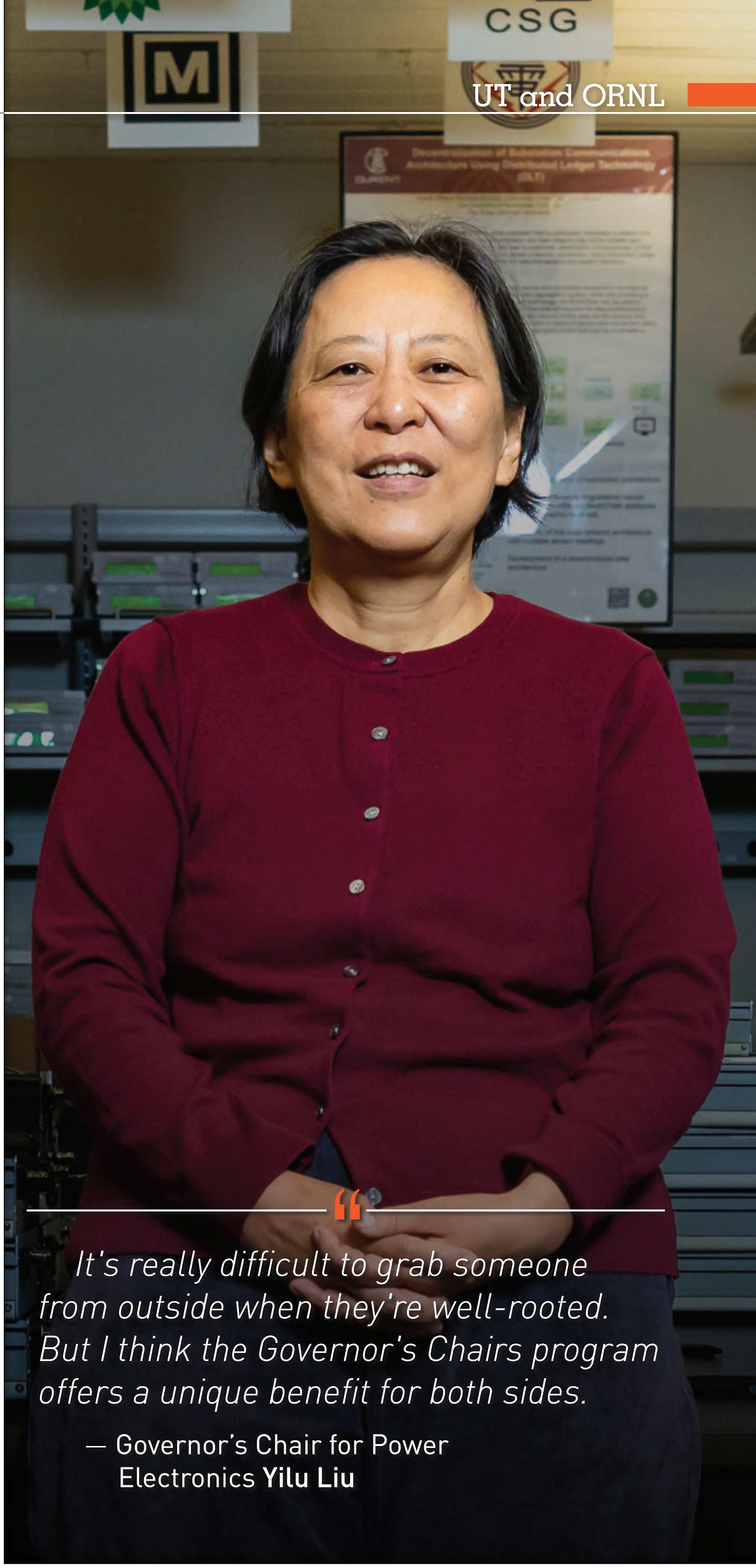
"For me, it's environmental remediation," he said. "I've done a bunch of different things related to oil spills such as the Deepwater Horizon oil spill," referring to the 2010 Gulf of Mexico disaster considered to be history's largest marine oil spill.

"I showed that there were bacteria down deep that were basically consuming the oil just as rapidly as it was expelled from the deep. That means that we didn't need to do a lot of things related to injecting nutrients and trying to recover it, which potentially would have damaged the environment more."

The stature of existing Governor's Chairs helps attract impressive candidates, noted Brian Wirth, the Governor's Chair for Computational Nuclear Engineering.

Wirth came to UT Knoxville and ORNL from the University of California, Berkeley, where he was on the nuclear engineering faculty. His group focuses on computational explorations of materials and nuclear fuel, both in existing reactors and in advanced reactors.

"When I came in 2010 and was being recruited here, I felt like the Governor's Chairs professors were the best faculty line in the country," he said. "In areas where UT and Oak Ridge missions align, it's really been game changing in terms of recruiting some really stellar faculty that have made significant contributions."



It's really difficult to grab someone from outside when they're well-rooted. But I think the Governor's Chairs program offers a unique benefit for both sides.

— Governor's Chair for Power Electronics **Yilu Liu**

A boon to students

These accomplished researchers work at ORNL and are expected to lead research collaborations, but they also have the responsibilities and opportunities that come with being college professors. Many of the students working with the Governor's Chairs also work at the lab.

> *The Governor's Chairs program is coveted by many universities across the U.S. My students can become much better than me when they come to my age.*
>
> — Governor's Chair for Advanced Manufacturing **Suresh Babu**

For Rigoberto Advincula, Governor's Chair for Advanced and Nanostructured Materials and leader of ORNL's Macromolecular Nanomaterials group, both roles were attractive.

"For me, the Governor's Chairs program is the biggest reason I moved to the University of Tennessee at Knoxville and Oak Ridge National Lab," he said. "In the area of polymer science, I think Oak Ridge and UT lead worldwide in terms of citations and recognition, but in order to continue that leadership, we need to bring in experts and hire people at both institutions."

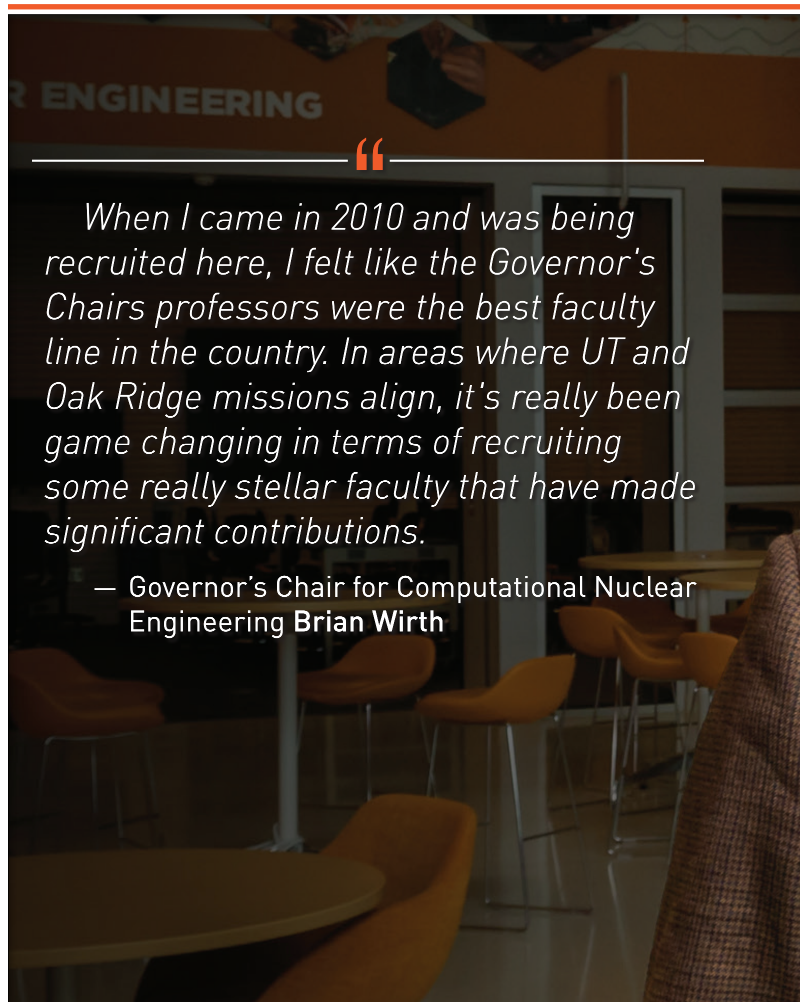
Advincula also values his role as a teacher, noting that he had mentored close to 150 undergrads as a professor before he came to Tennessee. He continues that focus with his undergrads at UT.

"They are involved in materials research, where they publish, together with my graduate students, and learn many skills that make them very eligible and sought-after in graduate school," said Advincula, who came to his position from Case Western Reserve University in Cleveland.

He noted that he encourages his postdocs and students to be mentors in their own right as well as skilled researchers, with students at each level working with others one level down.

"It allows me to distribute the mentoring, whether it's with undergrad, graduate or even high school students. The Ph.D. students I have are expected to mentor the undergrads. The undergrads then — in the past and maybe in the not-too-distant future — mentor high school students. So that type of outreach I've done all throughout my career.

"I've set up a lab that has ballooned out to about 24 students and postdocs. A majority of my researchers are undergrads, and I'm mentoring them to become future STEM advanced degree holders."



> *When I came in 2010 and was being recruited here, I felt like the Governor's Chairs professors were the best faculty line in the country. In areas where UT and Oak Ridge missions align, it's really been game changing in terms of recruiting some really stellar faculty that have made significant contributions.*
>
> — Governor's Chair for Computational Nuclear Engineering **Brian Wirth**

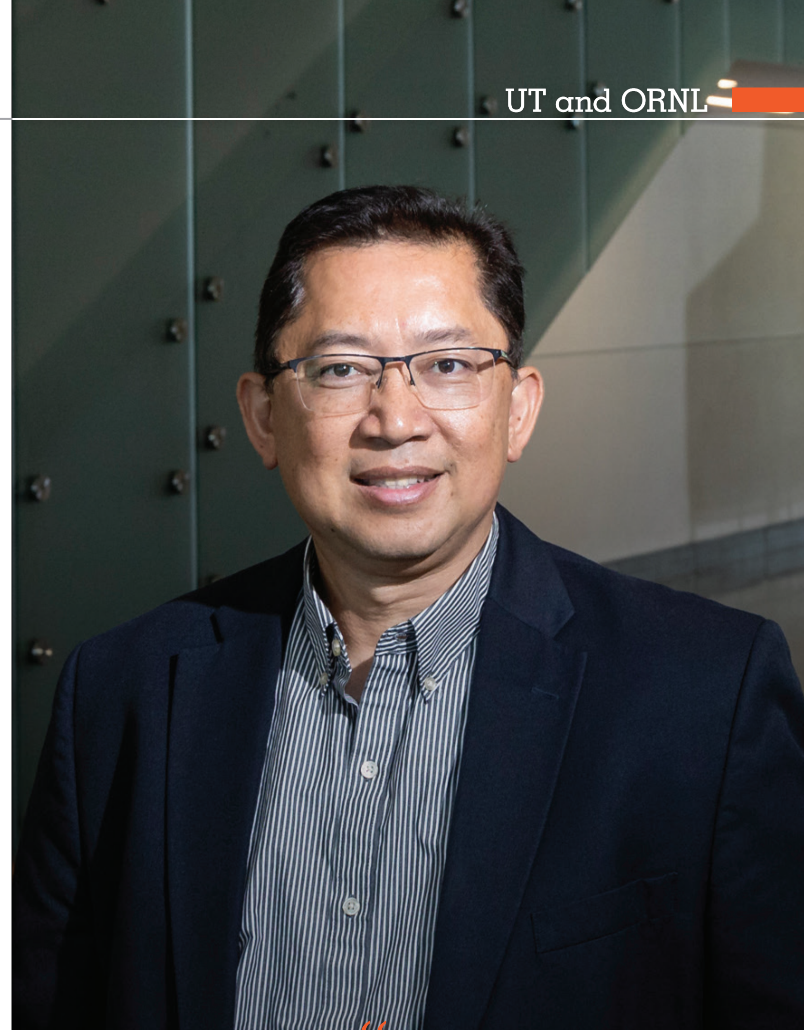
Suresh Babu, the Governor's Chair for Advanced Manufacturing, also values the unique educational opportunities that come with having a close relationship with a national lab. He came to his position from Ohio State University.

Babu was until recently director of the Bredesen Center for Interdisciplinary Research and Graduate Education, a collaboration — now under UT-ORII — that stresses entrepreneurship as well as science and engineering (see "Doctoral students look beyond academia," page 20).

Babu's goal is to mentor students and early career scientists so that their accomplishments eventually overshadow his own. He said the collaboration with ORNL — in which students learn from experts at the lab as well as from himself as their advisor — makes that a real possibility.

"The Governor's Chairs program is coveted by many universities across the U.S.," he said. "My students can become much better than me when they come to my age. When I did my Ph.D., there was no such mechanism; I was under one supervisor. There were not a lot of technical discussions from different perspectives. It's not easy for my students, but that is the best way to proceed to the truth."

For all its accomplishments, there is much the program can still accomplish, said nuclear engineering researcher Wirth. As UT and ORNL expand their connections, the Governor's Chairs are ideally situated to make the most of a growing collaboration.



For me, the Governor's Chairs program is the biggest reason I moved to the University of Tennessee at Knoxville and Oak Ridge National Lab. In the area of polymer science, I think Oak Ridge and UT lead worldwide in terms of citations and recognition, but in order to continue that leadership, we need to bring in experts and hire people at both institutions.

— Governor's Chair for Advanced and Nanostructured Materials
Rigoberto Advincula

"To me, this has been a great move," Wirth said. "I have no regrets about coming to East Tennessee from California. And I'm super excited to see what the next decade is going to bring, because I think there's so many opportunities to grow this partnership.

"It's been a tremendous place for me and my research group to work. But I think that there's so much more that can be done in the future."

Doctoral students look beyond academia

by Leo Williams
williamsjl2@ornl.gov

The integration of UT and ORNL may be best exemplified by the Bredesen Center for Interdisciplinary Research and Graduate Education, a 13-year-old Ph.D. program that places students at both the university and the lab.


Philip Rack

"The idea is that it sits right in the middle between UT and Oak Ridge," said UT materials scientist Philip Rack, the center's former director. "It's basically a virtual faculty, so there aren't tenure-track positions in this center; it's an amalgamation of University of Tennessee faculty and ORNL staff members."

The center is already a mainstay in the collaboration between UT and ORNL, and it's about to get much bigger. It has about 75 students supported at ORNL and another 25 to 50 located throughout the university, Rack said, but plans call for boosting the total number up to 500 in the coming years.

An interdisciplinary approach

Flexibility has been baked into the Bredesen Center approach since day one, said Lee Riedinger, the center's first director.

"Part of the idea was that this would be a fully interdisciplinary degree, where students could take courses from any department," he said. "The problem with a Ph.D. in physics or chemical engineering is you've got to stock up mostly on courses in that department, and there isn't time to take courses in other departments, whereas our students could take courses from any department."

"The Bredesen Center was created with interdisciplinary graduate student training in mind," agreed UT obesity researcher Brynn Voy, who in August 2023 became director of the center and education director of the UT-Oak Ridge Innovation Institute. "It recognizes that the big science problems that national labs in particular were created to address — the ones you read about on the front page of the paper — can't be solved by a single discipline."

Grad students at the Bredesen Center go into one of three Ph.D. programs: data science and engineering, energy science and engineering, or genome science and technology.

The program in data science takes advantage of ORNL's computing expertise as well as its world-leading supercomputers. Students in this program choose from among five focus areas: advanced manufacturing, climate science, biology, materials science and national security. For their part, students in energy science and engineering can focus on areas including nuclear energy, bioenergy, renewable energy, grid management and energy materials.

Genome science and technology is the latest program to join the Bredesen Center, although it's the oldest program of the three, dating back to 1998. Research areas in this program include molecular genetics and systems biology, structural and nanoscale biology, and computational biology and bioinformatics.

The idea is that it sits right in the middle between UT and Oak Ridge. It's basically a virtual faculty, so there aren't tenure-track positions in this center; it's an amalgamation of University of Tennessee faculty and ORNL staff members.

— UT materials scientist **Philip Rack**

Focuses beyond academics

The Bredesen Center is distinguished both by its interdisciplinary nature and by its insistence that students explore focuses outside the academic realm, Rack said. Known as breadth areas, these include entrepreneurship, policy and community outreach.

Voy noted that breadth areas are especially helpful to students who choose careers outside of academia.

"Most graduate programs that are thinking a bit forward recognize that their students don't just go into academia. We're no longer in a situation where we just train people to place in ivory towers. A lot of our students go to private industry, for example. That fact highlights the need for students to understand entrepreneurship."

Indeed, Bredesen Center students have a history of starting companies. Between 2012 and 2022, Bredesen Center students registered seven new companies, some while they were still students at the center.

> *Most graduate programs that are thinking a bit forward recognize that their students don't just go into academia. We're no longer in a situation where we just train people to place in ivory towers. A lot of our students go to private industry, for example. That fact highlights the need for students to understand entrepreneurship.*
>
> — Bredesen Center Director and UT-Oak Ridge Innovation Institute Education Director **Brynn Voy**

In the years since the center's creation in 2011, other UT graduate programs also allow students to become entrepreneurs, noted Deborah Crawford, UT Knoxville's vice chancellor for research, innovation and economic development.

"Students in Ph.D. programs outside the joint Ph.D. programs have the opportunity to focus on entrepreneurship," she said, "but there isn't such a strong focus on public policy in some of the other programs. So I think it's fair to say that the Bredesen Center led the charge, thinking about how the students that go through Ph.D. programs aren't all going to track into academic positions. In fact, we want to prepare students for a variety of career choices, and the Bredesen Center really was a pioneer at the university."

Encouraged by a physicist governor

The center was created at the urging of then-Gov. Phil Bredesen.

"This was all Phil Bredesen's idea, his last big idea as a two-term governor," said Riedinger, who served as the center's director until 2019. "Bredesen has a physics undergraduate degree from Harvard, and it was his idea to start some kind of interdisciplinary Ph.D., perhaps in energy, between UT and the lab."

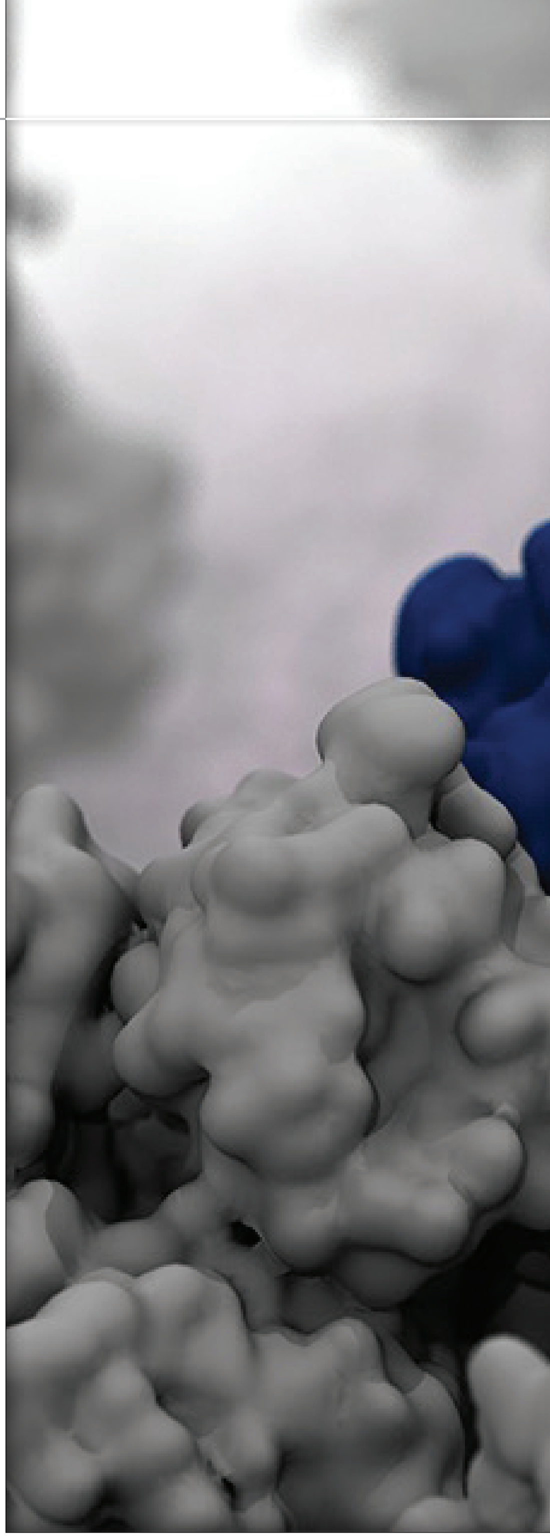
The Bredesen Center isn't ORNL's first venture into graduate education; UT grad students have been working at the lab for decades. In fact, the UT-ORNL Graduate School of Biomedical Sciences, based in ORNL's Biology Division, opened more than 50 years ago in 1967 and operated for 30 years.

In one sense, said Riedinger, the Bredesen Center formalized a relationship between the two institutions that had been going on for decades.

"We've had grad students at UT — some of my own and others — working at ORNL for decades. Indeed, I was a graduate student from Vanderbilt working here on my dissertation research. The difference about the Bredesen Center is that now, the people here are officially joint faculty at UT and mentors of the grad students, whereas before that, you'd have a research advisor here, but a faculty member at UT would have to be the real adviser and the real person to sign the dissertation.

"That was a big step forward," he added, "because researchers at ORNL really enjoyed having their own grad students and signing the dissertation and attending graduation ceremonies and putting the Ph.D. hood on the students."

ORNL's Titan helps simulate influenza virus



by Quinn Burkhart
ornlreview@ornl.gov

According to the World Health Organization, influenza infects an estimated 1 billion people worldwide annually.

The H1N1 simulation, created by Distinguished Professor of Chemistry and Biochemistry Rommie Amaro and her team at UCSD, contains 160 million atoms. To model such a complex system, the Amaro lab used ORNL's Titan supercomputer.

> *This research could be used to develop methods of keeping the protein locked open so that it would be constantly accessible to antibodies.*
> — University of California, San Diego principal investigator **Rommie Amaro**

Seasonal flu vaccines are reformulated each year to match dominant strains. When the vaccine matches the predominant strain, it is very effective; when it doesn't, it provides little protection.

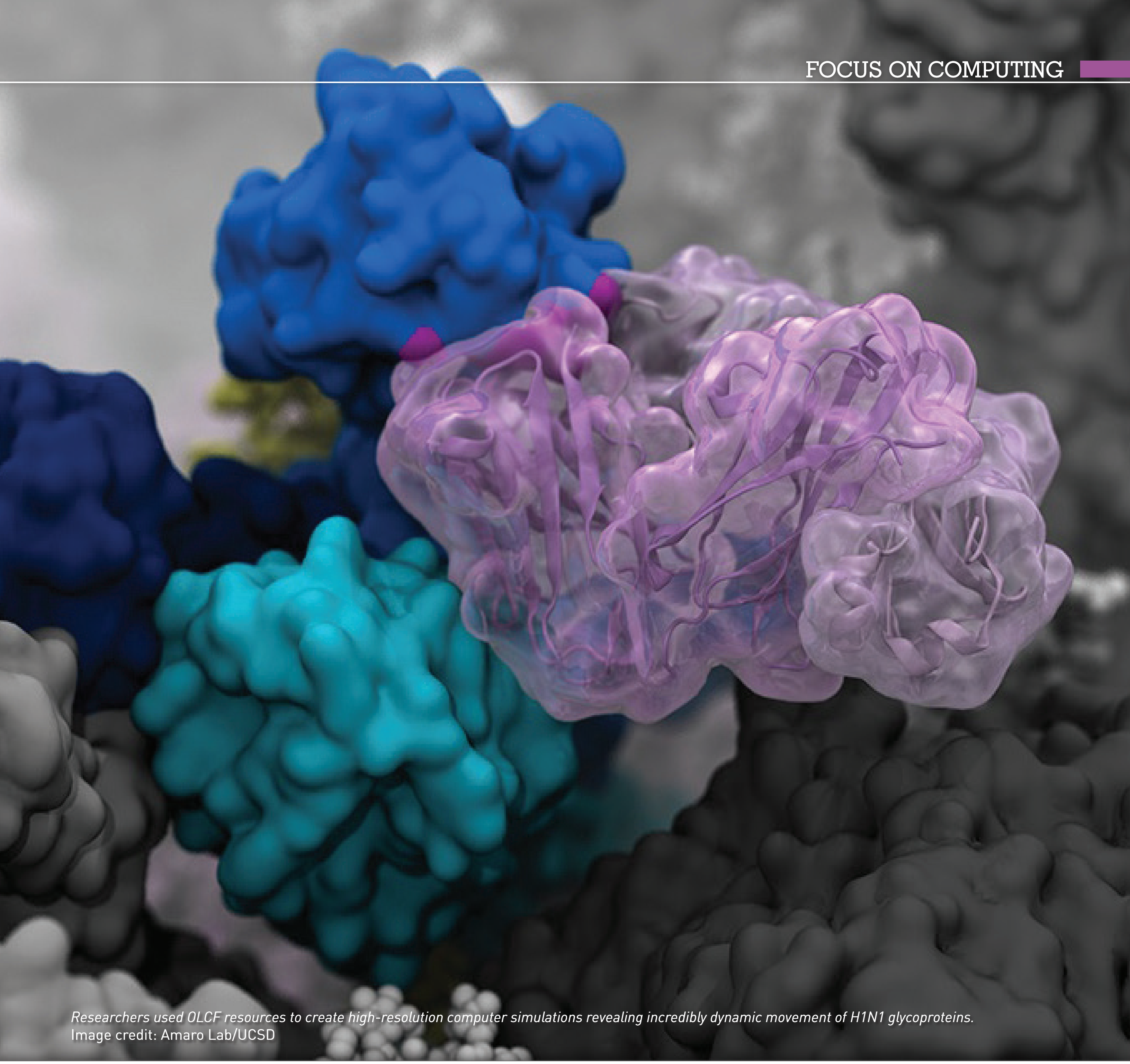
Researchers at the University of California, San Diego, have created an atomic-level computer model of the H1N1 virus that reveals new vulnerabilities in the molecular-level movement of two glycoproteins that are the main targets of the flu vaccine. This work, published in *ACS Central Science*, offers a new pathway for the development of vaccines and antivirals that target influenza.

Even though Titan is no longer in operation, researchers still benefit from data generated by the system.

"Titan was the first leadership-class hybrid (i.e., using CPUs and GPUs together) supercomputer. This work is a great example of how the impact from simulations performed on one-of-a-kind computational instruments such as Titan can be felt for years to come," said Bronson Messer, director of science at the Oak Ridge Leadership Computing Facility.

The main targets of the flu vaccine are two surface glycoproteins: hemagglutinin, or HA, and neuraminidase, or NA. While the HA protein helps the virus bind to the host cell, the NA protein acts like scissors to cut the HA away from the cell membrane, allowing the virus to replicate. Previously, the movements of these glycoproteins were not fully understood.

"This research could be used to develop methods of keeping the protein locked open so that it would be constantly accessible to antibodies," said Amaro, who is the principal investigator on the project.



Researchers used OLCF resources to create high-resolution computer simulations revealing incredibly dynamic movement of H1N1 glycoproteins.
Image credit: Amaro Lab/UCSD

Amaro's model showed the dynamic nature of the HA protein and revealed a molecular movement, or breathing mode, that exposed a previously unknown site of immune response known as an epitope.

"Titan's tremendous resources and vast amount of parallelism allowed us to achieve a remarkable amount of sampling — around 0.5 microseconds — with outstanding performance," said UCSD assistant project scientist Lorenzo Casalino.

NA proteins also showed a head-tilting movement at the atomic level. When Julia Lederhofer and Masaru Kanekiyo at the National Institute of Allergy and Infectious Diseases looked at convalescent plasma — that is, plasma from patients recovering from the flu — they found antibodies that specifically targeted what is called the "dark side" of NA, underneath the head. Without seeing the movement of NA proteins, it wasn't clear how the antibodies were accessing the epitope.

Amaro is making the data available to other researchers, who can uncover even more about how the influenza virus moves, grows and evolves.

"This paves the way for other groups to apply similar methods to other viruses," Amaro stated. "We've modeled SARS-CoV-2 in the past and now H1N1, but there are other flu variants and MERS, RSV and HIV — this is just the beginning."

Autocoding cancer

by Betsy Sonewald
sonewaldbv@ornl.gov

Researchers at ORNL and the National Cancer Institute have created an algorithm that speeds up the classification of cancer pathology reports.

Early results from the Cancer Moonshot program show that the algorithm dramatically reduces the time it takes for national cancer registries to process reports and, therefore, the time it takes for data to become available for public health monitoring and policymaking.

The network's development is supported through a collaboration between ORNL and NCI known as MOSSAIC — or Modeling Outcomes using Surveillance data and Scalable Artificial Intelligence for Cancer — that combines ORNL's computational and security resources with NCI's domain knowledge and population-level data.

The research is co-led by Heidi Hanson, leader of the lab's Biostatistics and Multiscale Systems group, and principal investigator Georgia Tourassi, associate laboratory director for computing and computational sciences.

The reduction in manual coding hours and the potential for near–real-time cancer reporting are promising for the future of public health surveillance.

— ORNL researcher **Heidi Hanson**

The new Case-Level Multi-Task Hierarchical Self Attention Network uses natural language processing to autocode cancer pathology reports submitted to Surveillance, Epidemiology and End Results, or SEER, registries across the United States based on data used for population-level surveillance of cancer, including cancer type, histology, laterality and behavior.

The 19 SEER registries collect and publish data gathered on every cancer case reported from 22 geographic areas in the United States. This data is a critical tool for tracking and understanding the nation's cancer trends and for informing public health strategy and policy. However, according to Hanson, public reporting of the data is usually about two years behind due to the volume of reports, which are traditionally classified by human registrars. That's where natural language processing algorithms can help.

Natural language processing algorithms are a type of machine learning trained to recognize patterns and keywords in human language by analyzing many target datasets — cancer pathology reports in this case. Often, a single cancer case leads to multiple reports that are not automatically linked to one another. For example, a metastatic cancer case can have reports from several tissue samples that don't reference the original diagnosis. Rather than report at the individual report level, the Case-Level Multi-Task Hierarchical Self Attention Network classifies at the case level by using data from a series of connected reports, boosting the algorithm's overall accuracy.

At ORNL, the team trains and tests its algorithms using two security frameworks, CITADEL and the Knowledge Discovery Infrastructure, which allow researchers to use the OLCF's high-performance computing systems for projects that include protected health information.

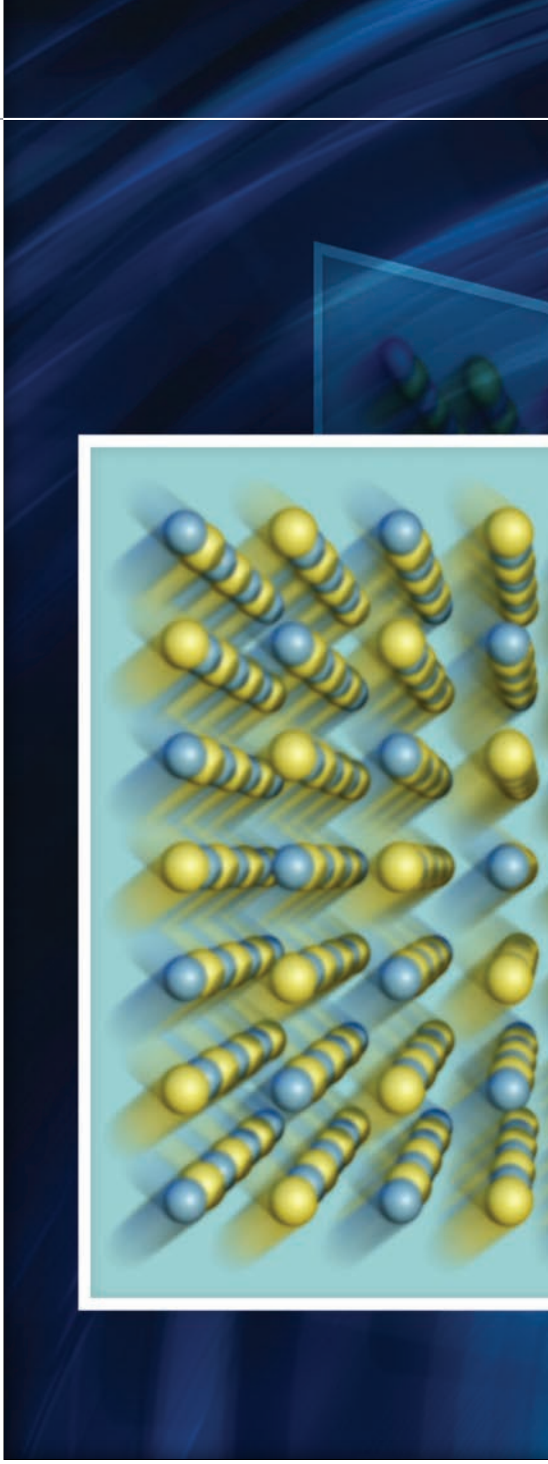
The algorithm is being used to classify thousands of reports per second in 12 SEER registries and one non-SEER registry. Working 18 times faster than a human registrar, the algorithm saves 46,000 person-hours per year, but it hasn't fully replaced human registrars. Of the millions of reports screened each year, 17.5 percent are autocoded at a predefined confidence threshold of 97 percent. Registrars then review a subset of reports that meet that threshold and conduct full reviews on reports that do not.

As the algorithm is adopted by more registries, the impact on population-level reporting could be significant. "The reduction in manual coding hours and the potential for near–real-time cancer reporting are promising for the future of public health surveillance," Hanson said.

'Neutron camera'

method captures atomic-scale activity in a flash

by Paul Boisvert
boisvertpl@ornl.gov



Scientists have long sought to better understand the arrangement and activities of the neighboring particles around each atom, known as the local structure of materials. In crystals, which are used in electronics and many other applications, most of the atoms form highly ordered lattice patterns that repeat. But not all atoms conform to the pattern.

We are tantalizingly close to having quiet, energy-efficient and thermoelectric solid-state refrigerators in our houses, replacing the noisy and energy-gobbling compressor fridges we have now.

— Columbia University and Brookhaven National Laboratory physicist **Simon Billinge**

When some atoms take up local arrangements that differ from that implied by the overall structure of the crystal, it becomes more difficult to study the local structure, especially when the atoms are moving. In fact, the inability to clearly see these local effects means researchers are often not aware that these effects can occur.

Now researchers using the Spallation Neutron Source at ORNL have developed a new method for studying the local structures of materials in detail and in real time.

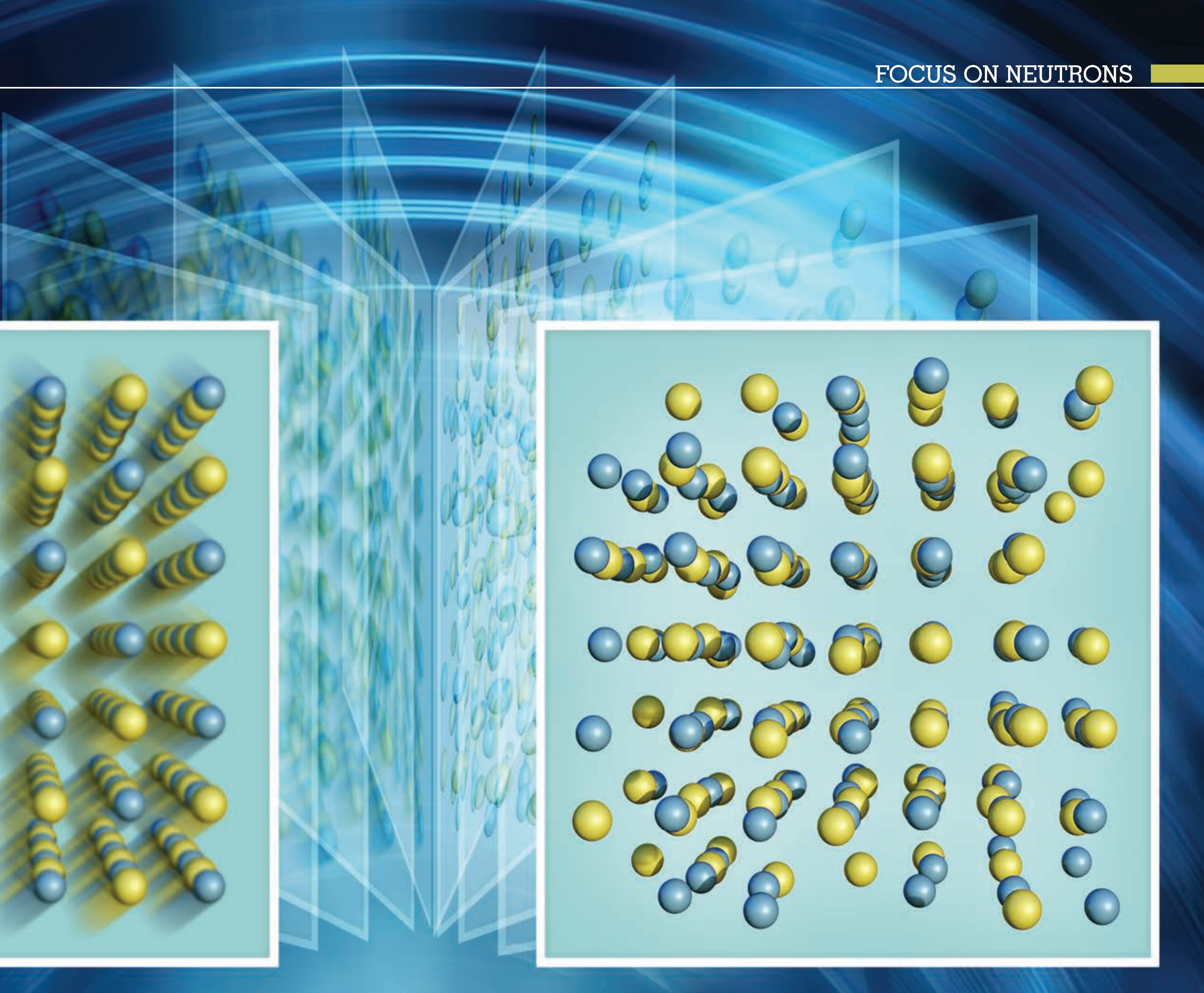
The team developed a variable-shutter pair distribution function, or vsPDF, technique in which neutrons function like a camera but at timescales a trillion times faster.

Results of the research, led by Columbia University, demonstrate a unique use of neutrons that could become a standard method for reconciling local and overall structures in energy materials. The research also revealed a key mechanism behind the thermoelectric effect, in which temperature differences in a material can be converted into an electric voltage or, conversely, the material can be used to heat or cool when a voltage is applied to it.

The new local structure analysis method uses the ultrabright flashes of neutrons produced by SNS. When these neutrons pass through a material, the resulting scattering patterns yield information about the material's atomic arrangement. The team used a novel energy-filtering technique to determine how to change the effective shutter speed of the energy to produce representations —or images—of the atomic arrangement. In conventional cameras, images of moving objects blur at slower shutter speeds. If the shutter speed is gradually increased, then the moving atoms will eventually freeze in an unblurred image.

The researchers were able to demonstrate the same effect on a timescale that allowed them to observe atomic motions in the material. This capability offered key insights into how the material produces its outstanding thermoelectric performance.

"Neutrons have exceptional properties as a probe of materials," said Simon Kimber, lead scientist on the project. "They have wavelengths comparable to the spacing between atoms, but they also



This illustration depicts the novel energy-filtering technique using neutrons that enabled researchers at ORNL to freeze moving germanium telluride atoms in an unblurred image. The images offer key insights into how the material produces its outstanding thermoelectric performance. Image credit: Jill Hemman, ORNL

have an energy similar to the vibrations of the atoms. This unique combination, along with the advanced instrumentation at SNS, allowed us to use the variable shutter speed method."

The team developed the new technique while investigating the material properties of germanium telluride, or GeTe, which is closely related to materials in thermoelectric-based generators such as those used to power deep-space missions like Voyager and the Mars rover.

"We are tantalizingly close to having quiet, energy-efficient and thermoelectric solid-state refrigerators in our houses, replacing the noisy and energy-gobbling compressor fridges we have now," said Simon Billinge, a professor at Columbia and physicist at Brookhaven National Laboratory. "Similar to the solid-state lighting revolution, we just need materials with slightly better properties for this to happen."

Thermoelectric effects are produced by a heat gradient — hotter to colder — in materials that resist heat flow while retaining electrical conductivity. Using the vsPDF technique, the research team found that at slower shutter speeds, the atomic structure of GeTe looks highly crystalline, yet faster exposures revealed an intricate pattern of dynamic displacements that disrupt heat flow.

Timmy Ramirez-Cuesta, SNS Instrument Development group leader, said "Using computer modeling, we calculated the motions of the atoms to visualize and understand how they are moving in the material. We used open-source software developed at ORNL to analyze the data and validate the experimental findings."

50 years after NASA Apollo missions,

moon rocks still have secrets to reveal

by Jeremy Rumsey
rumseyjp@ornl.gov

In 1969, astronauts of Apollo 11 were the first to set foot on the moon and to study the lunar surface. Over the next several Apollo missions, ending in 1972, astronauts brought back moon rocks for scientific research to unlock mysteries of the universe.

Now, nearly 50 years later, NASA scientist Andrew Needham is studying those same rocks with characterization tools and techniques light-years ahead of their predecessors. One such technique is neutron scattering.

Searching for clues to early planetary formations and where water might be stored on the moon, Needham studied a small collection of lunar and asteroid samples using the newly renamed neutron imaging instrument MARS — short for the Multimodal Advanced Radiography Station — at ORNL's High Flux Isotope Reactor.

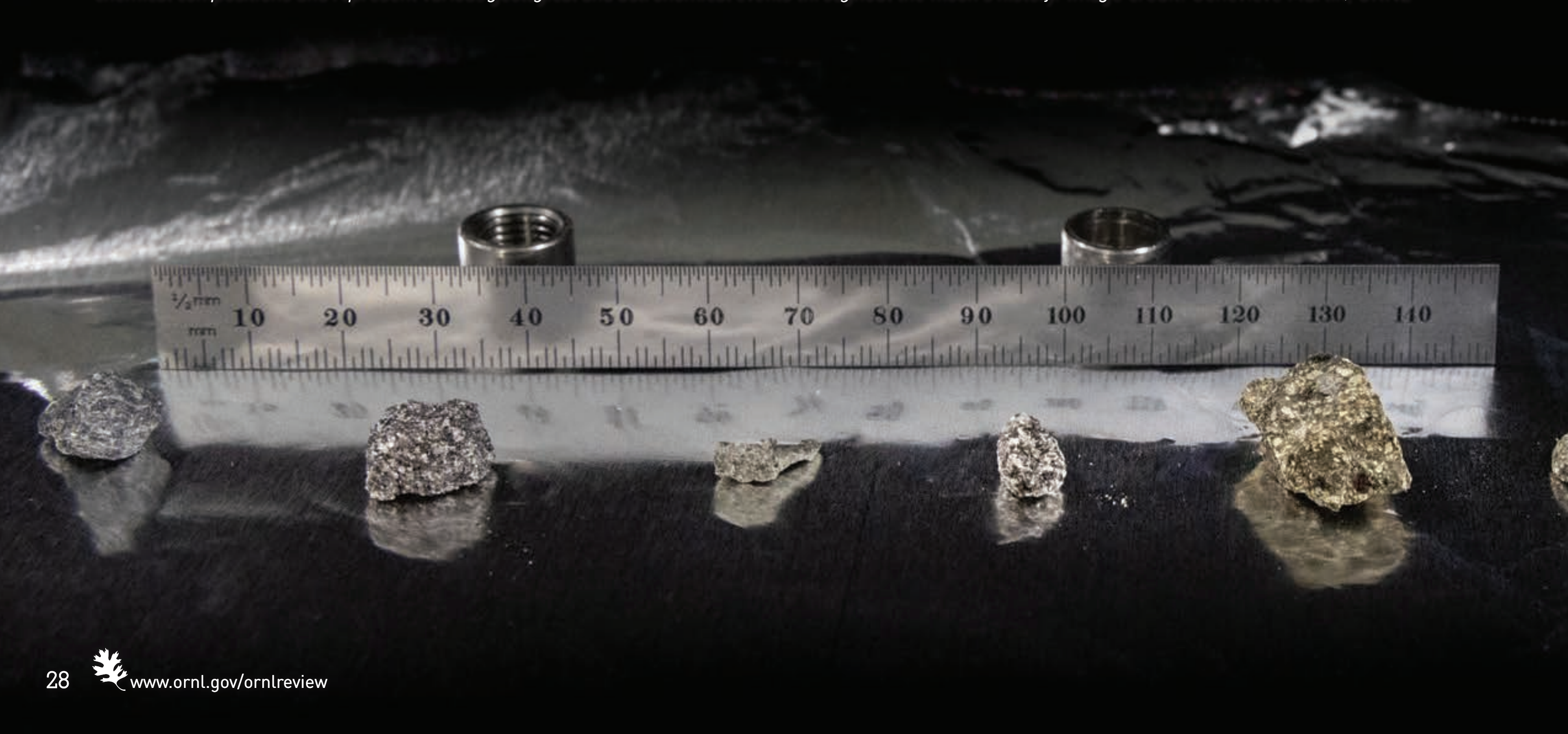
"In the past decade, there's really been a renewed interest in looking for water in places like the moon," he said. "We used to think the moon was very dry, but now we know that water is trapped inside the mineral content of these rocks. Studies have shown that water might be accumulating near the poles of the moon through impact events that are evidenced in these samples."

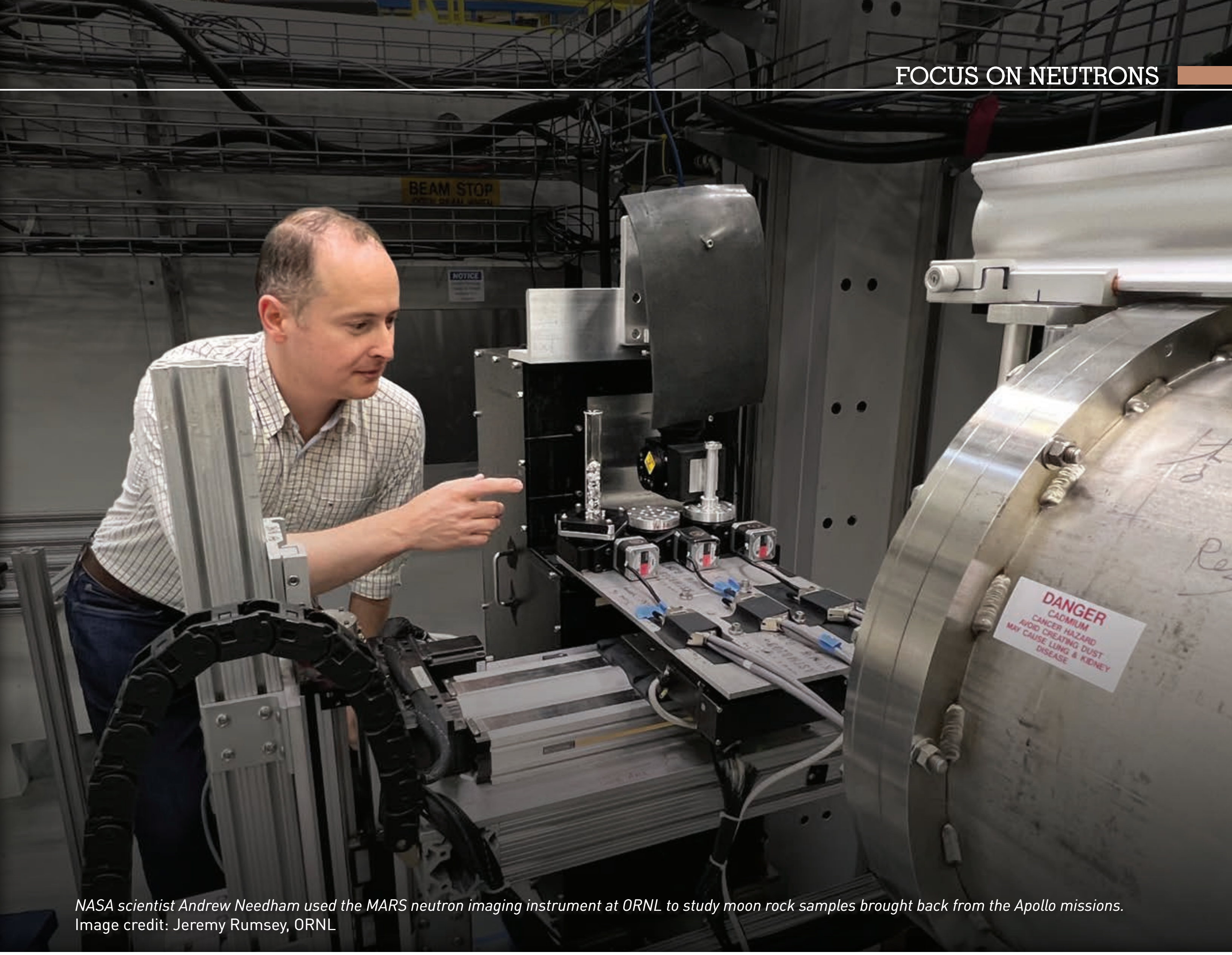
Needham says that if humans are going to further explore the moon, and one day Mars, it is essential to find new ways to fuel travel and survive without having to rely on resources from Earth.

"Understanding the composition of these rocks, where hydrogen atoms are, how they're stored and transported, really helps us understand the moon over its history and up to its present day, and how we might use that information to travel even farther."

The Apollo mission samples Needham is studying include impact breccias, which are made up of dust, rock fragments and melted particles mixed together after meteorites bombard the moon's surface. Needham explained that when the meteorites struck roughly 4 billion years ago, the impacts combined with and stirred up mixtures of materials from the moon's surface, as well as its deeper interior layers. In essence, he said, even one moon rock can contain a plethora of information from multiple astronomical events.

The lunar and meteorite samples consist of a variety of rocks, some more gravel-like and some similar to lava rock found in Hawaii. The samples have different chemical compositions and represent various geological and astronomical events throughout the moon's history. Image credit: Genevieve Martin, ORNL





NASA scientist Andrew Needham used the MARS neutron imaging instrument at ORNL to study moon rock samples brought back from the Apollo missions.
Image credit: Jeremy Rumsey, ORNL

Neutrons are ideally suited for use in studying the chemical composition of the Apollo moon rocks. They can pass through almost any material, but light elements such as hydrogen will block or deflect them upon contact.

Using the MARS instrument, which specializes in creating radiographic images similar to clinical X-rays, Needham loaded the samples into containers stationed on a rotating platform that allows measurements to be taken of the rocks in 360 degrees. Regions where hydrogen atoms are likely to be found are highlighted within the rocks as the neutron beam passes through the sample.

> *These are precious samples, so we can't go slicing and dicing as much as we want. Neutrons help us see inside the samples so that we can make the most precise slices to expose only the areas of interest. And it's really only neutron imaging that makes hydrogen atoms visually pop out, letting you know that, "Ooh! That's something I want to look at."*
>
> — NASA scientist **Andrew Needham**

In the neutron images, the hydrogen atoms show up as brightly colored spots in contrast to the rest of the sample. The more difficult it is for a neutron to pass through an element, the brighter that element will appear, resulting in a color scale that corresponds to different elements. The 360 degree measurements can then be used to create 3D models of the rocks that can in turn be compared with results from other research techniques, such as X-rays and electron microscopy.

"These are precious samples, so we can't go slicing and dicing as much as we want," Needham said. "Neutrons help us see inside the samples so that we can make the most precise slices to expose only the areas of interest. And it's really only neutron imaging that makes hydrogen atoms visually pop out, letting you know that, 'Ooh! That's something I want to look at.'"

Producing

biofuels for jets

by Stephanie Seay
seaysg@ornl.gov

To help the aviation sector reach a goal of zero carbon emissions by 2050, DOE's Center for Bioenergy Innovation at ORNL is setting its expertise and capabilities in plant science, genomics, microbiology and chemistry to the task of creating new low-carbon fuels for airplanes.

> *Using plants to produce fuels and bioproducts has multiple benefits in addition to being cleaner burning. During photosynthesis, as biomass forms, plants draw carbon dioxide out of the atmosphere. When we convert that biomass into fuels, carbon stored in the plant roots remains stored belowground. This means biofuel production contributes to carbon sequestration as well as fossil fuel displacement.*
>
> — CBI Chief Executive Officer **Jerry Tuskan**

Aviation is difficult to decarbonize. The weight and low energy density of today's batteries rule out electrification of large jets. The sector is looking instead to biologically sourced fuels to ultimately replace conventional petroleum-based products.

The need is urgent. The U.S. government has set a near-term goal of cutting life-cycle aviation greenhouse gas emissions in half by the year 2030, including emissions from fuel production and transport. To meet that goal, an estimated 3 billion gallons per year of a biomass- or waste-derived product known as sustainable aviation fuel, or SAF, is needed. By 2050, a full 35 billion gallons a year will be required to have all domestic flights running on SAF.

But the SAF industry is still in its infancy. According to the International Air Transport Association, only about 79 million gallons of SAF were produced worldwide in 2022, most from waste fryer oil. It is unlikely that the world will increase its consumption of fried foods enough to meet the grand challenge of SAF from waste resources.

Enter CBI, one of four DOE Bioenergy Research Centers across the nation with a mission of supporting a viable biofuels and bioproducts industry. The CBI brings together scientists from 17 national labs, universities and other partners to develop better biomass feedstock plants, along with custom-engineered microbes and catalysts to break down and convert the natural polymer lignin from nonfood crops like poplar and switchgrass into fuels.

"We've assembled as part the CBI team the world's best experts in many areas, including soil carbon sequestration, plant wall biosynthesis, microbial conversion of cell walls into fermentative intermediates, and catalytic chemistry for the conversion of these renewable feedstocks into hydrocarbons that can be used as a means of displacing current aviation fuel," said CBI Chief Executive Officer Jerry Tuskan.

In early 2023, CBI was renewed for five more years of funding by DOE's Office of

Science. The center's mission for the next five years is to focus on developing plant-derived SAF and certifying such blendstocks into an industry standard that verifies it has the same basic properties as conventional jet fuel.

The certification process is comparable to a pharmaceutical certification in that it's not just the end-product that's tested, but the steps taken to get to the final product, Tuskan explained.

CBI is working on initial fuel characterization using ORNL mass spectrometry and analytical capabilities for 18 fuel blendstock candidates derived collectively from poplar, switchgrass and corn stover feedstocks. Follow-on testing will be performed at the Federal Aviation Administration's fuel certification facilities at Washington State University.

Early results indicate a poplar-based CBI fuel will exceed many required parameters, one of which is reduced soot emissions. The soot emitted by jets that use fossil fuels acts as a condensation trigger that creates plane contrails — the white trails that appear behind aircraft. Those human-made clouds have been implicated in warming the Earth's climate by trapping heat that would otherwise be released into space.

"Using plants to produce fuels and bioproducts has multiple benefits in addition to being cleaner burning," Tuskan said. "During photosynthesis, as biomass forms, plants draw carbon dioxide out of the atmosphere. When we convert that biomass into fuels, carbon stored in the plant roots remains stored belowground. This means biofuel production contributes to carbon sequestration as well as fossil fuel displacement."

Displacing fossil fuels with bio-based alternatives has other benefits, Tuskan said. "If we can meet the U.S. goals for displacing fossil fuels and reducing atmospheric carbon dioxide, we will not only create green jobs here at home, but we will also benefit people around the world who live in at-risk communities like low-elevation environments in coastal regions or in urban heat islands."

ORNL supports Puerto Rican microgrids

Story and photos by S. Heather Duncan
duncansh@ornl.gov

Microgrid project leaders and solar advocates lead a parade in Adjuntas, Puerto Rico in March.

The streets echoed with the sound of drums and chants of support for community solar initiatives.

Sunshine puppets and flags, high school bands and beauty queens circled the town square as about 1,000 people marched to celebrate greater community independence through solar power.

A pizzeria is one of many local businesses with rooftop solar panels that will serve as a community gathering place during grid blackouts. The restaurant owner leads the co-op that owns the microgrids.

The region near Adjuntas, Puerto Rico, came together recently to celebrate the completion of solar microgrids that will support the area during blackouts. The celebration included a "Marcha del Sol" parade, concerts and a craft fair to demonstrate support for more solar and renewable energy projects in the U.S. territory.

Funded and installed by partnering nonprofits led by local conservation organization Casa Pueblo, the microgrids will improve lives of mountain residents by providing more reliable power in the wake of hurricanes.

ORNL researchers are creating an orchestrator tool to automate management of the microgrids, enabling them to shift loads to support each other if one is damaged. Businesses linked to the microgrids have committed to providing services to the community, such as refrigerating medicine and charging cell phones during broader outages.

An Adjuntas bakery connected to the microgrid will allow nearby residents to charge their phones and help provide food in the wake of hurricanes like Maria and Fiona.

ORNL researchers Max Ferrari (left) and Ben Ollis check different parts of the microgrid equipment in Adjuntas.

ORNL researcher Max Ferrari talks with the owner of the Adjuntas hardware store about his solar panels. Ferrari has worked with the businesses on the project since he was a college student.

Arturo Massol-Deya, executive director of Adjuntas conservation organization Casa Pueblo, discusses the microgrids with ORNL researcher Max Ferrari beneath a forest of solar panels in Adjuntas.

Simulation code

aids high energy physics research

by Dawn Levy
levyd@ornl.gov

ORNL scientists are leading a project to ensure that the fastest supercomputers can keep up with big data from high energy physics research.

"For scientific big data, this is one of the largest challenges in the world," said Marcel Demarteau, director of ORNL's Physics Division and principal investigator of the project, which first aims to address a data tsunami that will arise from a major upgrade to the world's most powerful particle accelerator, the Large Hadron Collider, or LHC.

"Each of its largest particle detectors will be capable of streaming 50 terabits per second — the data equivalent to watching 10 million high-definition Netflix movies concurrently."

The LHC sits deep underground at CERN, on the border between Switzerland and France. Smashing protons and heavier nuclei, it produces progeny particles that its detectors track. The detectors generate enormous amounts of data that is compared against simulations so that experiments can validate theories. The knowledge gained improves understanding of fundamental forces.

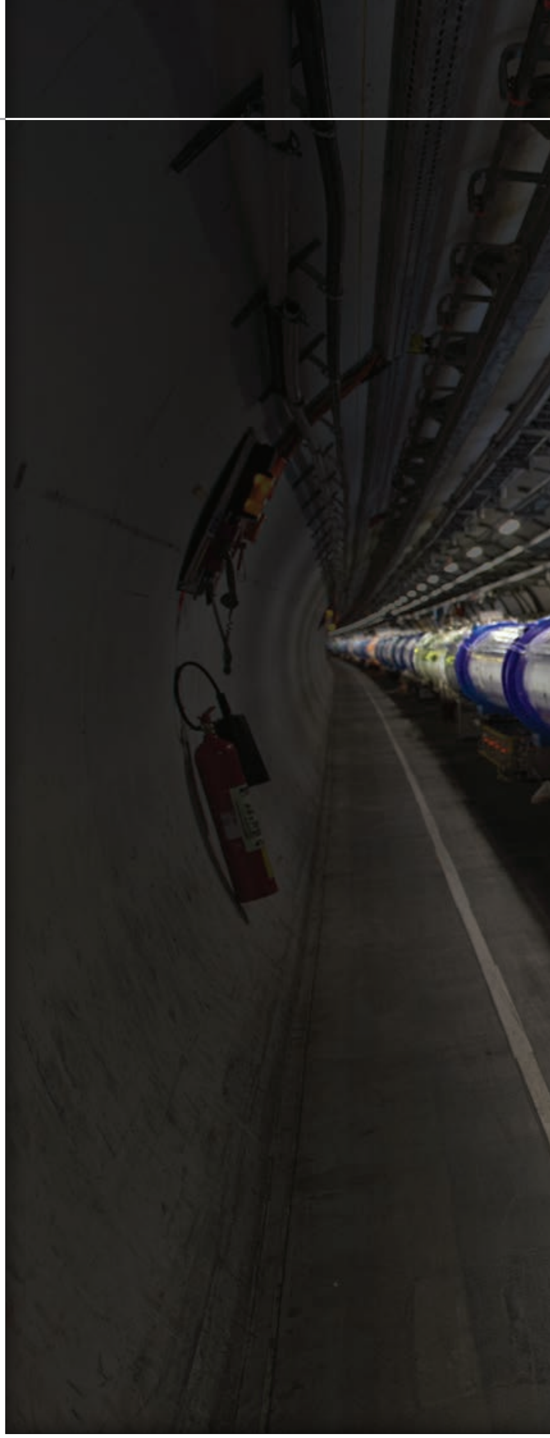
Researchers expect the upgraded particle accelerator, the High-Luminosity LHC, to begin operations in 2029. Luminosity measures how tightly packed particles are as they zip through the accelerator and collide. Higher luminosity means more particle collisions. The upgraded LHC promises discoveries but will create more data than simulations can manage.

"The High-Luminosity LHC will boost the number of proton collisions to 10 times what the LHC can produce," Demarteau said.

To address this challenge, partners in the new project are developing a simulation code called Celeritas — the Latin word for speed. Simulation codes calculate electromagnetic interactions as particles move through detectors. To vastly increase the data throughput from high-fidelity simulations of high energy physics experiments, Celeritas will use new algorithms that employ graphics processing units for massive parallel processing on leadership-class computing platforms such as ORNL's Frontier.

"Celeritas is an important step in reworking the entire way computational simulations and analyses are done in the high energy physics ecosystem," said ORNL's Tom Evans. He leads the multi-laboratory project, which includes scientists at Argonne National Laboratory and Fermi National Accelerator Laboratory, or Fermilab.

Evans uses Monte Carlo techniques that rely on repeated random sampling to step each particle through a virtual world and simulate the history of its movement.



"Think of it as a dice-rolling game, where we simulate particle tracks based on the best available physical models of their interactions with matter," Evans said. He works with ORNL's Seth Johnson developing methods and tools to optimize Celeritas. "We simulate tracks crossing a detector and compare them with data that comes out of the detector. These correlations are used to validate theories of the Standard Model of particle physics."

Currently, the Worldwide LHC Computing Grid manages the storage, distribution and analysis of LHC

Large Hadron Collider. Image credit: CERN

data. Its 13 largest sites, including DOE's Brookhaven National Laboratory and Fermilab, connect via high-speed networks.

"We want to incorporate DOE's leadership-class computing facilities into this network to bring to bear their rich computing power and resources," Evans said.

Celeritas collaborators also will develop tools to make DOE's federated computing facilities compatible with high energy physics computing centers. ORNL's Fred Suter and Stefano Tognini work with Scott Klasky, leader of the lab's Workflow Systems group, to integrate advanced tools and technologies that reduce the burden of high data traffic in and out of processors.

"As high-performance computing resources continue to grow in computational capability, we have seen much less growth in their storage bandwidth and capacity. That means that we must continue to optimize workflows to keep up with this imbalance," Klasky said. "This is absolutely necessary for scientific discovery, especially as we move to the Worldwide LHC Computing Grid. The conventional techniques that they have used there just will not be sufficient anymore for this compute challenge."

The team's first goal is to simulate the LHC's Compact Muon Solenoid detector on ORNL supercomputers. The detector's researchers are eager to integrate Celeritas into their existing software framework. Said Demarteau, "It is a highly sophisticated detector and an ideal test case for Celeritas."

For more information: bit.ly/47bAcb6

ORNL teams with Army to improve welds

by Dawn Levy
levyd@ornl.gov

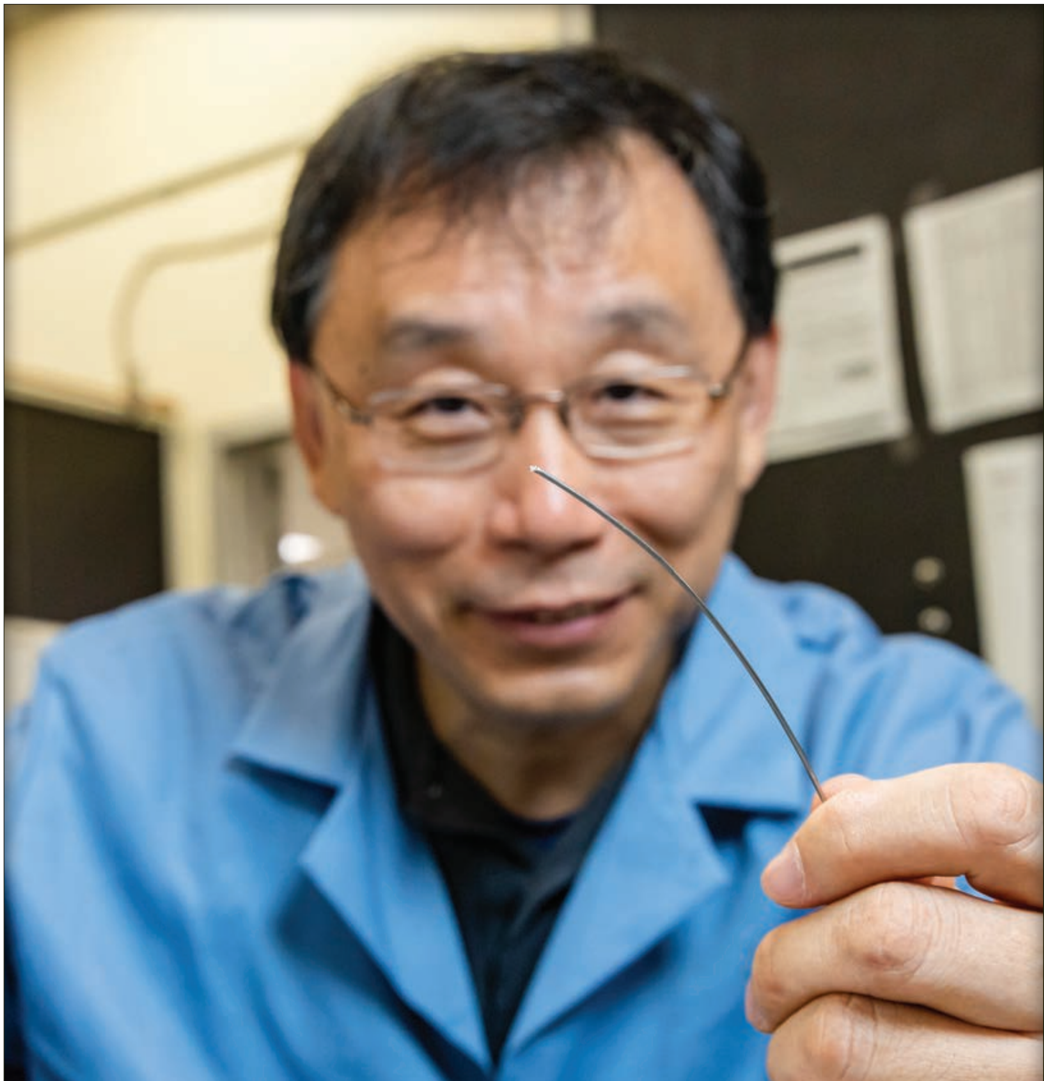
DOE and the Department of Defense have teamed up to create a series of weld filler materials that could dramatically improve high-strength steel repair in vehicles, bridges and pipelines. This novel weld wire could help revitalize America's aging infrastructures, which in 2021 received a C- grade from the American Society of Civil Engineers.

The invention from ORNL and the Army enables on-site welding without the costly, laborious heat treatments typically used to reduce residual stresses and material distortion. It solves a major problem that occurs when hydrogen atoms enter the steel during welding, reducing the metal's ductility, toughness and strength. Subsequent high tensile residual stress leads to perilous cracking.

"The filler material that ORNL and the U.S. Army invented is a unique and game-changing solution for residual stress control, distortion reduction and avoidance of hydrogen-induced cracking for a wide range of structural steels," said Zhili Feng, who leads ORNL's Materials Joining group.

"About 80 percent of welded structures in the United States are made of steels, so applications for our innovative fill metal are extensive," said Stan David, an ORNL corporate fellow emeritus who led the lab's welding program for 25 years. "It is cheaper to repair a structure than to replace it. Our filler provides high-quality weld joints for increased service life of welded structures in demanding environments. The invention could potentially save U.S. industry hundreds of millions to billions of dollars each year."

Strong steels are especially prone to hydrogen-induced cracking. To overcome this challenge, scientists at ORNL and DOD's former U.S. Army Tank Automotive Research, Development and Engineering Center — now called the Ground Vehicle



ORNL's Zhili Feng designs weld wire to match or exceed strengths of various steel alloys. In a weld, it counteracts stress caused by stretching with stress caused by compression. Image credit: Carlos Jones, ORNL

ORNL materials scientist Zhili Feng, left, looks on as senior technician Doug Kyle operates a welding robot inside a robotic welding cell.
Image credit: Carlos Jones, ORNL

System Center — partnered to invent an alloy with a unique chemical composition that can join strong steels while reducing residual stresses.

The alloy's ability to resist hydrogen-induced cracking comes from a novel phase transformation in the weld. As a weld cools, the filler material combats tensile stress, or "bad stress," which pulls at steel's crystalline microstructure to lengthen and break it. The phase transformation introduces compressive stress, or "good stress," to compensate for bad stresses as the weld cools.

This interagency success story began in 2011, when DOE's Office of Energy Efficiency and Renewable Energy's Vehicle Technologies Office funded ORNL scientists to work with multinational steel manufacturer ArcelorMittal on a cooperative R&D agreement. Automakers had begun reducing vehicle weight by using stronger steels to fabricate thin panels. However, thinner panels meant increased stress on the welds. ORNL's novel weld wire provided the solution they needed.

Wanting to reduce the weight of military tanks with ultrastrong armor to improve agility and fuel efficiency, the Army approached ORNL in 2013 to discuss hydrogen-induced cracking of armored steel components.

"We turned to ORNL because its welding research is world-class, and the partnership gave us access to the best-in-class experts and instrumentation of a national lab," said Demetrios Tzelepis, a senior materials engineer at the Army vehicle system center. "ORNL kept pushing the research envelope, and together we delivered a superb solution."

Feng added, "The requirements for tank steel and automotive steel are very different. ORNL had to change the chemistry of our weld wire to match the steel strength for the Army's applications." The resulting technology won an R&D 100 Award in 2017.

The chemical composition of the weld wire was initially developed to repair cars and later evolved to fix tanks; it has since progressed to mend pipelines and other critical infrastructures.

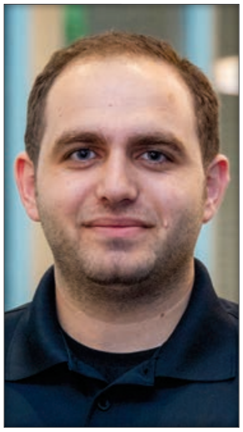
Moreover, the novel weld wire may also prove useful in additive manufacturing, or 3D printing, which employs localized melting to add layers one at a time and can create profound stresses in a fabricated part. The Army and ORNL again teamed up to explore the ability of innovative materials to avoid distortion and increase strength in printed steel parts.

"Huge economic benefits could come from eliminating cracking and post-fabrication distortion in welded or 3D-printed steel structures," Feng said.

For more information:
https://bit.ly/3UNi55h

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

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



Ozgur Alaca

Graduate Student, Electrification and Energy Infrastructure Division
Ph.D. student, Electrical and Computer Engineering, Texas A&M University
Hometown: Istanbul, Turkey

What are you working on at ORNL?

I work in the Grid Communications and Security group at EEID. My research focuses on investigating novel approaches for detecting and identifying anomalies in power grid signals. We developed a feature extraction method using statistical signal processing approaches to observe the characteristic distinctions between anomaly signals.

What would you like to do in your career?

I want to develop innovative mathematical approaches and signal-processing algorithms that touch on new and emerging areas containing massive measurement data. However, one of the most worthwhile goals of my career is to write a book in order to share my knowledge and experiences with future generations.

Why did you choose a career in science?

My interest in engineering and physics has been sparked by noticing the counterparts of theoretical studies in nature. Upon realizing that my education was merely a grain of sand in a vast desert, I became increasingly interested in learning more about science.

Pratishtha Shukla

Postdoc, Computational Sciences and Engineering Division
Ph.D., Electrical Engineering, North Carolina State University
Hometown: Bhopal, Madhya Pradesh, India

What are you working on at ORNL?

My research focuses on developing models and algorithms for improved control and coordination of energy systems, specifically the electric power grid. I also work on designing models for planning and assessments for future events that affect the grid, whether positive developments such as high penetration of renewable sources or threats associated with solar storms.

What would you like to do in your career?

I want to help build a clean, self-sufficient and resilient power grid to ensure a sustainable future. I hope to contribute my research and work at ORNL to this goal. I am also enthusiastic about sharing knowledge with future generations who are willing to work toward a similar long-term goal.

Why did you choose a career in science?

I have always asked the question, "Why?" Science can answer most of these questions, so I decided to get invested in science. The idea that developments in science and technology have a direct impact on all living things, people and animals makes me excited to work every day.

Jordan Stomps

Graduate student, Nuclear Nonproliferation Division
Ph.D. student, Nuclear Engineering and Engineering Physics, University of Wisconsin-Madison
Hometown: Detroit, Michigan

What are you working on at ORNL?

My research focuses on novel data analytic applications to national security over a variety of measurement modalities. I currently work on semi-supervised machine learning methods to leverage large volumes of radiation data with limited contextual information to produce interpretable estimates and accurately monitor, detect and characterize radiological material.

What would you like to do in your career?

I hope to continue supporting the missions of the National Nuclear Security Administration through research here at ORNL. Developing monitoring systems for nuclear fuel cycles combines my background in nuclear engineering with advances in data science. I expect a career in nuclear nonproliferation to be both fulfilling and impactful.

Why did you choose a career in science?

Science to me has been about a pursuit of discovery in the service of humanity. I have always wanted to be involved in nuclear science because I learned early on about all its exciting societal applications. Success in science for me is making incremental contributions that promote advanced technology utilization.

Briana Schrage

Postdoc, Chemical Sciences Division
Ph.D., Inorganic Chemistry, The University of Akron
Hometown: Strongsville, Ohio

What are you working on at ORNL?

My current research efforts are driven toward the development of novel chelators (molecules) that bind to alpha, beta and Auger-emitting radioisotopes to be utilized in targeted radionuclide therapy. My primary project investigates new chelators for the Auger-emitting radioisotope antimony-119. These chelation platforms can then successfully deliver antimony-119 to micrometastases and single-cell diseases in the body.

What would you like to do in your career?

Demand for high-end isotope production capabilities is continually on the rise, and I am interested in continuing a career working on isotope R&D and production. Additionally, I have an interest in mentoring students who are attracted to a career in science.

Why did you choose a career in science?

Children are naturally curious about science and the wonders of nature. My father holds a Ph.D. in mechanical and aerospace engineering, and it inspired me at a young age to pursue a career in science. After one high school chemistry course, I knew it was the field for me.

Abhijeet Dhakane

Graduate Student, Center for Nanophase Materials Sciences
Ph.D. student, Data Science and Engineering, University of Tennessee Knoxville (Bredesen Center)
Hometown: Pune, India

What are you working on at ORNL?

My research primarily focuses on understanding the static and dynamic properties of ferroelectric materials using atomistic simulations. I extensively use AI and deep learning techniques to understand the atomistic simulations where dynamic properties are influenced by defects and order parameter.

What would you like to do in your career?

I'm interested in being part of a team where I use my computational materials and data science knowledge to develop the next generation of materials needed for a fast-paced, growing society.

Why did you choose a career in science?

Since childhood I have been fascinated by scientific discoveries, reading biographies of the scientists and watching Nat Geo, Discovery and TV science shows. I was an active participant in science exhibitions during my school days. After pursuing an applied science degree in undergrad and grad school, now I'm switching to more fundamental science.

Huixin (Anna) Jiang

Postdoc, Chemical Sciences Division
Ph.D., Energy and Environment Science, Nagaoka University of Technology, Japan
Hometown: Laiyang, Shandong Province, China

What are you working on at ORNL?

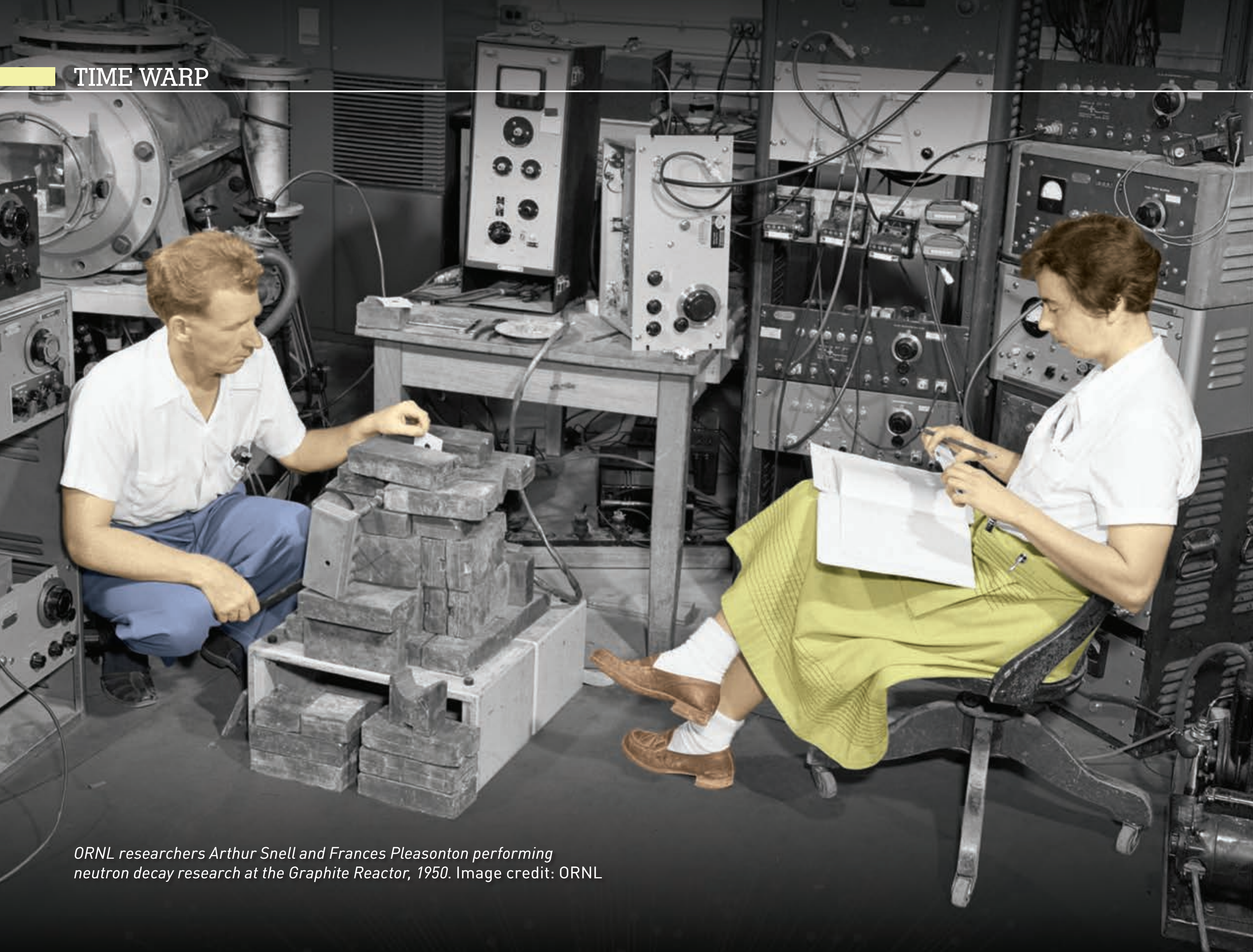
My research is centered on the development of ultraconductive copper composites with Dr. Tolga Aytug and scalable antibacterial filters with Dr. Kashif Nawaz. Integration of UCCs in energy systems is expected to increase energy efficiency. The antibacterial filters will play a crucial role in enhancing indoor air quality and mitigating the risk of respiratory infectious diseases.

What would you like to do in your career?

I aspire to make a positive impact on global challenges, including climate change, ecology, energy crises and future pandemics, through conducting R&D. While my primary focus is advanced material development, I am eager to contribute across diverse research areas to assist others and create meaningful solutions for pressing world issues.

Why did you choose a career in science?

I am driven by the exhilaration of continuous learning and the energy derived from conducting research. Devoting myself to science and contributing to solutions for global challenges fills me with pride and brings me immense satisfaction. Additionally, sharing my profession with my son to foster his interest in science is very uplifting.



ORNL researchers Arthur Snell and Frances Pleasonton performing neutron decay research at the Graphite Reactor, 1950. Image credit: ORNL

Physicist Frances Pleasonton joined early ORNL studies of the neutron

by Bill Cabage
cabagewh@ornl.gov

The old photos show her casually writing data in a logbook with stacks of lead bricks nearby or sealing a vacuum chamber with a wrench. ORNL researcher Frances Pleasonton was instrumental in the earliest explorations of the properties of the neutron as the then-named X-10 site was finding its postwar footing as a research lab.

Neutrons are one of two particles found inside an atom's nucleus, along with protons. In 1950, Physics Division Director Arthur Snell reported that he and Pleasonton had measured beta decay in neutrons, a process in which the subatomic particles — naturally short-lived outside the stability of a nucleus — emit a proton and an electron.

Pleasonton joined the project under inauspicious circumstances. Snell had been working with colleague Leonard Miller, and the two used the lab's Graphite Reactor — the world's first permanent nuclear reactor and only its second nuclear reactor of any type — to observe the decay by focusing a neutron beam. After publishing that observation, they intended to measure the decay, but Miller died in a vehicle accident.

Snell then enlisted Pleasonton and fellow physicist Reuben McCord to build a detector to count neutron decay products.

In an article headlined "Proof of Neutron's Radioactivity Obtained by Physicists at ORNL" from September 1951, Snell described how he and Pleasonton "opened a hole in the 7-foot-thick concrete shield" of the Graphite Reactor. "A stream of neutrons then came through the hole in a well defined beam."

In the early 1930s, neutron discoverer James Chadwick had realized that neutrons were slightly heavier than protons. He theorized that neutrons could turn to protons through radioactive beta decay. Snell, Pleasonton and McCord's complex experiment essentially confirmed Chadwick's prediction.

"The observations we have been able to make appear to us to constitute experimental proof beyond reasonable doubt that free neutrons are not 'fundamental' particles, but that they spontaneously transform themselves into protons," Snell wrote in the ORNL publication Lab News. He estimated neutron half-life at 10 to 30 minutes. Researchers are still trying to pin down the exact half-life.

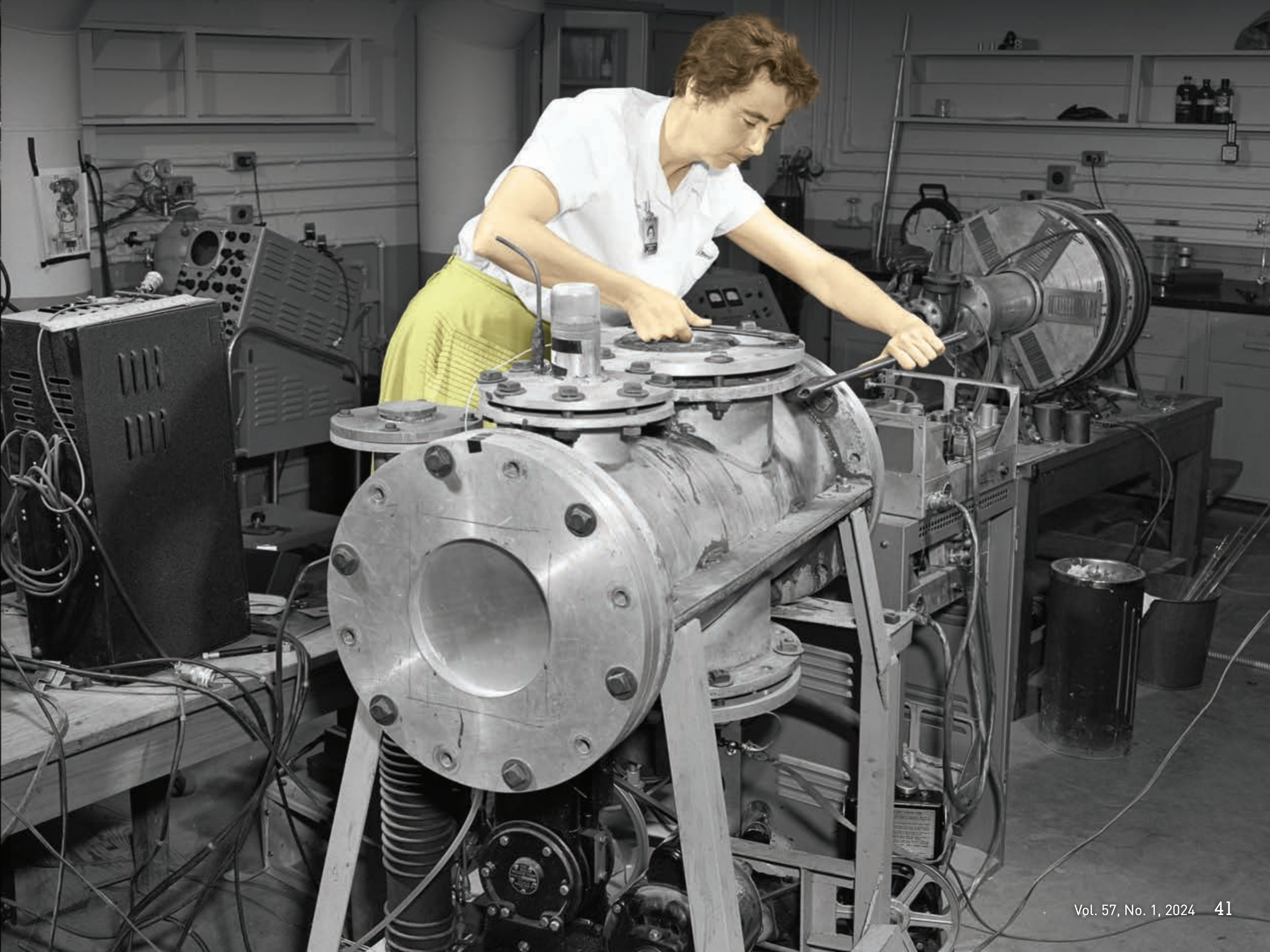
Snell valued working with Pleasonton.

"While I was director of the Physics Division (early 1950s), the bureaucracy had not matured, and I had time to leave the office and join my able colleague, Frances ("Tony") Pleasonton in our experimental laboratory," he wrote in 1985 in the journal *Nuclear Science and Engineering*.

Snell then describes two pursuits: the observation of neutrino recoil and charge spectrometry of radioactive rare gases, of which he wrote, "The charge spectra were qualitatively new; nobody had seen them before, and Tony and I were quite excited in seeing them for the first time."

Pleasonton authored and co-authored a number of scientific publications. In 1958, she and Snell studied the decay of the helium-6 isotope and confirmed the electron-neutrino theory of beta decay. After retiring from the laboratory, she remained in Oak Ridge and was active in local environmental causes. She died in 1990.

ORNL researcher Frances Pleasonton performing neutron decay research at the Graphite Reactor, 1950. Image credit: ORNL



Welcome to Research Insights

Additive Manufacturing the Future Part II: Improving the Process

ORNL Review is pleased to present the sixth issue of *Research Insights*, a collection of research articles from our scientific and technical staff. *Research Insights* was created to showcase the world-leading science being performed at ORNL, with each issue addressing an important theme.

This issue highlights recent advances by ORNL staff in additive manufacturing. During the last decade, ORNL has developed a substantial fundamental and applied research program as part of our Additive Manufacturing Initiative. Within this initiative, ORNL is working to improve energy-efficient metal and polymer additive methods, reduce the wastage of feed materials, attain properties compa-

rable to conventionally manufactured parts, lower cost, develop rapid prototyping and sustainable recycling, create automated manufacturing and tools for in-situ monitoring, take novel 3D-printing approaches, improve functionality, and create new high-efficiency applications.

Articles in this issue of *Research Insights* reflect these efforts, addressing technologies that focus on digital design and parts qualification of large-scale AM processes through controlled microstructure, distortion, and residual strain/stress prediction for improved process efficiency; slicer software for improved pathing and visualization of the additive process; fabrication and testing of ebeam melting of Titanium-vanadium alloy for turbocharger turbine wheels; AM digital twin with machine learning and simulation towards improved AM processing; design of new aluminum alloys for AM processing through detailed microstructural characterizations; and rapid X-ray tomography studies for understanding and improving AM methods.

The articles presented in this issue of *Research Insights* represent a small fraction of the ORNL research portfolio dedicated to helping achieve the nation's AM goals. We hope that you enjoy reading about the exceptional work being performed by ORNL staff.

Next-gen pathing and visualization for industrial additive manufacturing

M. Borish

Manufacturing Science Division

borishmc@ornl.gov

INTRODUCTION

The manufacturing industry is far from static. In fact, it is currently in its fourth revolution, Industry 4.0 [1]. This revolution is primarily characterized by a rise in smart manufacturing as represented by the continued digitization of manufacturing coupled with cutting-edge technologies such as sensor feedback, data analytics, and machine learning. One specific technology described in Industry 4.0 is additive manufacturing (AM), more commonly called 3D printing.

Oak Ridge National Laboratory's Manufacturing Demonstration Facility (MDF) focuses on developing AM technologies for industrial applications. One well-known example of an industrial AM machine at the MDF is the Big Area Additive Manufacturing (BAAM) system [2] shown in Figure 1, which is recognized for its construction of the world's first 3D printed car. The BAAM is a large-format, gantry-style polymer system like the small desktop systems familiar to most people, but scaled up to a much larger size.

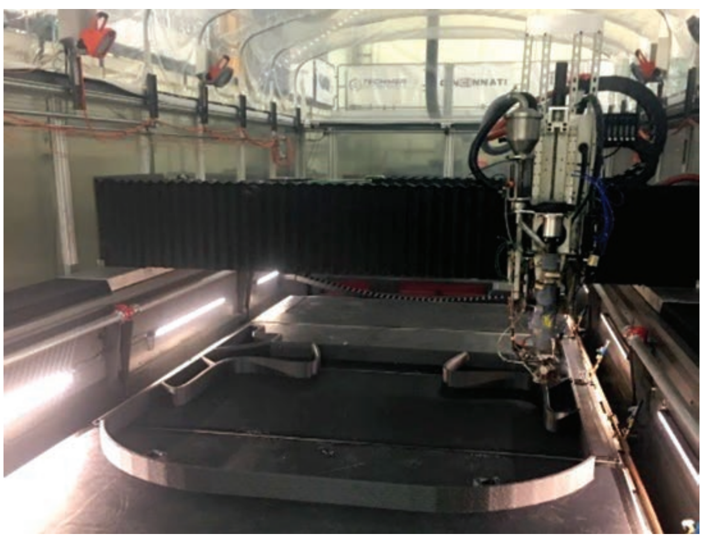


Figure 1. BAAM—interior example of large-format gantry-based 3D printer. (Credit: Borish, ORNL).

Like other industrial AM machines, the BAAM system is the result of significant technological progress, especially in the area of hardware development. However, despite the development of many impressive AM machines, software development for AM has lagged, and each stage of the object construction pipeline is lacking in software support. As a result, software support for AM is now a major area of research.

Slicing software is one such form of software support. Slicing is the fundamental AM process that converts a digital 3D object into g-code, which is the standardized human-readable format for the machine commands used to build an object. Since the advent of AM technology, the slicing pipeline has been the same. First, a 3D object is created using computer-aided design (CAD) software. The CAD representation is then exported as a stereolithography or STL file, which is a triangulated representation of the object's surface. The STL file is then imported into slicing software, which converts the object into a series of layers and fits the machine motions, called paths, to each layer.

The slicing process generally has three steps: cross sectioning the object at a specific height, fitting paths to the resulting 2D cross section, and optimizing the planned paths. These steps are repeated until the entire 3D object has been cross sectioned, resulting in the layers characteristic of 3D printing. The paths produced from these steps are then translated to g-code commands and written to a file. Finally, the g-code file is input into the appropriate machine, which should construct the originally designed object.

This pipeline has several issues, one of the largest being the sequential monolithic workflow. From design to construction, there is no feedback or iteration. In AM, this can be an issue because slicers assume a perfect construction process when evaluating geometry and fitting paths. In reality, the construction process is far from perfect. There are many variables beyond object geometry that play roles in 3D printing. This disconnect between slicing and reality has led to the colloquial phrase, "slice and pray."

Another major issue is the representation of geometry. Most 3D printing should really be called 2.5D printing because it is a stack of 2D paths without any real information about the third dimension. As a result, truly controlling the geometry of 3D printed objects can be challenging. Furthermore, because STLs are composed of triangles, they provide a faceted approximation of smooth surfaces. If an object has curvature in CAD, then that information is lost when converting to an STL. This presents a challenge when constructing objects with smooth surfaces or contours.

To address these and other challenges, slicing software must evolve and be designed with the next generation of hardware in mind. To that end, the MDF has been developing ORNL Slicer 2.0 (Slicer 2), which is currently used by nearly 60 organizations spanning government, academia, and industry. This software package incorporates new design principles to overcome the shortcomings of traditional slicing packages and also

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supports experimental research conducted at MDF. This article examines the design of Slicer 2 and its impact on the object construction pipeline.

A NEW SLICING PARADIGM

The first challenge for any next-generation slicer is to overcome the traditional sequential pipeline. Slicer 2 represents a new slicing paradigm in which the slicer is an active participant in the construction process, replacing the sequential process with an iterative one by incorporating sensor feedback [3]. This system allows construction that would otherwise be impossible and enables true path replanning based on feedback. This new paradigm is referred to as "slice on demand" or "slice on the fly" and is illustrated in Figure 2.

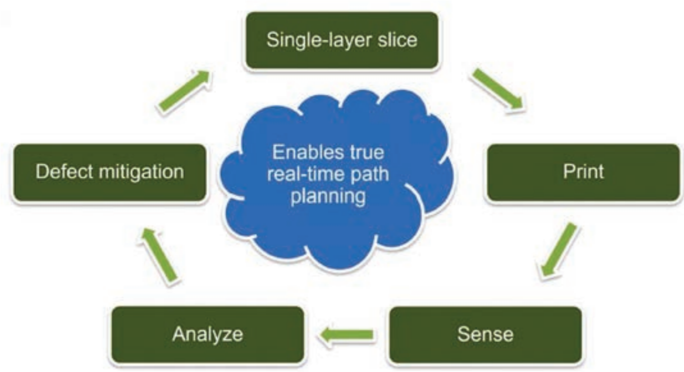

Figure 2. Slice-on-the-fly workflow. The slicer is involved with the construction process and feeds sensor input back into subsequent pathing decisions. (Credit: Borish, ORNL).

In this new paradigm, the slicer produces only the commands immediately necessary for the beginning of construction rather than producing all the commands as a single monolithic g-code file. For example, Slicer 2 can produce a single layer of pathing commands and then feeds this information to a machine's control system. The machine then constructs this layer, uses sensors to inspect the layer, and then feeds the layer information back to Slicer 2 for subsequent pathing. This method introduces adaptability to the slicing process that was impossible to achieve with traditional slicing.

That adaptability enables some of the experimental AM machines currently at the MDF, such as the rotary powder bed system shown in Figure 3 [4]. Unlike traditional AM machines that use a gantry or robotic arm to move, a rotary powder bed system uses a continuously rotating donut-shaped table. The continuous spinning allows much faster construction than traditional machines, thereby overcoming some of the tradeoffs between the size and resolution of an object that are typically inherent to AM. Generally, as an AM machine scales up in size, the resolution of the machine scales down because the layer height increases. However, a rotary powder bed system can build large objects with a very high resolution because its speed allows the addition of more layers instead of increasing each layer's height.

Such a system requires an enormous amount of g-code to build large objects because of the number of layers involved. The traditional sequential slicing approach would require hours to generate the necessary pathing. Therefore, the slice-on-the-fly paradigm is necessary; a single rotation's worth of g-code can be computed, optimized, and output in a second.

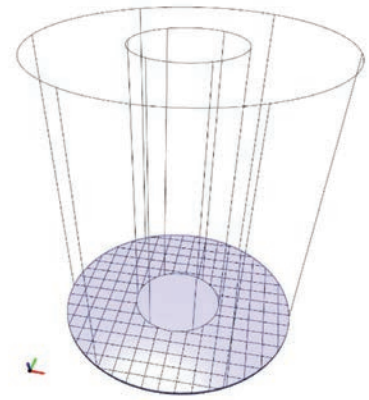

Figure 3. Rotary powder bed fusion volume visualization. The torus rotates to allow construction by lasers placed on opposite sides of the volume. (Credit: Borish, ORNL).

Naturally, to allow such capabilities, the slicing software package must have networking functionality to connect to other pieces of software and accept information. Thus, Slicer 2 is not just a standalone software package, but rather, it is one piece of a software ecosystem. The most obvious component of this ecosystem is sensor feedback, which helps overcome the slicer's assumption about the "perfect" nature of the build process. However, this ecosystem is not composed entirely of machine and sensor feedback. Slicer 2 is pushing the boundaries of geometry evaluation by connecting to other relevant software. For example, Slicer 2 can incorporate simulation information such as data from a finite element analysis to optimize pathing with considerations for thermal energy and stress.

In general, the adaptability and connectivity built into the slice-on-the-fly paradigm provide critical support for advanced manufacturing research. Additionally, slicers that use this paradigm can be seen as a platform or service as opposed to a singular piece of software, ultimately increasing the potential for novel AM software support.

HUMAN–COMPUTER INTERACTION

One novel form of AM software support enabled by Slicer 2's connectivity involves integration of human–computer interaction research. Like most technologies, AM has many problems associated with equipment operators. For example, the large number of variables that affect a 3D print make the operation, calibration and maintenance of 3D printers difficult. Equally difficult is the transfer of that knowledge to new operators. For many metal-based AM systems, this difficulty is compounded by the fact that the view of the current print must be occluded owing to the energy from the lasers or welders. Furthermore, many AM processes are now paired with a subtractive process such as milling or lathing and are often occluded by the coolants and fluids that keep the object cool while the subtractive processes are applied.

All these issues revolve around the need to transfer domain knowledge from the expert to the novice or the need to provide contextual and situational awareness to the user. These problems fall under the umbrella of workforce development, and Slicer 2 can specifically address this broad topic via connectivity with augmented reality solutions.

The Sensory Assistive Manufacturing Augmented Reality Artificial Interface (SAMARAI) project is an alternative way to visualize the information produced from Slicer 2 [5]. SAMARAI uses augmented reality to display relevant and spatially important information such as machine feedback or the pathing the machine will take for construction. A simple example is shown in Figure 4.

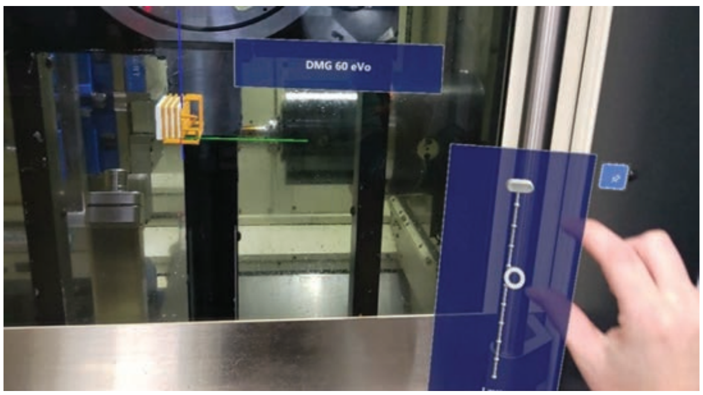

Figure 4. Example visualization of SAMARAI view. The stock to be machined is represented as the white block, and the yellow segments surrounding it represent the G-code pathing. (Credit: Borish, ORNL).

SAMARAI aims to standardize visual communication of information, just as g-code standardized the readability of machine commands. Information on the machine's status can be incorporated into the visualization to provide a clearer view of what is happening during construction. Moreover, various procedures that can be conducted on a machine—such as calibration or maintenance—are all merely a sequence of steps that can be illustrated using media, perhaps via combinations of visualized objects, text, audio, or video.

There is no reason that this information must only be viewed by local users. SAMARAI and its connectivity to Slicer 2 provide the possibility of remote collaboration. For example, an object designer may be using CAD/Slicer 2 at some remote location while the user or technician running the machine receives the g-code visualization overlaid onto the machine at a different location.

Ultimately, this visual feedback can be used to help users take nonintuitive steps to successfully complete construction of an object. For example, many hybrid systems have acoustic sensors, and specific pitches gathered by these sensors indicate build status to expert users. However, novices may not react the same way. Certain pitches indicate that the mill needs to be quickly moved into the object, but the instinctual reaction of a novice is to slow down and move away, which causes the tool to snap because of the forces involved. By introducing contextual visualizations, the hope is to allow novices to react more like experts.

These examples are just some of the problems faced by users of AM and subtractive technologies. These user-focused problems will only continue to increase as AM processes grow more complex. Software solutions like SAMARAI can help bridge the gap between design, path planning, user feedback, and visualization.

ADVANCED PATHING SOLUTIONS

Traditionally, 3D printed layers are produced by a horizontal plane intersecting an object at various heights. This approach has functioned well, but it is limited. A natural extension is to allow the intersecting plane to be rotated and applied along any axis. This strategy is called off-axis slicing and allows construction at any angle along any axis. An example is shown in Figure 5. This style of printing is particularly useful for new types of AM machines called belt-fed printers. Such printers have a rotary belt instead of a static build table, which allows potentially infinite printing because the belt can continuously offset the printed object. Building at an angle and rotating this belt allows objects much longer than the volume of the machine to be built.

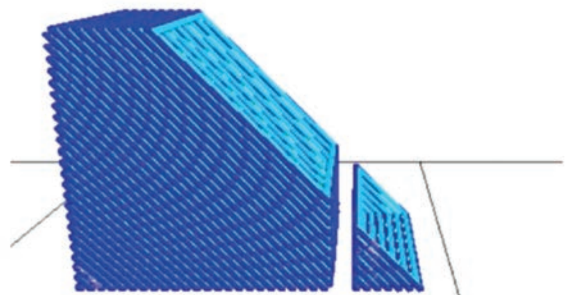

Figure 5. Example printing of a cube at a 45° angle down the x-axis. (Credit: Borish, ORNL).

The next obvious evolution is to move away from planar techniques. Nonplanar construction has been achieved via conformal mapping. A conformal map is a conversion from a curved to flat surface and is a form of texture mapping. Texture mapping is used by computers for various applications, such as video games. A real-world analogy is illustrated by the concept of wrapping a present with gift paper and then unfolding that gift paper to be flat again. By doing so, each point on the surface of the gift is mapped to a point on the paper. In terms of slicing, conformally mapped pathing exploits all the strategies available in 2D and then uses this mapping to apply the pathing in 3D (Figure 6).

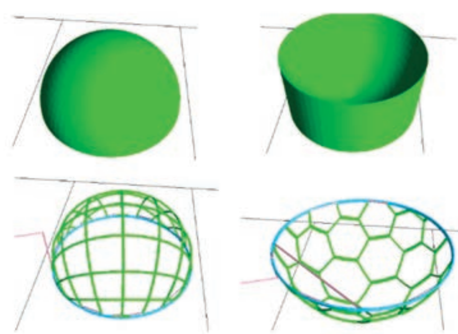

Figure 6. Conformal map of top surface used to transform pathing to match the surface. (Credit: Borish, ORNL).

Finally, there is the push to move away from the concept of layers and planes entirely. The newest representations include a voxelization of the object for the slicing process. By using such a representation, along with computations called level sets, it is possible to reconstruct curvature information that was lost in the conversion to an STL. An example is shown in Figure 7. This method is very important for subtractive operations because milling processes perform best using smooth sweeping motions. Such a representation also aids in the construction of objects with smooth surfaces or contours. An additional benefit is the ease with which sensory feedback information can be applied to 3D models. Such sensors typically rely on computer vision algorithms, and data from such algorithms are often represented as voxels. If both the model and sensory feedback information are represented in voxels, then the slice-on-the-fly paradigm can be more easily implemented.

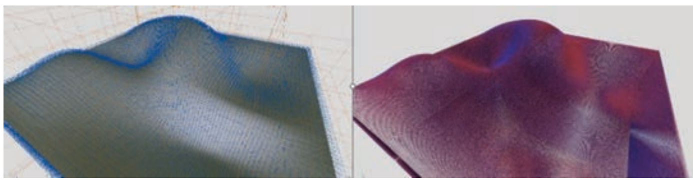

Figure 7. Object voxelization (left) and curvature computation using voxelized representation (right). (Credit: Borish, ORNL).

Ultimately, the problems and research presented here are only a small portion of the software issues that affect additive and subtractive manufacturing. As presented, this work touches on numerous disciplines within computer science. Significant work must be done to create a more integrated pipeline beginning with object design and progressing through construction and beyond. Staff at the MDF work constantly to push the bounds of AM to encourage the new paradigms described here.

COLLABORATE WITH ME

M. Borish, 850-543-4592, borishmc@ornl.gov

ACKNOWLEDGMENTS

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Fabrication and engine testing of additively manufactured prototype turbocharger turbine wheels from Ti-48Al-2Cr-2Nb Alloy

E. Cakmak[1], F. Medina[2], P. Singleton[3], J.A. Haynes[1]

[1]Oak Ridge National Laboratory Materials Science and Technology Division, [2]University of Texas at El Paso, [3]BorgWarner Turbo Systems

cakmake@ornl.gov

INTRODUCTION

Titanium aluminide is an intermetallic alloy with high specific strength, good corrosion and oxidation resistance at relatively high temperatures (up to approximately 700°C–800°C) and excellent strength retention up to the brittle-ductile transformation temperature (~800°C). These attractive properties are particularly important for high-temperature rotating components such as gas turbine blades [1–4] and turbocharger turbine wheels [5–8] wherein the lighter material reduces the inertia for rotation [6,9] and the weight of the components. For instance, when traditional Ni-base superalloy turbocharger turbine wheels are replaced with TiAl, weight can be reduced by 40% to 50%, improving acceleration response and decreasing exhaust emissions and energy consumption (hence increasing fuel efficiency) [8–10]. Furthermore, the lighter wheel decreases spool time, thereby improving transient response and reducing turbo lag in such vehicles where this alternative material can be used, and it also reduces bearing friction [11].

Manufacturing TiAl is challenging, which has hindered mainstream adoption of this lightweight, high-temperature material. Complex, higher cost casting methods are necessary, and casting yields are typically low because of the limited defect tolerance of these intermetallics. Furthermore, the brittle nature of TiAl alloys at low temperatures makes it difficult to machine them into complex shapes. However, additive manufacturing, or AM, has the potential to revolutionize manufacturing of intricate components from TiAl alloys. The preliminary work in a previous U.S. Department of Energy Vehicle Technologies Office Propulsion Materials Program exploratory effort [12] established a baseline understanding of the relationship among build parameters, microstructure and mechanical properties for Ti-48Al-2Cr-2Nb alloys additively manufactured by electron beam melting, or EBM, and confirmed that this material and processing method provides properties that exceed requirements for targeted turbocharger applications. EBM is a powder bed AM method wherein the powder material is raked onto a build table, and an electron beam is scanned over the bed to melt the powder in a pattern. The build table is then lowered by a layer's depth, a new layer of powder is raked, and the process is continued until the part is fully built.

In this work, the ORNL Materials Science and Technology Division partnered with BorgWarner Turbo Systems, or BW, and the University of Texas at El Paso to produce and test prototype turbocharger turbine wheels out of the Ti-48Al-2Cr-2Nb alloy. Extensive characterization of these wheels was also conducted at ORNL.

BACKGROUND

The turbine wheel design supplied by BW was manufactured at the University of Texas at El Paso with EBM from a Ti-48Al-2Cr-2Nb alloy powder (obtained from Praxair).

Six prototype wheels were built by EBM one at a time at the center of a build plate surrounded by six cylindrical preforms. Figure 1 shows the build schematic. This approach focused the heat on the wheel and prevented cracking during cooldown caused by thermal stress. This approach is not conventional for AM but was necessary in this case because of the brittle nature of this alloy.

Following the build, hot isostatic pressing, or HIP, was performed by Quintus Technologies on the turbine wheels and the cylindrical specimens to minimize the internal porosity and eliminate any microcracks. The HIP process involves application of isostatic pressure via a gas medium in a pressure vessel at elevated temperatures to help close internal defects.

After HIP, the turbine wheels were machined using computer numerical control, or CNC, machines to remove the supports, to surface-finish the bottom, and to cut threads. The fins were then surface-finished using abrasive-flow machining.

To identify the distribution of pores and/or microcracks, 3D microstructural information from as-built and hot-isostatic-pressed samples was collected with a Zeiss Xradia Versa 520 X-ray computed tomography, or XCT, unit. High-temperature mechanical properties were measured using uniaxial tensile testing and low-cycle fatigue, or LCF, testing of specimens machined from the cylindrical specimens.

RESULTS

Sample Build. Additive manufacturing techniques can produce near-net-shape parts, but these parts still require some finish machining. This is particularly true for parts produced using EBM, which have rougher surfaces (like sand-cast parts) than parts produced using laser AM.

Figure 1 shows all the stages of the build process for the turbine wheels: the CAD model stage, the as-printed piece, initial machining and final machining and polishing of the fins with abrasive-flow machining.

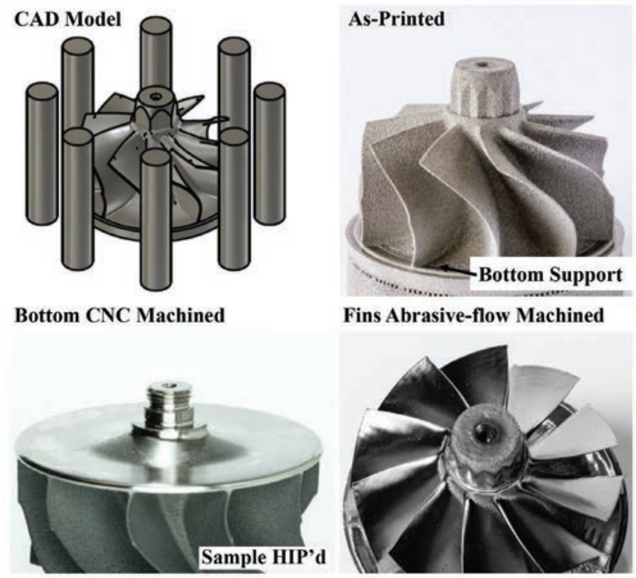

Figure 1. Stages of the turbocharger turbine wheel build process from the CAD model to the finished product. (Credit: C. Jones, ORNL).

As shown in the CAD model, the wheels were surrounded by cylindrical preforms. In addition to helping focus the heat at the center of the build plate, the preforms were later used to machine the mechanical test specimens. The machining steps were performed only after the samples were hot-isostatic-pressed to avoid failure during this step.

Initial density was measured using Archimedes' principle and optical imaging. These measurements showed that an average density of 3.943 g/cm^3 was achieved with a 0.33 vol.% average porosity.

XCT Results. The XCT images are presented in Figure 2. Figure 2a shows a 3D reconstruction of an as-built pillar (modeled using CAD as shown in Figure 1) with pores segmented and highlighted in green. In Figure 2b, a horizontal slice is presented that better shows the pores. AM parts are inherently porous because of gas porosity and lack of fusion. Gas pores are spherical, whereas lack-of-fusion pores are more lamellar.

EBM is performed under vacuum, and thus gas porosity originates from the gas trapped inside the powders. Lack-of-fusion pores are related to build parameters and, as the name suggests, occur because of insufficient melting or fusing. In Figure 2b, most of the pores are gas pores, but lack-of-fusion pores such as the one indicated by the yellow arrow were also observed. From the XCT data, the total pore volume was calculated to be 0.46 vol.%, similar to the values obtained based on analysis of optical images.

The sample was rescanned after HIP, and no pores could be detected within the resolution of the XCT instrument, indicating that full densification was achieved.

Mechanical Testing. Tensile tests were performed at room temperature, or RT, 700°C and 850°C. All of the tests were performed on hot-isostatic-pressed samples because as-built

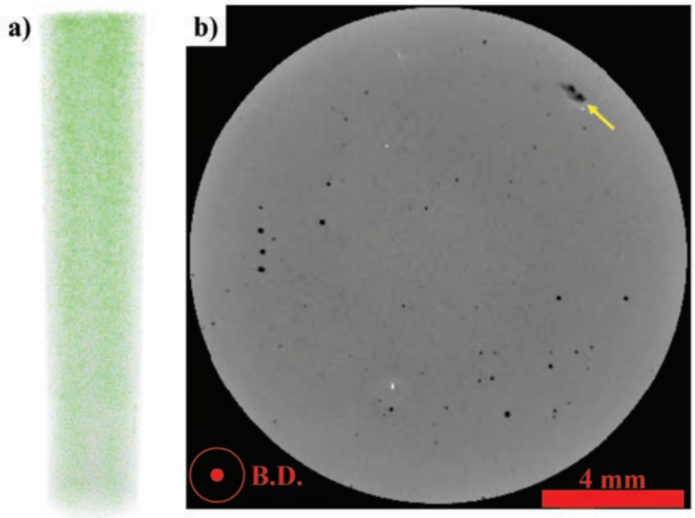

Figure 2. (a) 3D reconstruction of the as-built pillar with pores segmented in green and (b) a 2D horizontal slice of the as-built piece showing the pores in 2D. The yellow arrow indicates a lack-of-fusion defect. (Credit: ORNL).

samples did not show any plasticity resulting from porosity in previous observations [12].

The tensile test results are shown in Figure 3a: the RT-tested sample showed limited ductility as expected from intermetallic alloys. However, the ~2% engineering strain is deemed to be above the threshold necessary for machinability. As the temperature increased to 700°C, the ductility increased (~5% strain at failure) without significant loss of tensile strength (i.e., load at failure). At 850°C, the brittle-ductile transformation temperature was reached, and the sample failed at ~50% strain but at half the required stress compared with RT.

In Figure 3b, LCF results are shown from three samples. Two of the tests were finished before failure, and one was driven to failure. Testing was performed at 820°C (close to the expected operating temperature of the turbine wheel) under 240 MPa stress amplitude. Initially, an upper limit of 1 million cycles was established, but after the first sample reached 700,000 cycles, the grips on the test frame failed. The next specimen was tested to 1 million cycles and did not fail, so a third sample was tested to failure, which occurred at ~2.3 million cycles, far past the expected limit.

Duty-Cycle Testing. Two of the turbine wheels were shipped to BW for dimensional tolerance and duty-cycle testing. The duty-cycle testing will involve testing of the turbine wheel in an actual working environment in which the wheel will be subjected to the turbocharger's operating conditions. Similar or better results compared with traditionally manufactured turbine wheels will be a success criterion for this work and will enable more AM components to be manufactured for load-bearing applications.

CONCLUSIONS

This project investigates the feasibility of using EBM to additively manufacture lightweight turbocharger turbine wheels, particularly those used in the engines of heavy-duty freight vehicles, from a novel Ti-48Al-2Cr-2Nb intermetallic alloy.

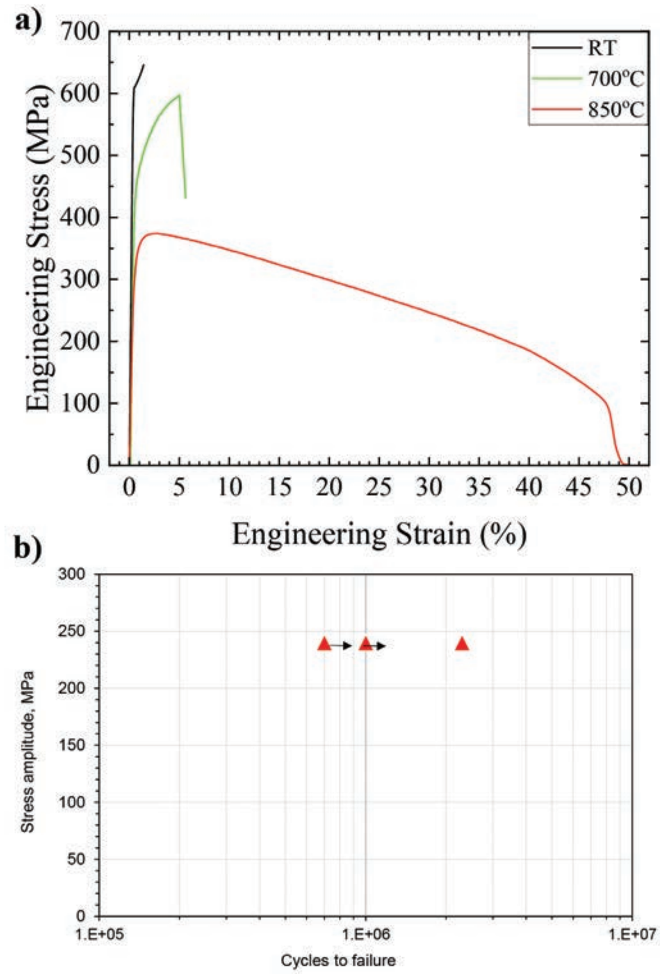

Figure 3. (a) Engineering stress- strain curves obtained from tensile testing of the TiAl specimens at RT, 700°C and 850°C, and (b) LCF data of three samples (shown as triangles) tested at an applied stress amplitude of 240 MPa at 820°C. Arrows indicate tests that finished before failure. (Credit: ORNL).

Prototype wheels were successfully manufactured to near-net-shape and post-processed with HIP to achieve full density. The samples were surface-machined to final shape and shipped for engine duty-cycle testing.

The mechanical and microstructural properties were characterized in detail up to 850°C, revealing acceptable results compared with the traditionally manufactured counterparts.

The project is currently in its final stage wherein successful demonstration of engine duty-cycle testing will be the final acceptance criterion.

IMPACT

This work lays the foundation for the commercial production and application of a difficult-to-cast intermetallic material via the alternative method of AM, resulting in a lightweight, high-temperature engine component that improves engine efficiency in a difficult-to-electrify transportation sector (freight). Longer term, these methods and results can be extended to other efforts to use AM to develop alloys for commercial components with previously unachievable combinations of superior properties and complex geometries, which will enable design of propulsion systems with higher efficiencies and reduced environmental impact.

COLLABORATE WITH ME

Ercan Cakmak, 865-574-6538, cakmake@ornl.gov

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Leveraging supercomputing to speed the development of new additively manufactured parts

G. L. Knapp[1,*], J. Coleman[2], M. Rolchigo[2], B. Stump[2], M. Bement[2], A. Plotkowski[1]

[1]*Materials Science and Technology Division,* [2]*Computational Sciences and Engineering Division*

**knappgl@ornl.gov*

INTRODUCTION

Metal additive manufacturing (AM) is transforming the production of energy-saving components by offering weight savings and performance benefits that surpass traditional manufacturing methods. One of the unique features of AM is its ability to tailor microstructures and alloy chemistries in intricate geometries to meet performance and efficiency requirements of various energy systems. However, designing and qualifying new parts presents several challenges owing to the multifaceted nature of AM [1]. A key issue is the presence of localized variations in the as-built material, even when the same AM system and feedstock material are used. This phenomenon is primarily attributed to fluctuations in melt pool behavior during the build process, which can be influenced by factors such as part geometry, material properties and heat source parameters [2].

Computational modeling can be an effective tool to illustrate the relationships between processing and microstructure evolution in AM [3]. However, the many physical phenomena occur over a wide range of length and time scales, posing significant modeling challenges. This article highlights ORNL's development of computational tools within a digital twin framework and their use to analyze the links between AM processing and material performance.

BACKGROUND

Laser powder bed fusion (LPBF) is a common type of AM process in which small metallic powder particles are melted by a focused laser beam to create a dense part. The microstructure that develops as the metal solidifies is governed by the local heating and cooling cycles. Therefore, prediction of the resulting microstructure requires (1) details of the AM machine operation, (2) estimation of the thermal conditions and (3) a model for microstructure evolution during processing. As described below, a multiscale approach for predicting microstructure distributions in actual AM builds uses a variety of ORNL capabilities. Figure 1 provides a diagram of the approach to generating an AM digital twin.

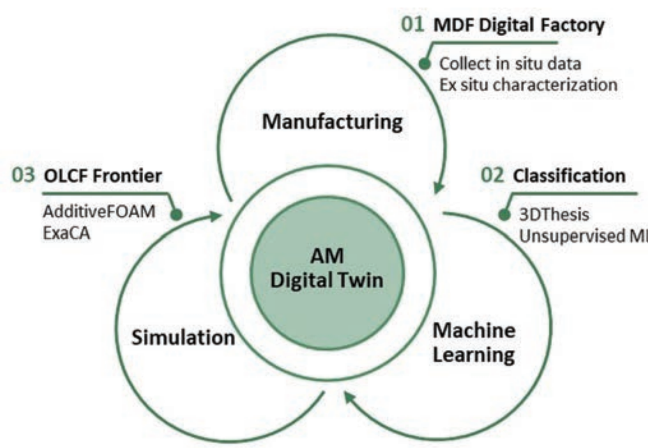

Figure 1. Process diagram of the AM digital twin utilizing ORNL's MDF and the Oak Ridge Leadership Computing Facility (OLCF). (Credit: J. Coleman, ORNL).

Process data. The Manufacturing Demonstration Facility (MDF) Digital Factory ecosystem was leveraged to simulate actual AM builds. The MDF Digital Factory is an interconnected network of AM machines, sensors, data storage, computational resources and software tools for data analysis. This network enables monitoring of AM processes, including the details of the process conditions, in situ process monitoring data and ex situ characterization data [4]. This infrastructure provides the necessary input information to run computational models, the results of which may be combined with experimental datasets for prediction of component quality.

Prediction of solidification conditions. A major challenge in predicting AM thermal conditions is the disparate length and time scales between the laser interaction with the material (~μm) and the heat transfer across the component (~cm), which requires a trade-off between physical fidelity and computational cost. To address this challenge, two distinct simulation approaches were developed at different model fidelities: 3DThesis [5–7] and AdditiveFOAM [8,9]. 3DThesis is an open-source code that uses a simplified representation of the heat transfer problem to approximate the conduction-driven heat transport such that the solution is computationally inexpensive. AdditiveFOAM uses a more detailed numerical model implemented within the OpenFOAM computational fluid dynamics framework, providing a more accurate representation of interactions between the laser beam and the material. This facilitates a more direct correlation between process parameters and the resulting solidification conditions.

Solidification microstructure. Using the thermal history predicted by process modeling, the solidification microstructure is determined by ExaCA, an open-source cellular automata model [10,11] that tracks the advancement of metal crystals in the wake of the melt pool using a rules-based approach. ExaCA predicts explicit representations of the as-solidified grain structure from which grain shape, size and crystallographic orientation distributions can be extracted. These modeling capabilities provide insight into how different processing parameters can affect the resulting microstructure and ultimately the mechanical properties of the printed part.

Leveraging ORNL supercomputing. Each of the codes described here uses ORNL's state-of-the-art computing resources to predict the melt pool behavior and resulting microstructure in AM-printed parts. AdditiveFOAM and ExaCA were developed as part of the Exascale Additive Manufacturing Project (ExaAM) [12], an initiative of the Exascale Computing Project that focused on development and validation of AM modeling tools and their use of exascale computing resources. These models can draw on the computing power of Frontier, the world's largest and fastest supercomputer, while also being portable to other high-performance computing resources.

RESULTS

Build-scale thermal predictions. Scan paths and process conditions from a Cr–Ni–Mo austenitic stainless steel (SS316L) build from a Concept Laser M2 LPBF machine were extracted using the MDF Digital Factory infrastructure, and 3DThesis was used for layer-wise heat transfer simulations of 36 parts printed under different processing conditions. The solidification temperature gradient, an important parameter for predicting the resulting microstructure, was then calculated from these simulations (Figure 2). Differences in the temperature gradient are apparent for different parts, providing an estimate of which parts may have the most different microstructures. These thermal data are registered to the build plate coordinate system, enabling correlation with experimental features observed in situ and via postprocess characterization and testing.

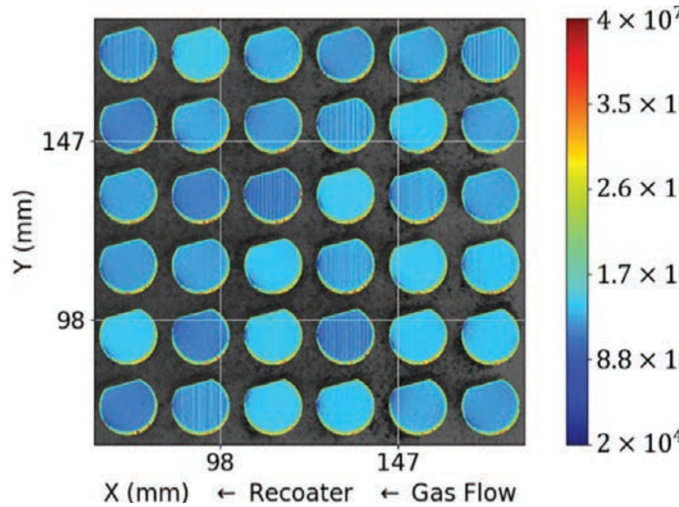

Figure 2. Layer-wise temperature gradients (K/m) predicted by 3DThesis, imported into the Peregrine AI software, a component of the MDF Digital Factory. (Credit: J. Stump, G. Knapp, ORNL).

Classifying build-scale thermal behavior. The thermal gradient distributions shown in Figure 2 are only ones of a variety of outputs of interest generated by 3DThesis across the build scale. Although trends in these thermal conditions are reasonable, the conditions are not sufficiently resolved for accurate determination of microstructure. Therefore, localized representative volume elements (RVEs) must be selected for higher fidelity thermal simulations using AdditiveFOAM. These regions were identified using Gaussian mixture models (GMMs), an unsupervised machine learning algorithm that divides data into distinct groups that are internally self-similar. The 3DThesis thermal data were classified in two steps. First, local solidification clusters were calculated using the GMM based directly on the thermal behavior at a length scale smaller than that of the melt pool. However, because microstructure also depends on regional interactions between these local conditions, these clusters were further grouped into supervoxels, and a second iteration of the GMM algorithm was performed to assemble regional clusters (Figure 3a). This two-stage classification method effectively considers both the solidification conditions and their regional interactions on the scale of multiple melt pools and layers.

The classification process yields a representative set of thermal behaviors that are self-similar but distinct from each other. The final regional clusters may then be mapped spatially back to the part to identify regions for detailed characterization and RVEs for higher fidelity simulations. This approach was validated by measuring the experimental crystallographic orientations using electron backscatter diffraction (EBSD) for specific locations identified by the clustering algorithm (Figure 3b), indi-

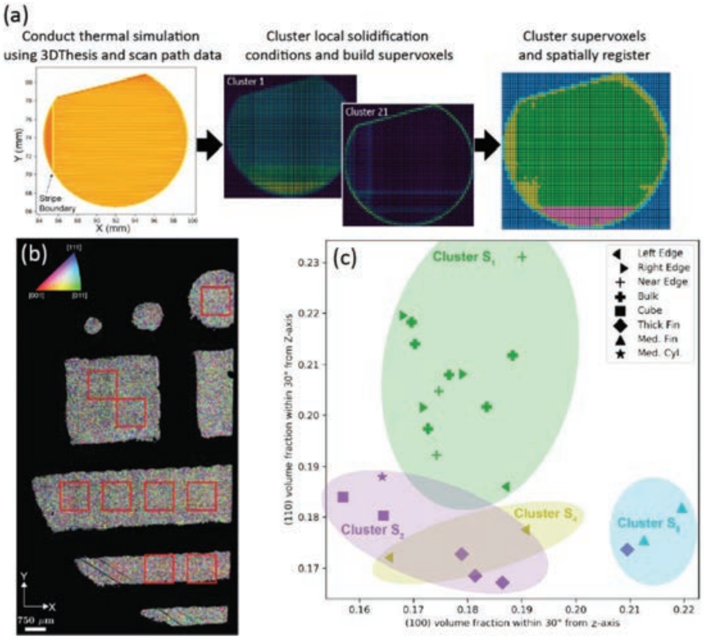

Figure 3. (a) Thermal data classification procedure flowchart, (b) example experimental data for grain structure and (c) clusters identified by the relationship between the local thermal gradient orientations with respect to two reference orientations. (Credit: G. Knapp, A. Plotkowski, ORNL).

cating that similar, distinct textures corresponded to the clusters (Figure 3c).

Detailed prediction of AM microstructures. The clustering analysis results were used to select RVEs for which AdditiveFOAM and ExaCA simulations were performed. An example of this approach is shown in Figure 4, corresonding to the bottom-right part shown in Figure 2 for a 1 × 1 × 0.5 mm RVE. An AdditiveFOAM simulation predicted the thermal conditions and incorporated the part geometry, dynamic behavior of the laser interactions and nonlinear thermal effects (Figure 4a). The simulation was significantly accelerated by locally refining the mesh only within the region immediately surrounding the selected RVE. The results of this simulation describe the thermal conditions at each location within the RVE during the solidification process. These data are stored in a reduced format that minimizes the necessary data transfer required for microstructure predictions.

The grain structure resulting from printing 20 layers of deposited material was then simulated using ExaCA based on these solidification conditions (Figure 4b). The RVE is large enough to produce statistically significant numbers of grains from which pole figures and inverse pole figure maps may be constructed (Figure 4c). This procedure was repeated for the other RVEs identified by the clustering analysis, providing a complete dataset describing the variability in the component's microstructure, which may be spatially mapped to the correlate with complementary in situ sensing or postprocess characterization data.

CONCLUSIONS

The modeling framework presented in this study offers a powerful tool for gaining valuable insights into the microstructure and performance of as-built AM parts. By directly interfacing with in situ data from powder bed fusion AM builds and leveraging

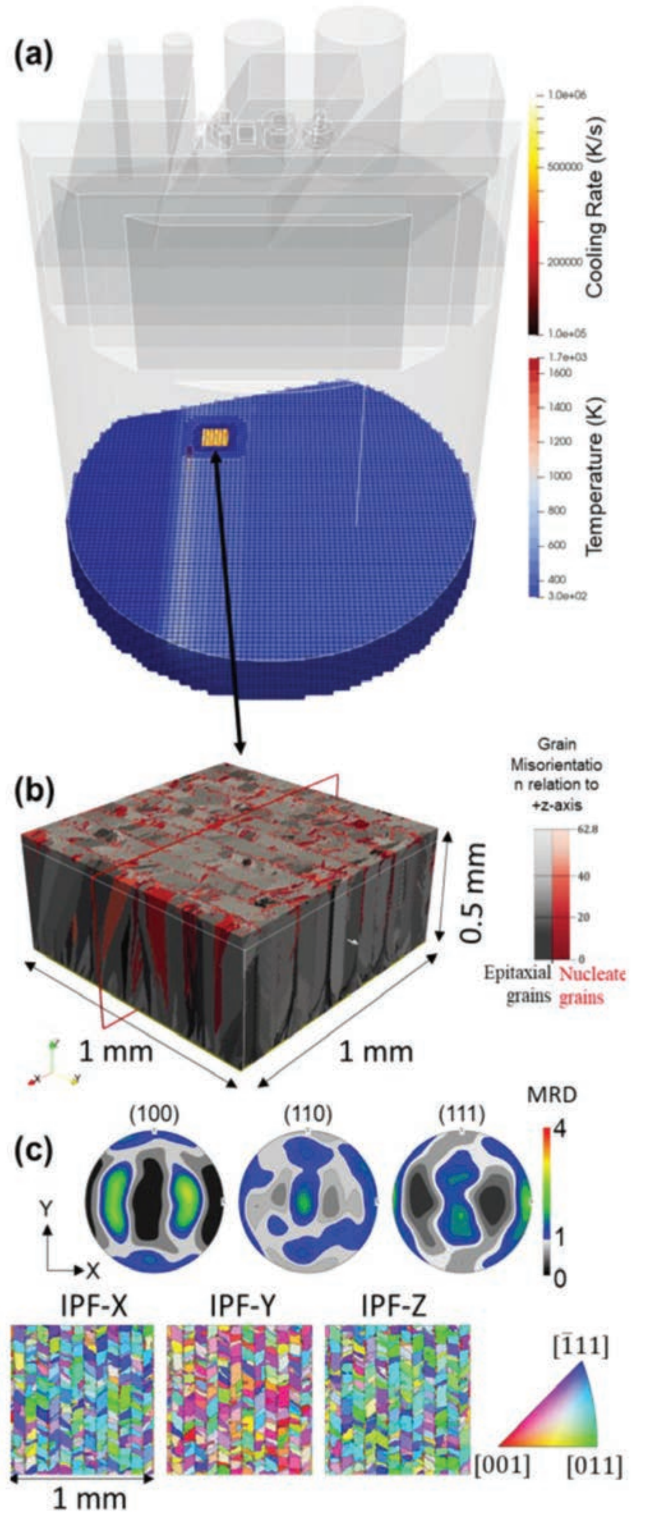

Figure 4. Simulating the microstructure for a region within a real part. (a) The in situ scan path data for a real part geometry (gray geometry) are extracted from the MDF Digital Factory platform and fed into the AdditiveFOAM melt pool solver. (b) Solidification data from the melt pool solver are passed to ExaCA, a solidification microstructure model, to predict (c) an explicit description of the as-solidified grain structure along with the corresponding inverse pole figures (IPFs) – quantified using multiples of a random distribution (MRD) – looking down on the XY-plane. (Credit: J. Coleman, M. Rolchigo, G. Knapp, ORNL).

high-performance computing, this open-source software can provide information about thermal evolution during an AM build and its interaction with the melt pool characteristics. These insights can be used to improve defect formation predictions and may help reduce current requirements for extensive experimentation. Continued improvements and automation of this computational tool set could enable prediction of part conditions before printing, thus enhancing the efficiency of AM processes. Overall, this framework represents a significant step toward improving the efficiency and reliability of AM processes.

IMPACT

The computational tools described herein provide valuable insights into AM experiments, offering a promising avenue for developing energy-saving parts. For example, the demonstrated modeling workflow is already being implemented at the MDF to identify appropriate process conditions, avoid defects, understand microstructure variability and increase printing efficiency. Furthermore, the detailed model predictions help define specific mechanisms for the development of unique microstructures in AM and will help to tailor desirable microstructures and even new materials or processes. By incorporating modeling into the Digital Factory ecosystem, the development and qualification of new materials and part geometries will be accelerated using AM.

These tools are readily available as open-source codes to the broader AM research community and are performance portable such that they can run on computing systems ranging from small workstations to the world's largest supercomputers. These features will help enable these tools to accelerate the development and adoption of new AM materials and designs through future scientific investigations.

COLLABORATE WITH US

Gerry Knapp, lead, model integration, knappgl@ornl.gov

John Coleman, lead developer of AdditiveFOAM, colemanjs@ornl.gov

Matt Rolchigo, lead developer of ExaCA, rolchigomr@ornl.gov

Benjamin Stump, lead developer of 3DThesis, stumpbc@ornl.gov

Matt Bement, principal investigator of ExaAM, bementmt@ornl.gov

Alex Plotkowski, senior R&D staff, plotkowskiag@ornl.gov

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Digital Design and Part Qualification for Large-Scale Additive Manufacturing

Y. Lee[1*], S. Simunovic[1], A. Nycz[2], T. Feldhausen[2], P. Nandwana[3]

[1]Computational Sciences and Engineering Division, [2]Manufacturing Science Division, [3]Materials Science and Technology Division

**leey@ornl.gov*

INTRODUCTION

Additive manufacturing (AM) is transforming industrial design and production, supply chains, and material consumption, offering design flexibility superior to that of conventional manufacturing technologies by creating near net shapes with minimal postprocessing. To date, AM technologies have been limited to rapid prototyping and low volume production resulting from the focus on rapid technology development. However, AM processes are transitioning to mass production as the process and part qualification becomes more standardized [1,2] and the cost of AM technology declines. For instance, the average annual growth of the AM market reported by Wohler's associates in 2019 was predicted to increase by greater than 20% over the next five years, projected to reach 35.6 billion USD worldwide in 2024 [1]. Nevertheless, a lack of robust, standardized AM processes [3] is a barrier to the wide market's adoption of AM technologies, with particular limitations in CAD/CAM design, process control, modeling/simulation, part qualification, and real-time data acquisition, as seen in Figure 1.

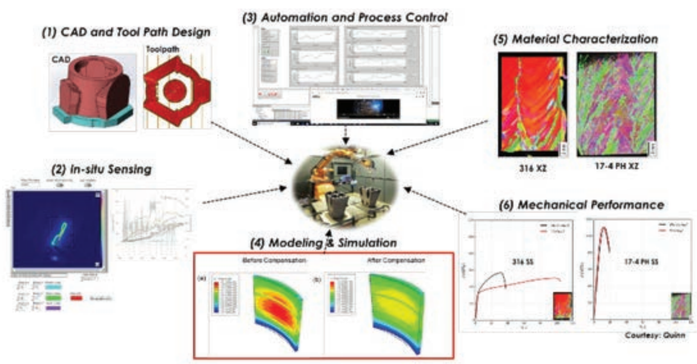

Figure 1. Large-scale AM is a multidisciplinary process including (1) CAD and tool path design, (2) in-situ sensing, (3) automation and process control, (4) modeling and simulation, (5) material characterization, and (6) mechanical performance. (Credit: ORNL).

BACKGROUND

Wire-based direct energy deposition (wire-DED) is gaining popularity to for fabrication of large-scale, near net shape parts. A near net shape part is a first-produced part that is nearly identical to the final part shape. Wire-DED provides a higher production rate than other AM processes, as well as low material cost and high material efficiency. The printable part size can be 10 feet (3,000 mm) tall or more (Figure 2).

Figure 2. Additively printed large-scale parts of ~5–10 ft. (Credit: Lincoln Electric).

However, dynamically varying printing conditions and geometries lead to complex thermal signatures which affect the temporospatial evolution of plastic deformation, thus resulting in internal stress buildup. This can lead to unfavorable part distortion during printing and consequently may cause part failure in critical service conditions. Internal stresses and deformation in large-scale AM scale with part size, so mitigation methods developed for welding and powder bed fusion have limited effectiveness [4–6]. Moreover, knowing the residual stress of an AM fabricated part a priori is necessary in wire-based hybrid (additive/subtractive) manufacturing to ensure that proper machining conditions and dimensional tolerances are used for the final part [7]. Residual stress can be experimentally measured using X-ray or neutron diffraction at ORNL and other facilities. Even though the accuracy of these measurement methods has been proved for many AM fabricated parts, the methods are best utilized for verification and development in computational models. Moreover, measurement is limited to a relatively small area of a relatively small part, so printing multiple parts and taking iterative stress measurements may become infeasible for large-scale part qualification, which may take weeks to complete. This analysis demonstrates methods and workflows for digital design and part qualification for large-scale AM components.

RESULTS

Model development. A practical thermomechanical simulation was developed at ORNL in collaboration with Lincoln Electric and Dassault Systemes [8]. The model was first evaluated on a planar wall to predict and manage temperature profile, distortion, and residual stress in wire-arc DED and then extended to the wire-based hybrid manufacturing. The prediction accuracy in distortion and residual stress was successfully confirmed using neutron diffraction at the high-flux isotope reaction (HFIR) of

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ORNL. We started the large-scale part simulation first and then found microstructure variations corresponding to the thermal cycles from the continuum-scale model. This workflow can result in a practical and rapid process optimization/automation and part quantification for large-scale AM. Additional discussions follow with real-world examples.

Prediction and validation of residual stress. Lincoln Electric used wire-DED to print a thin wall to validate the ORNL-developed thermomechanical simulation. The temperature profile was recorded during printing and used for model calibration. The residual stress was measured at ORNL's High Flux Isotope Reactor (HFIR) and compared to the model prediction [8]. The results agreed well qualitatively and quantitatively in relation to the neutron measurements presented in Figure 3a. The measurements capture the spatial variation of part deformation and residual stresses with high computational efficiency and accuracy. A similar, more advanced validation was made for hybrid manufacturing, as shown in Figure 3b. A wall was printed in five sections that were 25.4 mm tall using an interleaved printing strategy in which machining is conducted immediately after each section is deposited. The unique hybrid process led to development of a comprehensive, practical simulation for realization of fully coupled AM and machining operation with the interleaved printing strategy. This method, which is not available via traditional manufacturing or AM technologies, is presented in experimental literature [7] but not in simulation to because of the difficulty in modeling. The predicted residual strains agree well with the neutron diffraction measurement given in Figure 3b. Spike-like tensile strains developed along the build direction (z-direction), whereas strong compressive strains occurred around the center region. These characteristic features are well documented in the model. In the future, a robust, reliable method for distortion and residual strain prediction could be used widely to qualify and certify hybrid manufacturing.

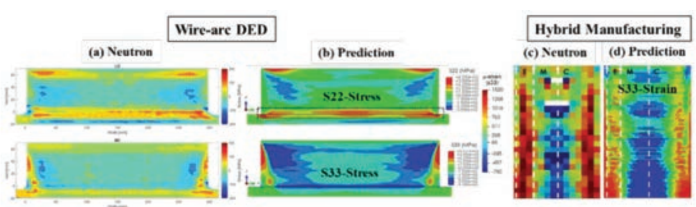

Figure 3. Validation of predicted residual stress to neutron diffraction measurement: (a) stress distributions along x- and z-directions (wire-DED), and (b) strain distribution along z-direction (hybrid manufacturing). (Credits: Nyx et al., Lee et al.).

Transient microstructure evolution. The characteristics of a part's microstructure should be examined to guarantee quality. Experimentally, the part should be sectioned, mounted, and then the scanning electron microscope (SEM) can be used to identify each phase of Ti-6Al-4V, including α and β phases. Additionally, electron backscattered diffraction (EBSD) is used to identify β grain morphology and texture. Although full area microstructure characterization is valuable, it requires a significant amount of time and is not feasible for large-scale parts because of cost and interference with rapid qualification [10, 11]. Therefore, numerical modeling can be an effective alternative to obtain 3D spatial and temporal microstructure information in physical experiments. A realistic thermal cycle from the continuum-scale model was incorporated into the microstructure prediction of Ti-6Al-4V under different process conditions of tool paths and interpass temperatures. Figure 4a shows how the microstructure evolution corresponds to the thermal history. The variation of microstructure evolution can be mapped over the part to create a full linkage of process-microstructure-property-performance. The Ti-6Al-4V can be digitized as α fraction, α lath thickness, β fraction, and β grain size. The information can be transferred to a synthetic microstructure, as shown in Figure 4b, thus linking microstructure to performance simulation for part certification.

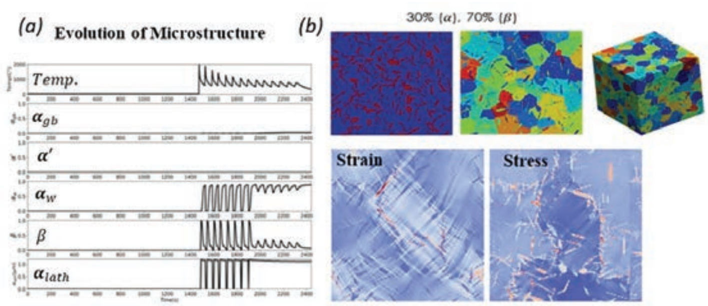

Figure 4. Prediction of microstructure evolution of Ti-6Al-4V: microstructure can be reconstructed based on the digitized characteristic features of Ti-6Al-4V. (Credit: ORNL).

Practical applications of digital design. Developments such as those described above triggered an extension of the prediction capabilities to larger parts (> 2.5 ft^2) with increased geometric complexity, to the use of multi-heat source system (MedUSA) and to emerging hybrid manufacturing methods. For instance, the integration of additive and subtractive models was demonstrated for the first time, to the best of the authors' knowledge, for interleaved hybrid manufacturing with high-fidelity neutron validation. The unique prediction capability opens a new area of process and property design in the hybrid manufacturing process.

Operando. Residual stresses are formed during printing and remain in a part even after printing. In many cases, the residual stresses degrade the part performance and reliability. However, the observation of residual stress evolution during printing is highly difficult not only because of limited accessibility to available facility, but also because of the limited area of measurement. A project recently initiated by laboratory directed research and development (LDRD, principle investigator, A. Plotkowski), performed in-situ residual stress measurement of low transformation temperature (LTT) steel using the VULCAN beamline at ORNL's Spallation Neutron Source. A combined thermo-mechanical phase-transformation model and operando neutron characterization revealed that highly temporospatial variations in thermal and phase transformation result in tensile-compression pattern in an LTT wall build. This demonstrated a pathway to control residual stress distributions through controlling thermal gyration and resultant phase transformation. Figure 5 shows development of alternating tensile-compression stresses with time-evolving phase transformation.

Interactive distortion control in large-scale parts. One major challenge in large-scale AM is management of part distortion. To reduce distortion, an intelligent optimization algorithm was developed using a combined environment of field-emission

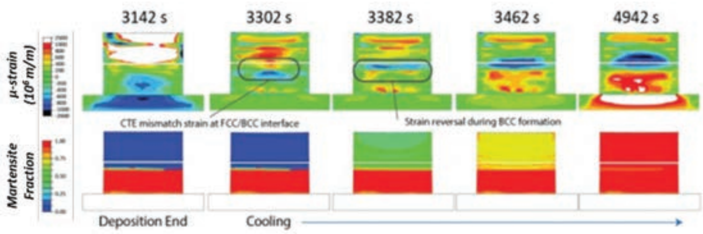

Figure 5. Integrated thermo-mechanical phase transformation model shows development of alternating tensile-compression stresses with time-evolving martensitic phase transformation. (Credit: Plotkowski et al.).

microscopy (FEM) and the Python library to automate and accelerate the distortion prediction and optimization. Another part of SS316L was printed with the STL file format with model-suggested geometry for proof of concept. The resulting wall is shown as compensated in Figures 6a and b. The wall is visually straight, and the maximum distortion was reduced by >75% compared to the original part. The developed framework could be incorporated into the part design process through integration with CAD packages, and it could also be incorporated into the process control frameworks for AM systems. Furthermore, extensions of the algorithm through the use of faster and/or higher fidelity simulations and by leveraging advances in machine learning could further enhance the algorithm's utility for complex geometry as shown in Figure 6c.

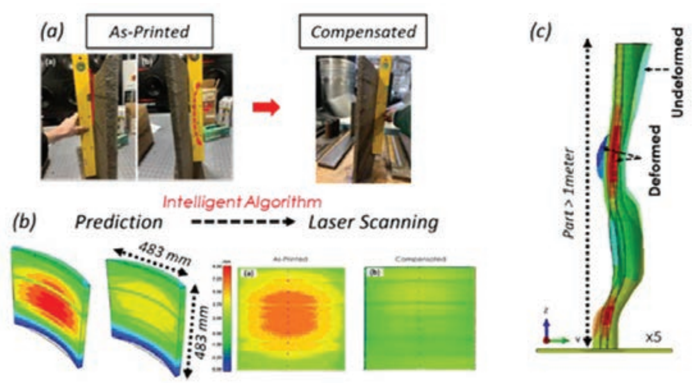

Figure 6. Interactive distortion control using intelligent algorithm: (a) as-printed and distortion compensated wall, concave distortion observed, (b) predicted and measured results (laser scanning) before and after distortion compensation, (c) further extension of distortion mitigation strategy to actual complex geometry. (Credit: ORNL).

Multi-Agent AM System (MedUSA). Many industries have attempted to increase manufacturing productivity by increasing production rate in an existing design with a single robot. However, this approach encounters a serious limit on printing speed. Parallel deposition can be thought of as having multiple robots on a single object. Using this calculation, the printing time becomes 63% shorter when using a multi-agent system (MedUSA at 5,400 s vs. Singe at 14,600 s). In practice, parallel, simultaneous printing is far too complicated to describe here because sophisticated control of process parameters and tool paths must be ensured to avoid robot crashes and to obtain good part quality. For instance, multiple simultaneous depositions occur to fabricate a part or multiple parts within a designated tool path. The tool paths can produce different areas of melting, leading to changes in melt pool physics and resultant thermal conditions in the build. Eventually, the distribution, level of distortion, and residual stress differ from that of a part fabricated with a single heat source. Cylindrical parts were printed to (1) determine the optimal sequence of printing, (2) decide how the tool path is split to each robot, and (3) define the influence of the tool path on part quality. This was accomplished using an identical tool path in each single robot, and multi-robots were employed to set and check distortion using a laser scanner. Although part distortion does not seem to be affected by the number of robots used, further investigation is still needed to determine material property and residual stress distribution. Figure 7 shows (a) the MedUSA system, (b) the heating zone assignment of each robot, and resultant distortion in (c) measurement and (d) prediction.

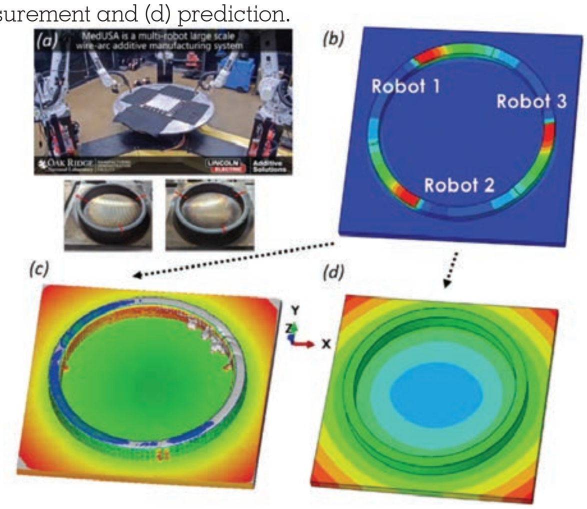

Figure 7. Printing time becomes 63% shorter when using a multi-agent system: (a) multi-agent AM system (Credit: MedUSA), (b) heating zone assignment of each robot, (c) measured distortion, and (d) predicted distortion. (Credit: ORNL).

Interleaved printing strategy in hybrid manufacturing. A simple combination of additive and subtractive operation is not a new concept in the AM industry, because a part produced by wire-DED often requires machining after printing to improve surface quality and part performance caused by fatigue. A distinctive benefit of hybrid manufacturing derives from an interleaved printing strategy not available via traditional manufacturing or AM technologies. The effectiveness of this printing strategy was demonstrated by a 68% reduction of overall manufacturing time compared to the traditional sequential AM and machining process, as well as a 97% reduction in material cost compared to that of CNC machining. Furthermore, this unique printing strategy enables surface machining of internal cooling channels, consequently reducing fluid/gas pressure drop, and it also increases cooling efficiency. A complete analysis of interleaved printing strategy is complicated. For instance, two parts were printed with and without a fillet geometry, as shown in Figures 8a and c; other conditions were identical. The observed microstructure is significantly different: one shows fine equiaxed microstructure (EBSD) and high plastic deformation (kernel average misorientation [KAM]) at the intersection depicted in Figure 8b, whereas neither fine grain nor high plastic deformation is found at the part without fillet shown in Figure 8d. This indicates that machining following fillet printing induces stronger plastic deformation that in turn influences grain recrystallization at activation temperature. These results show enormous potential for geometry-driven microstructure control within identical geometry after machining.

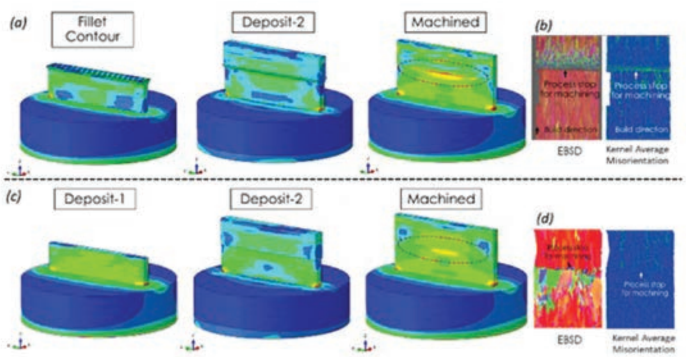

Figure 8. Geometry-driven microstructure control using hybrid manufacturing: (a) printing sequence for a geometry with fillet, (b) fillet geometry: fine equiaxed microstructure and plastic deformation at the interface (EBSD and KAM), (c) printing sequence for a geometry without fillet, and (d) no fine equiaxed microstructure and no plastic deformation at the interface (EBSD and KAM)— different microstructures can be created in identical geometries. (Credit: ORNL).

CONCLUSIONS

A workflow for comprehensive and practical modeling/simulations has been demonstrated for realization of digital design and part qualification in large-scale AM processes. Because printing of a large-scale part requires sophisticated control of part distortions and residual stresses, the thermo-mechanical model was initially developed and validated using neutron diffraction measurement in wire-arc DED and laser-wire hybrid manufacturing. A microstructure evolution model was incorporated into the residual stress simulation and was validated with in-situ neutron diffraction measurement. The results indicate that stress distribution can be manipulated by using LTT steel. The model and intelligent algorithm were coupled and demonstrated for distortion compensation in a large component. Results show that numerical modeling and advances in machine-learning further enhance the utility of this approach for complex part fabrication. A multi-agent AM system in wire-arc DED and an interleaved printing strategy in hybrid manufacturing show promise for high productivity, stress control, and material property manipulation. However, challenges remain in design tool path/printing sequence, in-situ sensing, and lack of understanding the influences of process parameters and geometry on microstructure and mechanical properties. For instance, high hardness of material (e.g., 17-4 PH) increases machining time, but this metric is difficult to know a priori in interleaved hybrid manufacturing. Ultimately, the overarching goal is to develop an integrated, incorporated, practical optimization workflow for the process control / design stage to allow for tailoring material/mechanical properties and digital design using computational models, experiments, and data analysis.

IMPACT

A robust, reliable method of microstructure, distortion, and residual strain/stress prediction has wide applications for enhancing AM design efficiency. The workflow described here for large-scale component design and analysis presents a unique opportunity to redesign and qualify AM control processes with enhanced operational capabilities in digital design and manufacturing.

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Yousub Lee, 865-241-2647, leey@ornl.gov

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Advanced characterization for metal additive manufacturing leveraging deep learning and rapid X ray computed tomography

A. K. Ziabari

Multimodal Sensors Analytic Group

Electrification and Energy Infrastructures Division

ziabariak@ornl.gov

INTRODUCTION

Metal additive manufacturing (AM) is a promising technology that enables the creation of complex components in a cost-effective and energy-efficient manner. However, metal AM comes with its own set of challenges, especially in ensuring the quality and consistency of the printed parts. The quality and consistency can be affected by factors such as incorrect printing conditions and suboptimal parameters, which may cause issues such as flaws (porosity, cracks, etc.) in the parts, affecting their performance and properties.

To solve these problems, X-ray computed tomography (XCT) is used. XCT is a nondestructive method that captures images of the printed parts from various angles, and these images are then used to construct 3D representations of the parts. This method enables assessing the quality of the parts to identify defects and understand their physical properties without damaging them.

However, XCT is not without its problems. The process can be time consuming and expensive, and the quality of the images can be compromised if the process is streamlined to be faster or cheaper. One particular challenge is a phenomenon known as the *beam hardening effect*, which occurs when the X-ray photons pass through dense materials such as metals. The lower energy photons are absorbed more easily, leaving only high-energy photons which can cause distortions in the resulting images.

In addition, XCT scans can be very time consuming, laborious, and expensive, so using them to characterize hundreds of parts being manufactured every day at a manufacturing center is unfeasible. Reducing the scan time has a major impact on the cost, labor and energy efficiency of the systems.

BACKGROUND

To address these challenges and enable XCT to become practical for high-throughput, scalable characterization in metal AM, deep learning–based algorithms are being developed to leverage knowledge about printed parts such as their computer-aided design (CAD) model and physics-based information and properties. Under the Simurgh framework, which is the software package licensed under U.S. Department of Energy ID number 90000193, two deep learning–based algorithms are being developed, as described below.

2.5D CAD-DLMBIR [1,2]. The CAD-assisted, deep learning–based, model-based iterative reconstruction (CAD-DLMBIR) approach uses a model-based iterative reconstruction (MBIR) algorithm that employs the CAD model of the parts and the physics of the process to produce high-quality 3D reconstructions. The MBIR algorithm is initially time consuming but can produce excellent reference reconstructions for later use.

A convolutional neural network (CNN) was developed and trained to learn the relationship between the XCT reconstructions and the high-quality reference reconstructions. Instead of CNN learning using fully 3D CNN or learning slice by slice in a 2D CNN, this approach uses multiple neighboring slices of 3D volume as input and maps them to a single slice from the 3D volume as output: hence, *2.5D*. The process is significantly faster than training and testing a 3D CNN and is comparable to a 2D CNN), producing output with a quality similar to that of a 3D CNN. This learned relationship can then be applied to new samples to generate high-quality 3D image reconstructions quickly and efficiently. The proposed approach has allowed for fast, high-quality 3D image reconstructions of the parts while reducing the scan time (by as much as 12 times from 2 h/part to 10 min/part), and it also reduces cost and labor. With a higher technology readiness level, CAD-DLMBIR is a research product designed to address the immediate needs of industry partner ZEISS Industrial Metrology and to immediately improve the characterization quality at ORNL's Manufacturing Demonstration Facility (MDF).

Simurgh [3,4]. In the second approach, generative adversarial networks (GANs) are used, along with a library of defects and a physics-based XCT simulator and CAD model of the metal components, to create a realistic synthetic dataset. The GAN model is trained to style transfer the noise and artifacts to the simulated synthetic X-ray images (a process similar to generating fake face images and transferring face images between different people and celebrities, for example). Pairs of synthesized data are created based on GAN-generated (corresponding to low-quality XCT data with artifacts and noise) input and their corresponding high-quality ground truth (i.e., the simulated XCT data without any noise and image artifacts). These synthetic data are then used to train the CNN architecture to learn how to suppress the artifacts and noise and to produce high-quality reconstruction.

Once the network is trained, it works on real datasets. This is a state-of-the-art approach that addresses challenges with CAD-DLMBIR because it does not require performing high-quality measurements to generate ground truth. The results demonstrate that the Simurgh algorithm can produce even higher quality reconstructions compared with CAD-DLMBIR, and in the long

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term, Simurgh is expected to become the go-to algorithm for ZEISS Industrial Metrology and for parts being scanned at the MDF.

RESULTS

The ultimate goal of the developed algorithm is to reduce the scan time while maintaining the high-quality and speed of reconstruction even for denser materials.

Scan time can be reduced by reducing number of scan angles or by reducing the duration of acquisition at each angle. Both of these measures will introduce artifacts and noise because the required data are being sacrificed at the expense of reducing the scan time, making it more challenging to perform reconstruction accurately, and in turn making it more difficult to extract meaningful information. The problem of metal artifacts, particularly beam hardening, is more pronounced for parts made of denser and thicker materials such as metals.

Numerous results demonstrate the performance of the proposed approaches. As the density and/or thickness of materials are increased, the algorithms supersede the standard algorithm, even when the scan time is reduced 3 to 12 times, and high-quality reconstruction is produced from these very fast scans.

Fast, high-quality reconstruction in Al alloys (thick, lower density metals). The top image in Figure 1 shows the results for thick Al alloy parts with complex features. For this lower density alloy, the scan time was reduced by a factor of three, and the quality improved significantly. This scan would typically take 40 min to 1 h but was complete in only 13 min. Recently, the scan time was reduced to under 10 min (results not shown here), and the new setting is now being used at ORNL's MDF to scan lower density metals.

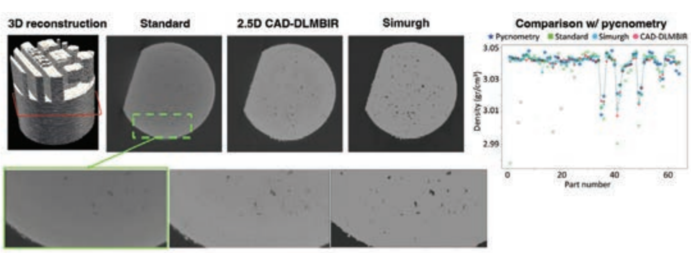

Figure 1. Top left: 3D object made of an Al alloy reconstructed after an XCT scan. A slice through the object shows the comparison between the standard algorithm and the subject algorithms, along with expanded images of a region of interest selected inside the slices. The density of the parts was extracted from the reconstructed volumes of 64 objects using all three techniques, and results were compared with a reference density measurement approach as shown in the graph on the right. The dark black spots in the images are pores and defects in the printed part, and those spots are smeared in the image obtained by the standard algorithm. (Credit: A. Ziabari, ORNL).

Fast and high-quality reconstruction in thick, high-density metals. The subject algorithms were also tested on several high-density metal components, including Ni alloy and stainless steel. Both CAD-DLMBIR and Simurgh produce very high-quality reconstruction of the parts from very fast and sparse scan data. The high-quality reconstruction can be used to extract information about defect distribution and characteristics in the printed components and to analyze how the printing processes affect the quality of the printed part.

However, ground truth data must be produced, and the performance of XCT algorithms must be ensured. As shown in Figure 2, high-quality reconstruction was verified by cutting a printed component and using high-resolution optical microscopy at 1 μm pixel size to evaluate the flaw detectability performance of the Simurgh algorithm. Analysis of these data demonstrates that 100% of flaws 100 μm or larger can be extracted, and about 40% of flaws that are even smaller than 1 voxel (i.e., 17.3 μm) can be extracted using a scan that takes approximately 10 min (also shown in Figure 4b). A typical scan for such a sample size takes approximately 2 h, and when using the standard algorithm for a 10 min scan, only 100% of flaws larger than about 400 μm can be detected.

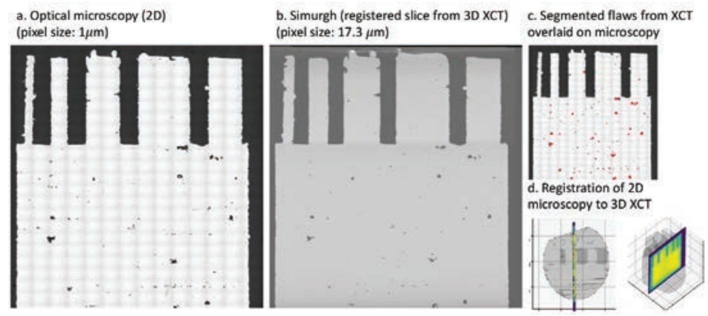

Figure 2. To verify the high-quality reconstruction, the sample was cut using high-resolution microscopy to compare the detected flaws from XCT to microscopy data. (a) 2D optical microscopy cross section, (b) corresponding registered slice from 3D volume reconstructed using Simurgh, (c) extracted flaws from XCT overlaid on 2D microscopy, and (d) diagram showing registration process. (Credit: A. Ziabari, ORNL).

Figure 3 shows an example of reduction in scan time from 1 h to only 10 min and the effect it has on the subject algorithms vs. the standard algorithm. For a thick stainless-steel alloy, a standard scan for such a thick part can exceed 1 h. Performing a 1 h scan to characterize hundreds of components being manufactured every day is computationally prohibitive and very expensive. Reducing the scan time to 10 min per component lowers the cost and labor and enables holistic characterization of hundreds of parts. Moreover, the standard algorithm introduces significant artifacts and noise (see Figure 3b), resulting in loss of quality and inaccurate characterization of components. However, the proposed algorithms produce high-quality reconstruction of components, even with a 10 min scan, allowing for high-throughput, scalable characterization of parts at reduced cost and labor.

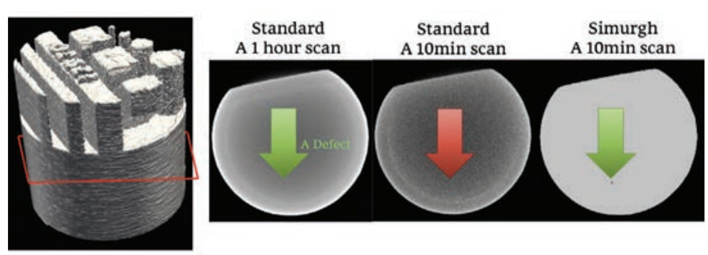

Figure 3. Left, 3D object (made of stainless steel, 316L) reconstructed after an XCT scan; right, comparison of standard algorithm and Simurgh as scan time is reduced from 1 h to 10 min. (Credit: A. Ziabari, ORNL).

Figure 4 depicts the improved detection capability of the proposed algorithms for low- and high-density metal. Figure 4a presents a comparison for Al alloy, showing that even after reducing the scan time by a factor of 3, the proposed algorithms out performs the standard algorithm and can detect 100% of defects that are 50 μm or larger, and can also detect 3.5–4 times more defects that are at voxel size in a single scan (i.e., 17.3 μm in the examples shown). For a high-density metal, Simurgh can detect 100% of the flaws greater than 100 μm, even when scan time is reduced by a factor of 12 from 2 h to 10 min. Compared with the standard algorithm's 100% detection of flaws greater than 400 μm, these algorithms provide more than 4 times improvement in detection capability while reducing the scan time by a factor of 12.

The results shown in Figure 4 are based on the available standard flaw detection algorithm at the time of the analyses. Flaw detection algorithms have been further improved but are not reflected in the figure.

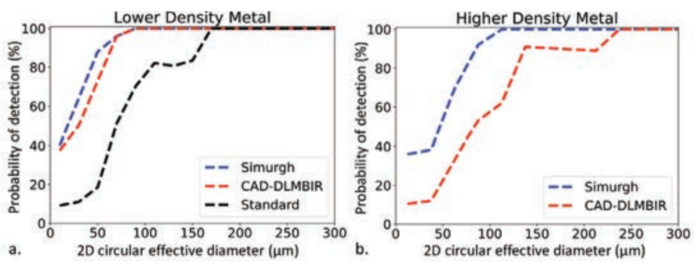

Figure 4. Probability of flaw detection for different algorithms based on comparing flaws detected from reconstruction of fast (sparse) XCT measurements to high-resolution microscopy at 1 mm (a) for lower density Al alloy, and (b) for high density metal alloy. Both plots demonstrate detection capabilities of the proposed algorithms. For the high-density metal alloy, the result of the standard algorithm is omitted because it appears above 400 mm or so. For the lower density alloy, the result of Simurgh is estimated based on previous work [3] and on the similarity of results between Simurgh and the densely scanned CAD-DLMBIR presented in another study [1]. (Credit: A. Ziabari, ORNL).

High-throughput and scalable characterization. The high quality of the proposed reconstruction algorithm from very fast scanning acquisition has paved the way for high-throughput, scalable characterization at the MDF and for identifying the ideal process parameters for consistent and repeatable printing of the components. An example process is shown in Figure 5. In this process, hundreds of components, each printed with a separate printing process parameter, can be scanned, and then information can be extracted to show how these process parameters affect the quality of the printed part.

The algorithms developed under the Simurgh framework enable each part to be quickly scanned and quickly reconstructed, and because of the very high quality of reconstruction, each part can be quickly analyzed using simplified postprocessing algorithms. Once all the parts are characterized, data are analyzed to extract optimum process parameters for printing consistent parts. A recent publication [1] demonstrates for the first time that the optimum process parameters can vary depending on the geometry of the printed part using XCT reconstruction of objects with complex geometric features.

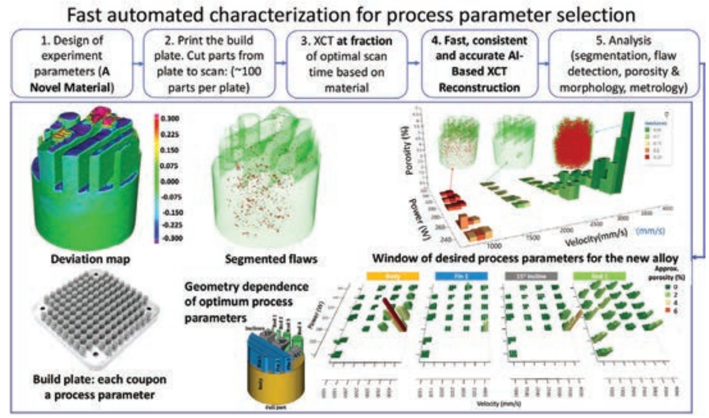

Figure 5. Fast automated characterization for process parameter selection. A build plate is designed, and each component is printed with a separate printing process parameter. The components are quickly scanned, reconstructed and characterized using the algorithms provided. This test allows for quick evaluation and analysis of the effect of process parameters so that the region of ideal process parameters can be located, resulting in minimum porosity and deviation as a metric for the ideal printed component. Furthermore, by analyzing these ideal components and their individual geometric features, the effect of geometry on the selection of the ideal region of process parameters was evaluated. (Credit: A. Ziabari, ORNL).

CONCLUSIONS

The proposed XCT reconstruction algorithms offer several key advantages that make it a powerful tool for industrial applications. First, they enable scans up to 12 times faster than previously available, even for high-density materials such as Inconel 718 and stainless steel with thick, complex geometry. This accelerated scanning process results in lower costs and less labor associated with XCT scanning and analysis. Second, these algorithms deliver higher quality results without imposing additional computational burdens, as demonstrated by the significant improvement in total characterization time by cutting the scan time, reconstruction time and postprocessing data analysis time. Simurgh also relies only on AI-generated synthetic data, thus eliminating the need for extensive data curation. These features allow for high-throughput, nondestructive characterization of multiple components, therefore streamlining the overall process. They also enhance detection capabilities and reduces analysis complexity. When compared with high-resolution microscopy, the proposed algorithms show an improvement that is four times more effective in defect detection, thus simplifying the analysis process and increasing the accuracy of defect identification. Overall, the developed XCT reconstruction algorithms offer a comprehensive solution for faster, more accurate and cost-effective industrial computed tomography imaging.

IMPACT

AI-based nondestructive evaluation (NDE) characterization, particularly through these advanced XCT reconstruction algorithms, plays a pivotal role in supporting the Advanced Materials and Manufacturing Technologies Office's (AMMTO's) mission of fostering clean energy transition and enhancing manufacturing competitiveness. By leveraging AI in NDE, this cutting-edge technology enables rapid, high-quality characterization of complex parts, which is essential for the qualification and certification of advanced materials and manufacturing processes. This advanced characterization promotes material and energy efficiency in manufacturing and bolsters the resilience of domestic supply chains for clean energy technologies.

Furthermore, these AI-driven XCT reconstruction algorithms contribute to the development of advanced materials, processes and digital systems that enhance the economy's overall efficiency. By significantly improving image resolution and defect detectability and reducing scan time, this technology streamlines the manufacturing process and reduces associated labor and costs. This innovation results in more sustainable and efficient manufacturing practices, which ultimately align with AMMTO's focus on driving clean energy transition and strengthening manufacturing competitiveness across various industries.

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The proposed approach can be applied to XCT reconstruction in different scientific imaging applications outside computed tomography and in other 3D nondestructive imaging applications with some modifications.

Amir Koushyar Ziabari, 831-334-9296, ziabariak@ornl.gov

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Development of new high-performance Al alloys for additive manufacturing

A. Plotkowski[1*], S. Bahl[1], Y. Yang[1], D. Splitter[2], A. Perrin[1], J. Poplawsky[3], L. Allard[1], A. Shyam[1], J. Haynes1, R. Dehoff[4]

[1]Materials Science and Technology Division, [2]Buildings and Transportation Science Division, [3]Center for Nanophase Materials Science, [4]Manufacturing Science Division

**plotkowskiaj@ornl.gov*

INTRODUCTION

Aluminum alloys, an important class of structural materials, are in demand because of their excellent combination of specific strength, conductivity and corrosion resistance. Aluminum alloys are a natural fit for use with emerging additive manufacturing (AM) processes and their associated design freedom to fabricate lightweight, high-performance components. However, conventional Al alloys present two significant challenges for AM: they are susceptible to cracking during processing, and their properties tend to degrade rapidly with increasing temperature.

These limitations have prevented adoption of conventional Al alloy compositions for AM, and only a few have been successfully industrialized compared to thousands available for conventional processing. The purpose of this work is to develop new alloys that turn the complex thermal conditions found in AM from a limitation to an advantage. For this purpose, AM's rapid cooling conditions were exploited to design and manipulate unique microstructures. By combining AM with computational techniques for alloy design and advanced characterization, it may be possible to not only match conventional processing but also to improve performance.

BACKGROUND

A significant issue with processing conventional Al alloys is their propensity for hot tearing, which occurs when stress (e.g., thermal contraction) is exerted on the partially solidified metal [1]. This problem is especially limiting when the solidification of high-performance wrought Al alloys creates deep dendritic networks prone to cracking. This issue can be countered by designing alloys to form a eutectic solidification microstructure in which multiple solid phases simultaneously form from the liquid [2]. This approach has been successfully adopted for shape casting and has been adapted to AM with the commercialized AlSi10Mg alloy, for example, but only a few such alloys have been tested.

High-performance wrought alloys also tend to lose much of their strength at high temperatures [3]. These alloys derive their strength primarily from nanoscale precipitates formed during solid-state heat treatments. In service near the aging temperature (approximately 200°C), these precipitates coarsen and dissolve. Secondary phases are also formed in the aforementioned eutectic reactions, but in conventional processing, they are very coarse (>10 μm) compared to solid-state precipitation reactions and are therefore not as effective for strengthening. However, the length scale of the eutectic microstructure is sensitive to the solidification rate [4], and processing with fast cooling reduces the size of reinforcing particles, leading to increased strength.

The approach described herein was to design Al alloys with compositions that encourage eutectic solidification and to refine the microstructure by using high cooling rates in AM. In this way, designing alloys that are simultaneously printable while also achieving desirable mechanical properties may be possible. Furthermore, for the alloys to operate successfully at high temperatures, the types of secondary phases that form to maximize their thermal stability must be carefully selected.

RESULTS

AM microstructures offer unique properties. In previous research, ORNL designed Al-Cu-Mn-Zr (ACMZ) alloys for excellent castability and high temperature stability. Strengthening in these alloys comes primarily from metastable formation of θ' precipitates upon heat treatment, which are stabilized by additions of Mn and Zr. These alloys rely on a high Cu content (up to 9 wt %) to avoid hot tearing by increasing the volume fraction of the stable θ-Al_2Cu intermetallic phase during solidification. However, increased castability comes at the cost of ductility because the θ particles preferentially form at grain boundaries and act as fracture initiation sites without contributing to strengthening.

A similar alloy was processed by laser powder bed fusion AM (Figure 1). Unlike the cast alloy the θ particles are distributed uniformly in the microstructure from a nonequilibrium eutectic solidification reaction, and their size is refined by several orders of magnitude. Their reduced size strengthens the alloy through an Orowan mechanism that is not significant for their large size in the cast microstructure. In situ studies during deformation revealed the relationships between microstructure and mechanical behavior. X-ray diffraction (XRD) analysis during tensile testing showed the small particles avoid brittle fracturing, which is a key failure mechanism in castings, and that the small particles in AM carry a much higher fraction of load by comparison [5]. However, neutron diffraction during creep shows that for slower deformation rates at elevated temperatures, this load is increasingly transferred back to the Al matrix through a mechanism called *load shuffling* [6].

Design of eutectic alloys opens up processing and performance space. Although the ACMZ alloy demonstrated interesting microstructure and properties, its processing range was narrow. Some conditions produced sound material, whereas others caused substantial hot tears to form [7]. Additionally, although the properties at room temperature were attractive, Cu diffuses relatively quickly through the face-centered cubic (FCC) Al matrix at elevated temperatures, and the θ particles that strengthen the material coarsen rapidly [8]. Therefore, other near-eutectic Al-based systems that form thermally stable phases should be identified. For this purpose, Ce is an attractive alloying addition because its low solubility and diffusivity in Al help to slow coarsening kinetics.

High-throughput computational thermodynamics helped identify that Al-Cu-Ce alloys feature a eutectic reaction that produces a high volume fraction of Ce-containing intermetallic phases. The solidification temperature range is also narrow,

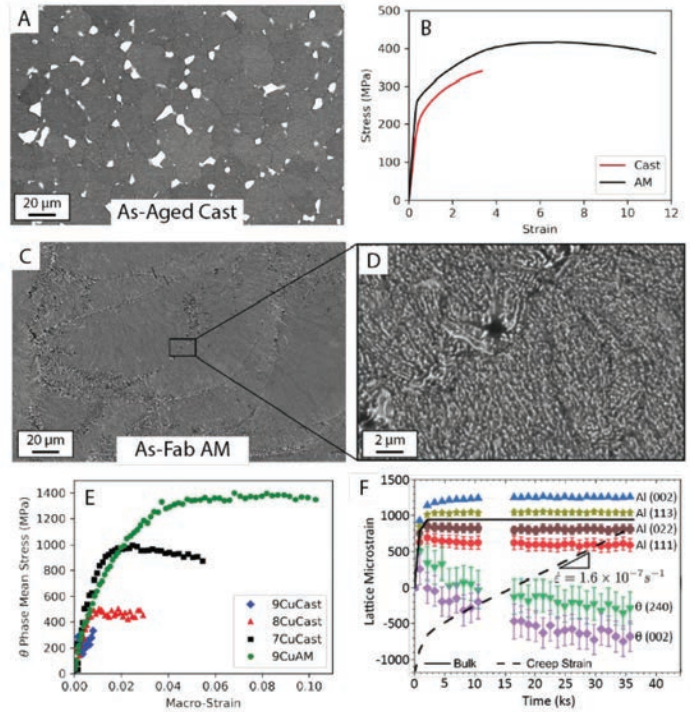

Figure 1. (A) Microstructure of an aged ACMZ casting [7], (B) comparison of room temperature tensile curves for cast and AM samples, (C) microstructure of an AM sample showing (D) significant refinement of intermetallic particles, (E) room temperature in situ high energy XRD showing the difference in θ phase stresses in cast and AM alloys [5], and (F) in situ neutron diffraction data during creep at 300°C showing shedding of load from the θ intermetallic particles to the Al matrix [6]. (Credit: Plotkowski).

which is desirable to avoid hot tearing (Figure 2A). Two alloys were fabricated: a ternary alloy (Al-9Cu-6Ce) and a quaternary alloy (Al-9Ce-6Ce-1Zr) in which Zr was added to serve as a grain refiner and to form stable $L1_2$-type precipitates during post-process heat treatment [9,10]. Both alloys formed a refined eutectic microstructure, making them printable across a wide range of AM conditions. The Zr addition enabled grain refinement through nucleation of FCC Al grains on primary Al_3Zr particles.

The addition of Zr also plays an important thermodynamic role. The eutectic solidification structure of the ternary Al-Cu-Ce alloy contained FCC Al and the metastable Al_8Cu_3Ce intermetallic phase, which transformed into Al_8Cu_4Ce upon heating, with an associated spheroidization and coarsening of the microstructure. The addition of Zr stabilized Al_8Cu_3Ce within the range of 300°C–400°C and significantly improved the coarsening resistance of the microstructure [11,12].

Atom probe tomography revealed that the high solidification rates also provide extended solubility for Zr far beyond what is possible in the near-equilibrium conditions of conventional solutionizing heat treatments (Figure 2C and D). The higher solubility allows for precipitation of a large fraction of $L1_2$ Al_3Zr nanoparticles when age hardened at 350°C for 8 h. The combination of nanoscale eutectic microstructure and nucleation of $L1_2$ particles resulted in increased room temperature strength while retaining ductility, making the static mechanical properties of the alloy comparable to conventional wrought materials while

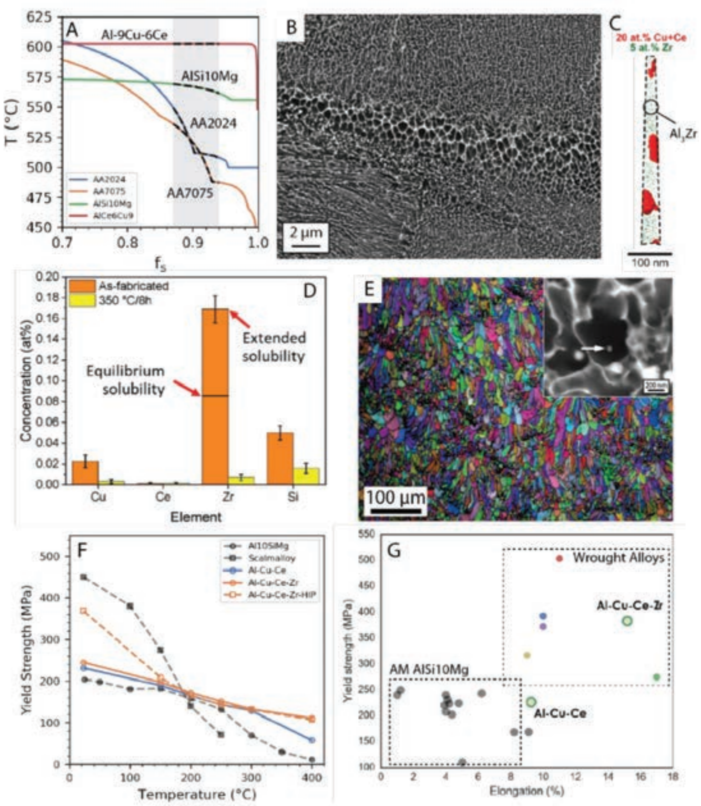

Figure 2. (A) Schiel simulations of Al-Cu-Ce showing a narrow freezing range [13] and (B) an example AM microstructure for Al-Cu-Ce-Zr. (C) Atom probe tomography data show Al_3Zr precipitation caused by aging [11] (D) in response to extended solubility caused by high solidification rates. (E) Electron backscatter diffraction data show that Zr addition also causes grain refinement through formation of primary Al_3Zr particles. (F) Yield strength with temperature as a function of composition and heat treatment are compared to some benchmark alloys. (G) The properties for aged Al-Cu-Ce-Zr are competitive with conventional wrought alloys. (Credit: Plotkowski).

being highly printable. Compared to benchmarks, the Al-Cu-Ce alloys showed good thermal stability and superior strength retention at high temperatures above 300°C.

New DuAlumin-3D alloy exhibits exceptional performance. The results for the Al-Cu-Ce alloys suggest that the high cooling rates in AM can be used to achieve refined microstructures with desirable mechanical properties. To take this design concept further, the Al-Ce-Ni ternary system was investigated which exhibits a ternary eutectic reaction in which three phases simultaneously form from the liquid. Computational tools were used to determine that the addition of Mn may stabilize desirable Ce-containing, coarsening-resistant intermetallic phases. Furthermore, Zr was added to aid in printability through grain refinement and to enable Al_3Zr precipitation.

The result of this design process, Al-9Ce-4Ni-1Zr-0.5Mn, was called *DuAlumin-3D*. The alloy was shown to be highly printable for complex shapes such as the high-efficiency internally cooled piston shown in Figure 3A. The alloy exhibits a nanoscale solidification microstructure consisting of multiple coarsening-resistant intermetallic phases. Like the previously described Al-Cu-Ce-Zr alloy, the Zr addition is largely trapped in solution because of the high solidification rates during processing. Direct aging causes precipitation of $L1_2$ Al_3Zr nano-precipitates which strengthen the Al matrix between the intermetallic particles formed upon solidification. The combination of these mechanisms results in a complex multiscale microstructure to achieve an exceptional combination of strength, ductility, and strength retention at elevated temperatures (Figure 3B–3D). The refined secondary phases in the microstructure provide significant strengthening, with room temperature strength exceeding that of Al-Cu-Ce-Zr.

The selection of thermally stable intermetallic phases enables the alloy to retain much of its strength at elevated temperatures, as shown by the comparison with a variety of benchmark materials in Figure 3E. This feature of the microstructure was caused by both the thermodynamics and the kinetics of the selected alloy composition. Specifically, ternary Al-Ce-Ni alloys tend to form Al_3Ni intermetallic particles which coarsen rapidly compared to the slow kinetics of Ce-containing phases. The Mn addition in this alloy was found to destabilize formation of Al_3Ni and instead encouraged $Al_{20}(Mn,Ni)_2Ce$ compounds. The Ce content of the latter intermetallic type becomes the limiting factor for microstructural coarsening, which is a function of both the solubility and the diffusivity of the solute, both of which are low for Ce in Al. Stabilizing these phases, for which coarsening is limited by Ce, significantly increases the mechanical performance of the alloy at high temperatures.

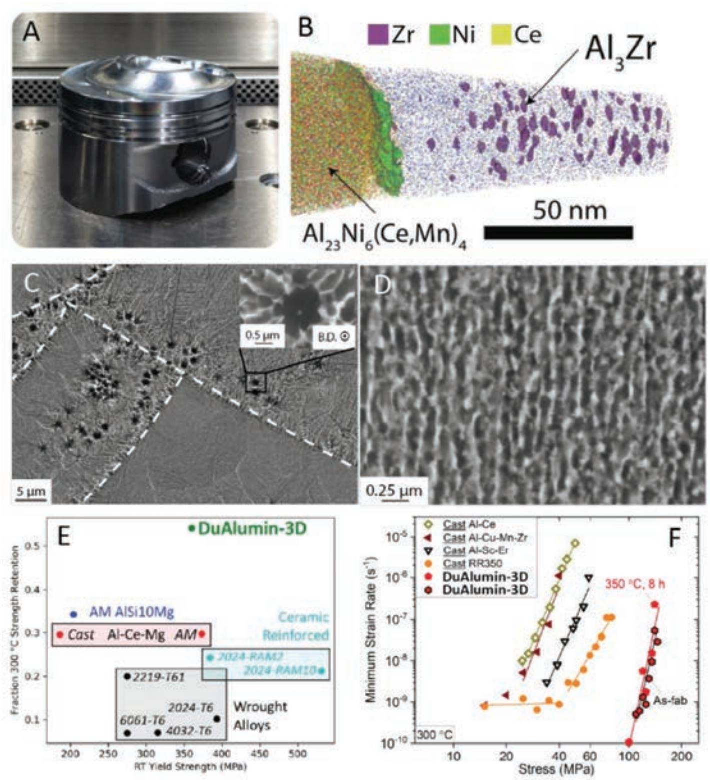

Figure 3. (A) An example high-efficiency internally cooled piston additively manufactured with DuAlumin-3D. (B) Atom probe tomography showing Al_3Zr nanoparticles dispersed in the Al matrix after heat treatment. (C) SEM micrograph showing the solidification structure, and inset showing grain refinement and (D) higher magnification of the refined intermetallic particles. (E) The alloy retaining a large fraction of its room temperature strength up to 300°C compared to benchmark alloys. (F) Tensile creep data showing that this is the most creep-resistant Al alloy at 300°C. (Credit: Plotkowski).

The highly stable microstructure at elevated temperatures is particularly important for creep deformation, for which loads are sustained for long periods. The thermally stable, refined intermetallic particles formed during solidification in the AM process are well suited for resisting creep deformation. Indeed, the alloy was found to exhibit the best known creep resistance of any Al alloy at 300°C (Figure 3F). Direct aging at 350°C for 8 h, which causes precipitation of Al_3Zr particles, did not significantly affect the creep rates at 300°C. This result indicates that although precipitation significantly affects room temperature strength for tensile testing, it is not significant relative to the solidification microstructure for slower strain rates at elevated temperatures.

CONCLUSIONS

Additive manufacturing processes exhibit unique thermal conditions relative to conventional processing. Although these conditions sometimes prevent direct use of existing alloys, they may also be exploited to produce unique microstructure and attractive properties, assuming that the alloy composition is suitably designed. In this work, ORNL researchers demonstrated an approach for designing and manufacturing near-eutectic Al alloys with AM that achieve properties that are not only comparable to existing alloys but also superior to those designed for conventional processing routes. By understanding the mechanisms for phase transformations during processing and mechanical behavior, performance can be improved further.

IMPACT

Additive manufacturing processes enable design freedom not possible with conventional subtractive manufacturing. However, the process features unique characteristics, and new alloys must be designed to suit these processes and to enable the fabrication of complex components with improved performance. The work described herein demonstrates a new class of Al alloys well suited for AM with properties that cannot be achieved in conventional alloys and processes. The research is published in a variety of articles and has resulted in numerous patents.

Moreover, these capabilities offer a significant industrial impact. First, the combination of excellent mechanical properties and AM printability enables lightweighting and performance gains in the automotive sector. Additionally, the properties at elevated temperatures far exceed the capabilities of current Al alloys. In many scenarios in the automotive and aerospace industries, components with applications at intermediate temperatures are overdesigned with Ti alloys. These alloys are significantly more expensive and heavier and exhibit worse thermal and electrical characteristics than Al alloys, but they are selected because of their capabilities at temperature. In these cases, these new Al alloys offer a solution for lightweighting, thermal management and cost savings. Because of these advantages, the alloys designed here resulted in collaborative U.S. Department of Energy (DOE)–funded projects with General Motors, Honda Performance Development, and Boeing.

Finally, the scientific understanding of the alloy design principles and deformation mechanisms suggests that further improvements in properties and performance are possible. The work presented here provides a rich scientific study of unique microstructures in AM and lays the groundwork for a growing community of researchers to develop a wide variety of new alloys for AM.

COLLABORATE WITH ME

Alex Plotkowski, plotkowskiaj@ornl.gov

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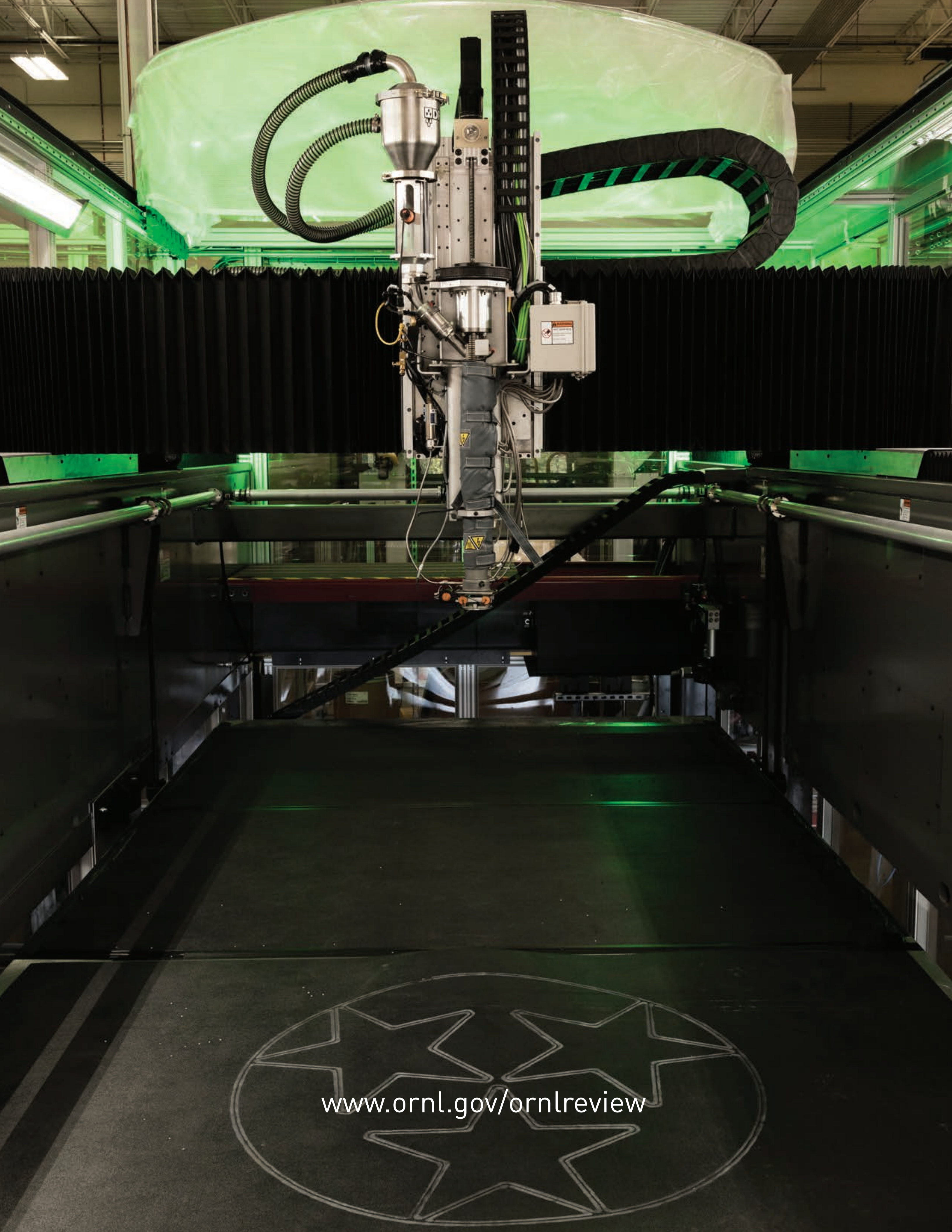

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