Livermore: Machine learning aids the dark-matter quest

Sandia: Applying theory to shore up fusion plasmas

Plus: Strength in powdered sugar, optical improvements and catching explosions in the act; final-year fellows’ research highlights; NNSA’s Marvin Adams on stockpile stewardship and achieving fusion ignition; and shock physics’ enduring allure

COMPATIBILITY TEST
Samantha Lawrence (SSGF 2015) and her Los Alamos team study how crucial metals perform in harsh environments
The Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship (DOE NNSA SSGF) provides outstanding benefits and opportunities to students pursuing degrees in stewardship science areas, such as high energy density physics, nuclear science, or properties of materials under extreme conditions.

The fellowship includes a 12-week research experience at Lawrence Livermore National Laboratory, Los Alamos National Laboratory or Sandia National Laboratories.

**ELIGIBILITY:** U.S. CITIZENS WHO ARE SENIOR UNDERGRADUATES OR STUDENTS IN THEIR FIRST OR SECOND YEAR OF DOCTORAL STUDY.

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The Department of Energy National Nuclear Security Administration Laboratory Residency Graduate Fellowship (DOE NNSA LRGF) gives doctoral students the opportunity to work at DOE NNSA facilities while pursuing degrees in fields such as engineering and applied sciences, physics, materials, or mathematics and computational science.

Fellowships include at least two 12-week research residencies at Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Sandia National Laboratories or the Nevada National Security Site.

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THE LRGF MAKES SOME HISTORY

WELCOME TO THE 14TH EDITION of Stewardship Science magazine, originally labeled “the SSGF magazine” for the DOE NNSA Stewardship Science Graduate Fellowship. It’s now our fifth issue to also showcase the outstanding researchers in the younger DOE NNSA Laboratory Residency Graduate Fellowship (LRGF).

It’s a big year for the newer program, and that’s reflected in these pages. For one thing, the composition on page 8 is the first by an LRGF recipient to win the annual Essay Slam competition that pits submissions from fellows and alumni of both programs. What’s more, LRGF welcomes a record incoming class of six recipients, pushing the total for both programs to a record 11 new fellows. You can meet them on the inside back cover. And, not least, our LRGF outgoing-fellow profile features a University of Nevada, Reno, physicist who, with a boost from Neil deGrasse Tyson, followed an unusual path to the world of Z pinches and plasmas.

We’re also pleased to present an interview with NNSA Defense Programs Deputy Administrator Marvin Adams, who played a prominent role in the fusion-ignition announcement that drew worldwide attention at the end of 2022. He discusses that milestone and more on page 7.

– The Editors, Stewardship Science: The SSGF/LRGF Magazine
Alumna Samantha Lawrence studies compounds exposed to harsh environments, seeking degradation solutions.
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Fusion breakthroughs support broader stewardship science experiments, NNSA’s Marvin Adams says.

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MESOSCALE DISLOCATIONS, UNFURLED URANIUM AND FLASHOVER
Fellows report on their research as they finish their programs.

Samantha Lawrence, SSGF class of 2015, works in Los Alamos National Laboratory’s Sigma Division, where she and colleagues study metals in exotic environments — hydrogen pipelines, nuclear reactors and weapons. She leads the Materials Compatibility Team, which develops substances and components in support of national security. Compatibility is an aspect of qualification, which ensures that materials are suited for particular uses. Los Alamos National Laboratory
PROTECTION CONFECTION

Your powdered doughnut’s coating could double as a veneer that withstands extreme impacts in space and the scorching temperatures in fusion energy experiments.

Researchers at Sandia National Laboratories’ New Mexico campus bake ordinary powdered sugar under zero-oxygen conditions to produce nanometers-thin layers of carbon black. The polycrystalline carbon is sandwiched between and atomically glued to thicker layers of silica, Earth’s most common material, in an architecture mimicking a seashell’s.

The coating is light and protective to 1,650 degrees Celsius, says Guangping Xu, a senior member of the Sandia technical staff who led the research. It’s made from an off-the-shelf ingredient — literally. “The sugar we used I purchased from a grocery store,” Xu says. “We analyzed this, and it’s pure sucrose,” a suitable carbon black feedstock.

*R&D World* magazine named the coating project one of its top 100 new technologies for commercial development in 2022. A patent is pending.

With support from Sandia’s Laboratory Directed Research and Development program, the team set out to improve shielding for instruments and samples in pulsed-power devices. Sandia houses the Z machine, the world’s largest such facility, which generates tremendous, exceedingly brief electrical discharges mainly for fusion and materials experiments.

Shots at Z and similar devices vaporize metals, Sandia physicist Chad McCoy says, “so you’re blasting essentially molten steel, aluminum, et cetera, all around the target chamber.” Fragments as large as an eighth of an inch can survive, traveling at kilometers per second. “We’ve seen some of this debris punch through quarter-inch-thick steel plate. That’s what we have to fight to do science on Z.” Meanwhile, chamber temperatures can reach up to 1,500 C. And future, more powerful pulsed-power machines will require even stronger shielding than the available options.

After tests showed the coating was 80% stronger than silica alone, the team tried it in Z experiments. The researchers placed the coating, just 45 microns (millionths of a meter) thick, about 10 millimeters in front of a polyethylene layer. For contrast, the team placed a bare silicon substrate in front of the polyethylene in another cassette.

Experiment fallout deformed the polyethylene layer by 0.144 inches behind the bare silicon. It distorted just 0.010 inches, 14 times less, behind the Sandia coating.

Beryllium, the standard shielding substance in pulsed-power devices, costs hundreds of dollars for a postage stamp-sized piece; materials for a similarly sized carbon black-silica coating wafer cost pennies.

Beryllium also is toxic, requiring special handling and post-shot cleanup. The Sandia team’s coating is environmentally benign.

The researchers describe their coating as a layer cake, with sugar-based carbon black, appropriately, replacing the frosting. They apply drops of a readily available silica precursor, mixed with ethanol, to a spinning substrate to spread the material evenly. Next they apply drops of sugar, dissolved in ethanol and water. The liquids are alternated to produce the desired layer count and then baked at up to 850 C in an oxygen-free atmosphere. The silica precursor decomposes to amorphous SiO2 layers. The sugar sheds hydrogen and oxygen atoms to become carbon black. Heat atomically bonds the sheets to each other.

Each layer of the composite coating helps the next mitigate shocks. “Carbon black is kind of a soft material,” Xu says. “When you have cracks in the silica layer, when they propagate to the carbon black, they will stop there.”

The coating, McCoy says, is hard but brittle, cracking as it absorbs energy from flying fragments. It’s typically applied to materials with high toughness — the ability to absorb energy by deforming. By covering tough materials, such as metals or high-temperature polymers, with the coating, “we’re taking the best of both worlds: this really high-hardness material that’s on something that is really tough and ductile.”

Xu says the coating process could be scaled up by immersing parts into alternating vats of silicon precursor and sugar solution.

The coating could have dozens of uses, including protecting spacecraft, such as satellites and capsules, from collisions with space junk and micrometeorites. It’s as strong as standard shielding of similar weight but far cheaper.

That’s pretty sweet. — Thomas R. O’Donnell

Guangping Xu uses a digital optical microscope to examine the unusually hard, sugar-based coatings his lab has produced. Bret Latter, Sandia National Laboratories.
GRATE EXPECTATIONS

Powerful and efficient lasers drive research in fusion, astrophysics, particle accelerators and stockpile stewardship. But today’s most energetic beams — operating on the petawatt scale — hit limits on the light intensity that their solid-state optical components can handle. Now, Lawrence Livermore National Laboratory researchers have described a way to replace some parts with plasmas, perhaps boosting current lasers’ power a thousand times without increasing their size.

High-energy lasers use chirped-pulse amplification, a Nobel Prize-winning technique that stretches focused light pulses, boosts their power, and then compresses them to produce ultra-short blasts of high-intensity light. The process requires two sets of optical gratings made from solid-state materials. But as shorter pulses are compressed and focused into a powerful laser beam, these components can fail.

“When light gets too intense, it burns things,” says Matthew Edwards, who started the project as a recipient of the lab’s Lawrence Fellowship. “And that includes the crystals and the pieces of glass that make up the lasers.” To counteract that problem, today’s petawatt beams are large and distribute the light intensity across optical components tens of centimeters in diameter.

Plasmas can handle higher intensities. For more than a decade, researchers have proposed using them in optics, Edwards says. But working with these ionized gases is tricky. “They’re hard to control. They don’t tend to do what you want them to do.”

Edwards, now a Stanford University mechanical engineering professor, and Pierre Michel, Livermore’s laser-plasma interactions group leader, started by seeking light-control mechanisms that could function despite plasma’s expected imperfections. It’s not just that “we have an optic that’s made of plasma. We want to be able to use the optic in a laser system so that the overall system is smaller, more efficient and behaves well,” Edwards says. They described this work in a 2022 Physics Review Applied paper.

To build the grating, the team aims two weak lasers into a gas. When the beams create the optimal interference, the gas ionizes into finely divided layers, a 10-micron-scale alternating pattern of charged and neutral molecules. This plasma grating changes the direction of a third incoming light beam just as a solid-state grating would — but it can withstand damage from light up to a thousand times more intense. Over the past three years, the researchers have dramatically increased the grating’s efficiency and have shown how basic plasma components could be built into an entire laser toolkit.

The gratings are about 100 microns in diameter, a bit larger than a human hair, but Edwards expects that millimeter-size gratings, which could boost laser power even more, are possible with their methods. Other innovations, such as improving the solid-state driving lasers to help stabilize plasmas, also could help researchers build more powerful beams, Edwards notes, but “the damage threshold of the optics is really the primary bottleneck.” — Sarah Webb
**THE K-MOD SQUAD**

A barrel-shaped, minivan-sized, X-ray-generating device called a Febetron has become an important national security tool.

“Because nuclear tests are banned, we have to rely on computer simulations to ensure that the weapons in the United States’ national stockpile will perform as intended,” says Kalpak Dighe, a Los Alamos National Laboratory physicist.

To feed data to and refine those simulations, experimentalists unleash conventional explosives against mock nuclear weaponry components. Multiple Febetrons capture data from these dynamic events, using X-rays to make images called radiographs that are “analogous to pictures you would take with a camera using visible light,” Dighe says.

Each Febetron — a trademarked name for field emission beta-ray device — contains a stack of electrical capacitors. “When triggered, the energy stored by each capacitor is released in a single, intense pulse of high-energy electrons,” Dighe says. “When this high-energy ray of electrons strikes stationary targets of high-atomic-number elements such as tungsten or tantalum, the sudden deceleration of the electrons generates X-rays.”

The Febetrons’ extremely short pulses “allow us to capture images that basically freeze the high-speed motion,” he adds, and can be captured on video that dramatically displays flying debris, accompanied by the thunderous boom from a test explosion. The Febetrons are 15 feet away, protected by barriers.

Besides validating nuclear weapons design simulations, Febetrons have other defense applications. In controlled laboratory environments, their intense electron beams bombard high-value electronic circuit boards such as those in missile-guidance systems, providing design criteria for shielding in high-radiation environments, Dighe says.

Febetrons have been a workhorse for 40 years. But the pulsed sections that comprise their capacitor module stacks are aging and often fail.

“Through mergers and acquisitions, the company that manufactured the original capacitor modules changed hands about five times,” Dighe says. “But nobody invested the time to redesign the pulsed power system.”

A couple of years ago, Dighe and his team of Robert Sedillo, Timothy Byers and John Wilson began the first module remake in decades, dubbing their result “K-module” after Dighe’s first name.

The original modules were monolithic units that encased all components in epoxy designed to prevent electric arcing. But the resin also made the old modules unserviceable. “Workers had to discard the whole defective module and needed to have enough spares on hand to replace the ones that suffered internal damage,” Dighe says. Otherwise, lead times for new ones could take months.

To design the K-module, Dighe used electric-circuit simulations, 3D modeling software and sophisticated electrostatic simulation software. The revised modules can store three times the energy as the originals and produce 1.5 times the output voltage, upping the X-rays.

“The higher X-ray dose allows deeper penetration into metallic objects and provides enhanced contrast and clarity for sharper radiographs,” Dighe notes. What’s more, one K-module has performed reliably in approximately 400 live explosive field events at Los Alamos during the past two years.

Unlike the original modules, the K-module fabrication process is simple; it does not require molds or tooling, which allows them to be reconfigured for a variety of applications.

Among those impressed: *R&D World* magazine, which conducts an annual global science and innovation competition. In 2022, the K-module team won one of the magazine’s R&D 100 awards.

– Monte Basgall

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*A Los Alamos National Laboratory-designed K-module that can generate 3.3 million volts and 10 thousand amperes, resulting in 33 gigawatts of peak power for 20 nanoseconds. Los Alamos National Laboratory*
How did your security-advising career develop?

When I went to Texas A&M in 1992, I continued to do technical work for Livermore. I started getting invited to join review and advisory panels, including a seven-person DOE blue ribbon panel on the future of nuclear engineering and research reactors. The nuclear power industry was in the doldrums; U.S. research reactors had dwindled from 70 to around 30. A lot of nuclear engineering departments closed. We wrote a report, and Congress passed legislation that implemented our recommendations. It was an epiphany: A professor can influence national policy. After this, I prioritized national-security service over other kinds of professional service.

What else prepared you for this job?

Thirty years as a professor working in national service involved frequently communicating to high-level decision makers who lacked a technical background. That’s not always easy. But I’ve worked very hard to communicate the whole truth — what we believe to be true, our uncertainties, and how we can address them.

The National Ignition Facility fusion achievement was a huge milestone. What does that mean for stockpile stewardship?

It helps us with the plain old science of stockpile stewardship and opens a broader range of experiments that will help us answer necessary and perplexing questions without resorting to nuclear explosive testing. The temperature, pressure and radiation conditions reached in a nuclear weapon are extreme, and the more fusion yield we can get out of these experimental targets, the closer we can approach those conditions. It allows us to do some really detailed investigations, test our computational tools’ predictive capability and refine them. This also demonstrates to the world that our technical expertise in weapons-relevant areas remains second to none, an important nuclear deterrent component. We don’t show the world that our weapons work by making the ground shake anymore. Instead, we execute our science-based stockpile stewardship and do careful assessment, and we are as public about that as we can be. The more we can do in the laboratory along these lines, the more confidence we will have and the less likely it becomes that we will ever have to return to nuclear testing. And avoiding testing is an important part of our entire nonproliferation regime, which in turn is a benefit to our national security.

In that fusion press conference, you mentioned that NNSA was hiring. How can aspiring scientists and engineers prepare for those jobs?

We’re having trouble hiring all the people we need — at the three national security laboratories, our production complex, the Nevada National Security Site and in NNSA. Anyone who might be interested in working at an NNSA laboratory should spend a few months at one, get a feel for what it’s like. There’s so much exciting work going on.

Any parting advice for early-career researchers?

Any day you learn something is a good day. Try to have a lot of good days. Whether you’re interested in influencing your field of study or broader policy decisions, you’re going to find — maybe to a surprising degree — that communication skills really matter. Communicate with people who are not like you. Don’t let your transmit button get stuck too often. Go into receive mode now and then. Personal relationships matter. They not only help you get things done but also make work life enjoyable. As an illustration, a friend once told me that people who fund research don’t want to give money to a person — they want to give their money to a person they trust.

We in the nuclear security enterprise are at an inflection point. We have more work than ever, and what we do today will define our capabilities for the coming decades. It really is a once-in-a-generation opportunity to make a long-lasting difference.
The Power of Pores

By Taylor Sloop

I’ve always wanted to understand how the world around me works, from learning about center of mass — when I asked my dad why there were extra pieces of wood across the bottom of a bedside table — to grasping how an entire field of physics is based on the observation that light always travels at the same speed. I’ve always loved chemistry and physics, so studying how a material’s chemical composition leads to its physical properties is fascinating. However, I didn’t know what field I wanted to study within materials science until I heard about shock physics. The cool notion of clashing compounds captured my imagination.

When people hear the word shock, many imagine situations in which something surprising happens. In materials science, shocks happen whenever objects collide.

Think about a car crashing into a wall. When the two make contact, an immense force stops the car abruptly. Whenever force is applied to an area, it creates pressure. In the case of the car, this pressure generates a shock wave that moves away from the impact and can change how fast atoms in a material move, pushing them forward in a way similar to how an ocean wave moves water droplets. Collision-driven shocks are like ocean waves in another way, too: If many of them interact, they can combine or cancel each other, like when a wave rolling toward the beach absorbs one rolling away.

To study these shock wave phenomena, materials scientists collide two objects at high speed. As you may remember from school, Newton’s third law of motion says that when this happens the two bodies must apply equal and opposite forces to each other.

Think of when you high-five someone. You and your partner both feel a slight sting on your hands because both experienced an equal and opposite force. It’s the same when two objects — a projectile and a target — meet, but instead of looking at a tingling feeling, scientists study the shock wave that moves away from the impact. For our experiments, we make the two objects from the same material.

When the projectile hits the target, equal and opposite shock waves move away from the impact point and through both objects at their original speeds and in their original directions until they encounter a new material. That means when the waves enter the open air behind the projectile and target, the resulting interaction resembles the initial impact because the air, in this case, functions as a new material.
At this point, the process starts anew: The waves collide with the air and rebound into the target or projectile. In my experiment, the target is thicker than the projectile, so the rebounded waves move back toward the target’s center from both objects and eventually pass each other. When this happens, the shock waves apply a pulling — tensile — force within the target. This only happens when waves pass each other, so we design the experiment so they’ll cross in the target. If the tensile force is big enough, it will pull it apart from the inside out.

My research focuses on disrupting these shock waves and making it so the pulling force is never applied in a material’s center and thus won’t pull it apart. Using our knowledge of shock behavior, I add pores to my materials, making them resist forces that would rend them in a crash.

I build my samples layer by layer on 3D printers, directing the machine’s laser to simply skip certain areas, leaving a hole — a pore — about half a millimeter long. My tests suggest this size is big enough to print without being so large as to weaken the material.

A shock wave coming across a pore collapses it and slows down. With enough pores, I can slow the wave so that the rebounds never interact and cannot pull the material apart. So far, I’ve found that 0.5-mm pores slow the shock wave enough that my material withstands impact at around 600 mph. It still fails at higher speeds. I’ve also seen that even one 0.5-mm pore will change wave interactions enough to lessen a collision’s effect.

You can probably guess why I study this. There are many instances when it’s helpful to know how much internal tension a material can withstand before it’s pulled apart. A car crash is one example: When two vehicles collide, each experiences these waves. We want to design bumper material that’s strong enough to stay intact under a shock, keeping passengers safe. To find the right material, we must know how it fails under dynamic conditions, like impact.

In this case, a shock shouldn’t be a surprise.
COVER STORY

MATERIAL
A former fellow now at Los Alamos studies stresses and strains in metals and other components sensitive to destructive elements.
Engineers rebuilding the San Francisco-Oakland Bay Bridge in 2013 were alarmed when new, high-strength steel rods — essentially long bolts — snapped soon after workers snugged them. The builders grew even more worried when they realized the same rods were used throughout the structure, which carries about a quarter million vehicles each day.

The culprit: hydrogen degradation from salty sea air and humidity. “That causes general corrosion of steels, and under the right situations you can evolve hydrogen gas” that diffuses into the metal and weakens it, Los Alamos National Laboratory’s Samantha Lawrence says. “Because it’s a metal under stress, that can promote cracking and ultimately failure.” Hydrogen trapped in the metal when the rods were galvanized also may have contributed to the problem.

California spent millions to correct the problems in a prominent example of hydrogen embrittlement, one of Lawrence’s key research areas. But rather than spans over the sea, she and her Los Alamos colleagues study metal in more exotic environments, such as hydrogen pipelines, nuclear reactors and weapons.

Lawrence, a Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship (DOE NNSA SSGF) recipient from 2012 to 2015, leads the Materials Compatibility Team. It’s based in the lab’s Sigma Division, which uses engineering and metallurgy to develop substances and components in support of national security.

Compatibility is an aspect of qualification, which ensures that materials are suited for particular uses. Compatibility can mean the interaction of multiple materials with each other and with their environment. An automobile’s gear box, for example, may include a magnesium housing, steel gears and a brass synchronizer, with all three metals exposed to the same gear oil. Researchers would want to know about possible reactions between the materials under a range of operating conditions, such as various oils, over time.

Lawrence and her colleagues, however, mostly study compatibility in the context of harsh environments and how metals, particularly stainless steels, high-performance superalloys and high-density metals such as uranium, behave in them. Her specialty is hydrogen exposure.

“If the United States and the world are to embrace an energy economy based on hydrogen, researchers must decipher degradation, which could erode facilities designed to store and move the gas. The challenge, Lawrence says, is creating inexpensive, long-lasting hydrogen-resistant materials.

But there also are present-day uses, such as oil- and gas-handling equipment, “an application where there’s hydrogen sulfide gas generated that can cause failures of these large infrastructure components that literally fuel our economy.”

Lawrence expanded her portfolio to include uranium when she joined Los Alamos in 2016. “From a fundamental metallurgical perspective, it has a crystal structure that is different from a common engineering alloy. It’s much more complicated.” Although uranium is a more difficult element, the information metallurgists gain about its fundamental interactions with hydrogen can provide clues to how the gas degrades standard bulk metals. Mary O’Brien, a postdoctoral researcher in Lawrence’s lab, is leading the studies.

Theoretical descriptions of atomic-scale hydrogen degradation abound — and compete — Lawrence says, but she explained three possible mechanisms for how this lightest of elements can affect a metal’s toughness or structural integrity.

Because hydrogen atoms are so small — in their most common form, just a proton and an electron — they can easily move through a metal’s atomic lattice, landing in preferred locations. Often, they settle at points where the metal is stressed, especially defects like dislocations, or irregularities in the crystal structure.

“Hydrogen will happily sit there, and it can influence the way that dislocations move throughout the metal,” Lawrence says, affecting how it deforms. “When hydrogen interacts with these dislocations and changes the plasticity of the metal, it can change how much it will stretch on the macro scale.”
Hydrogen atoms also can locate in a stress field just ahead of a crack's tip. With a hydrogen atom here, even a tiny fissure left from the metal's processing is more likely to spread under deformation.

Another place hydrogen can find a metal-based home: boundaries between the fine grains that comprise many substances. Here, hydrogen and metal atoms can bind into hydrides, which are new and distinct atomic arrangements, or phases, that differ from the parent metal.

Some hydrides are needle-shaped, Lawrence says, with atoms located on a boundary, disrupting how grains adhere. “You can promote failure along a grain boundary as a result of that hydride sitting in a particular spot.”

But when explaining how these and other general hydrogen degradation processes occur, metallurgists often disagree about the specific, atomic-level causes. Academic publications on the subject are flecked with acronyms such as HELP (hydrogen-enhanced localized plasticity), HEDE (hydrogen-enhanced decohesion) and AIDE (adsorption-induced dislocation emission), each representing a different theory.

“In the literature there’s been a healthy debate in communities saying oh, this observation suggests that HELP is the operative mechanism in this material under these conditions,” Lawrence says. “Or maybe with the same material, under the same conditions, someone else will have a result that suggests that HEDE is the active mechanism.”

In research dating back to her Purdue University doctoral studies, Lawrence suggested it’s “really a ‘both and’ effect.” For example, some metal failures show signs of brittleness. “When you look at a fracture surface, you can see flat facets where grain boundaries were,” meaning HEDE could be the operative theory. But closer examination can spot evidence of plasticity in the material’s subsurface, “which suggests that it really wasn’t a totally brittle failure. You had some plasticity prior to the fracture,” indicating a HELP-type explanation. “That maybe suggests that we have multiple mechanisms at play at the same time.”

To sort the complex factors influencing degradation and fracture, Lawrence and her colleagues test hydrogen-exposed metals’ strength under varying conditions. For example, to gauge the effect of grain size and temperature, the researchers heated pure nickel alloy specimens, some with larger grains and some with smaller grains, and subjected them to hydrogen gas under pressure.

The bar-like samples were then stored in an ultralow-temperature freezer at 223 Kelvin (-50 degrees Celsius). Then the researchers stretched them, with some bars chilled even further — to 77 K — and others at room temperature, about 295 K.

“We saw some change in the deformation behavior of the material, but that wasn’t enough to tell us what was happening,” Lawrence says. The scientists had to peer into the samples at a higher resolution, so they turned to two of the newer tools that have helped them plumb atomic-scale phenomena driving macroscale material behavior.

One, thermal desorption spectroscopy, measures the hydrogen that disseminates from a metal as it’s heated. The team put samples into a furnace under vacuum and used a mass spectrometer to study the samples as the temperature increases.

“Because you’re ramping this (temperature) over time, you also have a temporal signature for when hydrogen is extracted,” Lawrence says. By studying peaks in the spectra, the team could identify the total hydrogen loss and the tiny structures, such as grain boundaries or dislocations, it came from in the sample. That helped the scientists understand how hydrogen “was affecting the metal lattice, and then we scale that up to our macroscale mechanical behavior. Maybe we can understand why the behavior changed.”

Samantha Lawrence and colleagues used electron backscatter diffraction to acquire images of a steel subjected to a particular processing pathway and to highlight the orientation of grains (a) and the types and distributions of defects (b,c) within the structure. The technique helps them understand how processing affects the structure and performance of metals and alloys. Mary O'Brien.
The second tool, positron annihilation spectroscopy, gauges the lifetimes of positrons, the antimatter counterparts to electrons, to locate structural defects. A positron source, such as the isotope sodium-22, is sandwiched between identical metal samples. The positrons interact with features in the metal, and a detector measures those that emerge from the layered sample.

The results indicate hydrogen charging increased vacancy concentrations and vacancy cluster size (depending on the material and testing conditions) in the nickel samples, and that these were more likely to form at grain boundaries. Hydrogen-enhanced vacancy cluster distribution also made the metal stronger, but at the expense of ductility.

More recently, Lawrence and her colleagues have turned to particle beam technology, tapping facilities like the Los Alamos Neutron Science Center, or LANSCE, and the Advanced Photon Source (APS) at Argonne National Laboratory near Chicago.

“These beamline tools allow us to track very particular signatures of the material as we go through an experiment. We’re doing in situ experiments” — as materials change — “as opposed to postmortem characterizations.”

She could do such investigations outside a national laboratory, Lawrence says, but “being here makes it easier to access these tools, because I also have access to experts who know how to apply them.” Not only are lab colleagues trained to conduct these complex experiments, they’re also better able to interpret the results. “I don’t have to try to become an expert in neutron scattering techniques because I have colleagues who already are.”

Lawrence and her associates focus on specific metals, but these tools and observations are useful for studying other materials, too. “That’s one of the fun things about being a metallurgist,” she says. Most metals have, “for lack of a better term, basic rules that they follow — the underlying physics that determine their behavior are the same regardless of the class of alloys we’re talking about.”

Lawrence will apply and expand those lessons as she and her team focus on material qualification, using experiments to ensure metals are well suited for particular applications. She’s developing strategies for rapid material classification and “thinking through what type of information we need for materials qualification, particularly when we start thinking about the manufacturing pathway” for a substance.

At a fundamental level, Lawrence will continue collaborating on beamline experiments for challenging materials and manufacturing science questions, with more experiments planned at LANSCE, the APS and elsewhere.

Lawrence has a convenient sounding board for her ideas: Her husband, Paul Gibbs, is a metallurgist on a different Sigma Division team. His brother, John, a DOE NNSA SSGF alumnus, and John’s wife, Meghan, also are Los Alamos metallurgists.

“Sometimes it’s hard to leave work at work,” Lawrence laughs. “We have a nice little family network.”

In early 2022, Sigma Division managers asked Lawrence to lead the newly formed materials compatibility team, gathering existing staff and new hires. The problems and people keep her engaged and excited about her duties, Lawrence says.

“We’re frequently tasked with understanding complicated materials and manufacturing questions” few other labs face. “So we get to work on some pretty interesting problems, and I get to do that work with a really fantastic set of people.”

The important national security aspects of her work also are satisfying, Lawrence says. She cites Sandia’s motto, taken from a 1949 letter President Harry Truman wrote regarding the lab’s founding: exceptional service in the national interest.

“That resonates with me. There’s a reason that I do what I do, and that’s it.”
A fellow turns her machine-learning skills toward detecting dark matter and monitoring nuclear reactors.

By Sarah Webb
Sophia Farrell became fascinated by nature’s fundamental particles and chose to major in physics at the University of Dallas. A summer 2018 research project at the Texas A&M University Cyclotron Institute defined her next steps. While there, she used machine learning to improve methods that discriminate neutrons from gamma rays.

Farrell, finishing a Ph.D. at Rice University in Houston, was wary at first because she’d envisioned building particle detectors, not writing code. “But I loved it. And I didn’t know a thing about machine learning before or really that much about nuclear physics.” When Farrell presented the work at an American Physical Society meeting later that year in Hawaii, she delved into talks about both particle physics and nuclear security. “There wasn’t enough time in the world for me to go to all of the sessions I was interested in.”

Just a few years later, as a Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship (DOE NNSA SSGF) recipient, Farrell returned to these themes during a 2021 Lawrence Livermore National Laboratory (LLNL) practicum. Working with Adam Bernstein, she joined the WATCHMAN (WATer CHerenkov Monitor of ANtineutrinos) collaboration and focused her machine-learning lens on rare, antineutrino-generated signatures to track nuclear reactor activity from up to tens of kilometers away. This advance could make monitoring schemes more practical and politically viable.

“Sophia is a shining example of somebody with training in fundamental physics bringing her experience to bear on a practical problem,” Bernstein says. “She was able to bring her newly burgeoning skills as a machine-learning expert to a blend of applied and fundamental physics research.”

But Farrell didn’t discover physics immediately. Math “was my language,” she says. As a child, the return to school each year coincided with her birthday and felt like a present. At home, she designed experiments with a stereo to measure her younger brother’s hearing loss. “I would turn on a song and have him take out his hearing aids and see at what volume level he could hear different songs and try to piece together what his hearing loss was.”

Farrell took calculus and physics courses at Dallas. During her sophomore year, she also took humanities courses — philosophy, literature, art — during a semester in Rome. “The thing I missed most, surprisingly, was my physics classes.” She returned to Texas and chose to major in that subject.

Farrell’s undergraduate advisor and mentor Sally Hicks encouraged her to apply for summer research opportunities through the National Science Foundation’s Research Experiences for Undergraduates program. Farrell studied quantum optics for a few months after her sophomore year, but the Texas A&M stay the following summer set her graduate school course toward Rice and physics problems that rely on computing.

Farrell joined Aaron Higuera’s group to seek particles representing signatures of dark matter, the mysterious stuff theorized to comprise at least 25% of the universe. Researchers have inferred its existence from radiation patterns and galaxies’ gravitational spiraling. “It’s not made up of protons, neutrons, electrons — any of the stuff that interacts normally within the universe,” Farrell says. “But it has some mass. It just doesn’t seem to want to interact with light or with the strong force or with the weak force very much.”

To find dark matter particles, Higuera’s group works on the XENONnT (pronounced Zee-non en-ton) experiment. This collaboration of two dozen institutions and 200 scientists operates at an international laboratory deep underground in a mountainous region of central Italy.

XENONnT maintains nearly 10 tons of the inert element xenon, kept as an ultra-pure, supercooled liquid. With that unreactive material as a baseline, the team can study what happens when radioactive particles interact with the vat’s contents, measuring any changes via nearly 500 sensors. By using this pure material and isolating it from the many interactions above-ground, the physicists hope to measure and identify dark matter’s elusive signatures.

“They are all those pulses, on the top and bottom of the detector, we can reconstruct when an interaction happens in the xenon, where it happened, how much light and charge it saw,” Farrell says. “And then we’re able to infer from that whether the particle interacted with...
electrons in the xenon or with the nucleus, and how strongly and what energy it deposited.” With those results, the researchers then determine whether the reacting particle was dark matter.

Farrell helped with initial work to build the detector, which she discussed in a 2021 prize-winning essay, “Into the Darkness,” published in the 2021-2022 Stewardship Science magazine. The project hit a potential roadblock when the team discovered the electrodes that stabilized the xenon couldn’t be operated at the planned voltages. Using her data-analysis skills, Farrell helped the team troubleshoot the situation and model the next steps.

“That was really cool, getting to make statements about what my research simulations were showing about what the detector was capable of,” she says. Farrell had a say as the project’s principal investigators made key decisions based, in part, on her work. “It helped me gain my confidence that this research is accessible to second-year students. You find a project where there’s a need, and you fill that need.”

Farrell has combined curiosity, computer science skills and the ability to work through physics’ many abstract concepts, Higuera says, with “great communication skills, which is sometimes very hard to find in our field.”

As the project got back on track, Farrell continued working on urgent XENONnT challenges that required her data-analysis expertise. “I started to learn that that was my favorite way to help the experiment.” But she also remembers thinking, “I have to do machine learning on this, or my soul is going to die.”

That drive led to her core thesis work: using machine learning to filter the firehose of data from XENONnT’s hundreds of detectors. A typical research run might produce petabytes of data, but the elusive particles the team seeks are neutrinos that only weakly interact with the highly nonreactive liquid. No more than a couple hundred brief signals within that massive flood are worthy of further investigation, and only one or two signals might represent the dark matter particles they seek.

The detector changes had introduced noise into the measurements, so Farrell’s technique helped focus attention on the relevant data. Her code complements an array of noise-reduction algorithms without having to break the data into human-readable features. The good news: her machine learning results match traditional analysis methods involving humans, and they can help researchers verify their work.

The approach also uses a straightforward neural network to classify the data. It’s tempting to overengineer a solution to a problem, Farrell says. Achieving a reliable result with a simple approach engenders confidence, and “people will be more willing to incorporate that new technology in the analysis.”
The simple-solutions lesson came from Farrell’s Livermore practicum. Like her dark matter research, nuclear reactor monitoring involves seeking rare, interesting signals — in this case, antineutrinos that interact only weakly with surrounding matter. Unlike her Ph.D. work, these data are sparse with many small fluctuations, so detecting a relevant signal can take a lot of time — a limiting factor. In the past, that has required placing detectors relatively close — within several dozen meters of a reactor.

Traditionally, researchers use a method called cut-and-count to analyze many initial data plots, selecting for an energy threshold or proximity to other events and other defining features. It turns out, Livermore-collaborator Bernstein says, “that is not necessarily the most efficient way to do it.”

Farrell applied machine learning to accelerate the signals search. Initially, she wanted to use complex methods to solve the problem, she says, but Livermore staff encouraged her to start with a simpler approach. Farrell wasn’t convinced at first but found it worked. With the approach, the team can detect antineutrino signals up to 50% faster, which could allow monitoring agencies to maintain accuracy while placing detectors farther from reactors. Bernstein calls Farrell’s contribution “quite helpful because it motivated us to pursue these machine-learning techniques in more detail.”

Earlier this year Farrell continued her work on WATCHMAN, expanding and deepening that research to fill a chapter in her doctoral thesis and produce a paper for possible publication. She plans to complete her degree later this year.

Farrell brings tremendous focus to her work and is a self-starter, Bernstein says. “Working with LLNL machine-learning experts, Sophia really helped us on WATCHMAN come up to speed on this promising approach.”

To which Hicks, the University of Dallas advisor, adds: “She’s so good at helping others, especially women. Her work in getting mentoring done and getting tutoring done was really top notch.”

When not focused on physics, Farrell raises poultry, a project that began with 10 chicks and a coop in her in-laws’ backyard in 2021. “I’ve become a crazy bird lady, and I love learning about chicken science.” As a side benefit, the daily egg haul has made good gifts for friends and family.

Farrell hopes to continue applying machine learning to important physics problems at one of the national laboratories or in industry. “I really liked the dynamics of the national lab research group. They seem to enjoy their jobs and their lives a lot. The lab hires really outstanding researchers, so I had the best of the best available.”
UNMOVED BY PSYCHOLOGY, A LABORATORY RESIDENCY GRADUATE FELLOW SWITCHED TO PHYSICS AFTER AN ENCOUNTER WITH NEIL DEGRASSE TYSON. HE SOON FOUND A PATH TO REAL STAR POWER.
banks can store up to two trillion watts of power, all unleashed through structure repurposed to house the massive machine. Zebra’s capacitor Zebra, a two-story-tall apparatus in a four-story, Cold War-era generators to study plasmas’ high-energy-density (HED) physics.

As a UNR physics Ph.D. student, Childers has performed theoretical research on plasmas like those powering the stars and sparking to life in laboratory fusion experiments. One of his many presentations earned the 2022 Margaret Burbidge Award for Best Experimental Research by a Graduate Student from the Far West Section of the American Physical Society.

Childers wasn’t always on the physics track. As a UNR undergraduate, he first studied psychology, but while collaborating on a research project during his final semester, he realized the subject matter just didn’t fulfill him, he says. “I was considering what I was going to do here.” A new direction opened through an elective astronomy class. Childers met Neil deGrasse Tyson when the famous astrophysicist visited and delivered an evening lecture. “He showed images from Hubble,” Childers says. “I remember thinking to myself, I want to study black holes. I want to do astrophysics.”

Childers received his psychology degree in 2011, then enrolled as a physics undergrad the next semester. He had taken a class with Alla Safronova, research professor of physics, who leads an NNSA-funded group studying the radiative properties of high-atomic-number ions in plasmas. “Even then, it was obvious that he liked physics very much and had a solid knowledge of the subject,” Safronova says. Childers wrote his senior thesis under Safronova’s supervision and later joined her group as a master’s student.

Safronova and her team conduct theoretical research but work hand in hand with experimental teams that use powerful devices called Z-pinch generators to study plasmas’ high-energy-density (HED) physics.

In a Zebra Z-pinch, the million-amp, two-million-volt current super-heats the target, or experimental load, tearing atoms from one another and stripping away many of their electrons. That converts the load into plasma — the fourth state of matter. At the same time, the current also creates a powerful magnetic field that encircles the plasma, literally pinching and holding it together for tens of nanoseconds, until instabilities let it leak or the machine’s charge is spent. Researchers use various instruments to probe the plasma’s secrets during its brief life.

Zebra’s impressive capabilities complement even larger and more powerful DOE plasma-research facilities, such as Sandia’s Z machine at its New Mexico campus, and the laser-driven National Ignition Facility (NIF) at Lawrence Livermore National Laboratory. Both house operations aimed at triggering inertial confinement fusion (ICF).

In ICF, either a Z-pinching or a convergence of the world’s most powerful lasers at NIF creates a plasma of hydrogen isotopes and intensely compresses it long enough for nuclei to fuse, converting minuscule amounts of mass into large amounts of energy.

One of ICF’s long-term goals is to become a practical power source, and NIF recently reported an experiment that yielded more energy than the laser energy that went in, a hopeful harbinger. Experiments on Zebra aren’t meant to trigger fusion, but to study the properties of plasmas generally and advance ICF research.

With guidance from Safronova and Victor Kantsyrev, another UNR physics research professor, Childers wrestled with his lifelong tendency toward excessive ambition. “When you come into a program like this, you have all these possibilities,” he says. “To produce really compelling and effective science, you have to fine tune and focus on a small, little detail and work out from that.”

Childers chose X-rays, a small detail with big implications. “X-rays are key signatures of high-energy-density processes and atomic physics that are critical to ICF experiments,” he says.

X-rays offer a peek into plasmas because they are tossed off by electrons, which play important roles in plasmas. As they interact with each other and with ions and energy sources, electrons yield energy in the form of X-rays with spectroscopic fingerprints denoting the type of interaction that took place. X-rays can tell much of a plasma’s story, such as how hot and dense the plasma was, how many electrons were torn from atoms and how the plasma evolved. They may even offer insights into electrons’ roles in instabilities that inhibit ICF experiments. “So, studying the X-ray radiation properties provides a very powerful diagnostic tool for indirect investigation of otherwise difficult-to-observe microphysics,” Childers says.
Safronova and her colleagues are leaders in developing new ways to study plasma radiation, including X-rays. For his master’s research, Childers tackled detecting polarized X-rays, which carry clues to elusive electrons that are hotter than the rest of the plasma. They’re prime suspects in instabilities and other woes that frustrate ICF experiments.

Polarized X-rays are hard to detect, however, because the electrons that produce them are far outnumbered by cooler electrons emitting their own brand of X-rays. In an experimental plasma, most electrons are thermal; they gain their freedom from neutral atoms through elevated mass temperature. Their temperature is basically the same as the plasma’s ions and neutral atoms. Polarized X-rays come from rogue electrons called non-thermal because their higher temperature comes from some external source, such as an electron beam.

To capture more polarized X-rays, the group set up a unique experiment on Zebra. The target: four fine wires of molybdenum, which is known to shed hordes of free electrons under the right conditions, readily forming the electron beams needed to power hot, non-thermal electrons.

Instead of arranging the wires in parallel, the researchers crossed them in the middle, forming an X. This X-pinch produces a compact plasma where the wires cross. One of Childers’ tasks was helping configure a spectropolarimeter, a device Kantsyrev’s group developed with assistance from Safronova’s group. It captures both vertical and horizontal polarized X-rays, pinpointing the hot spots that emit them.

When Zebra discharged, molybdenum vaporized where the wires crossed. True to form, some of the atoms became neon-like molybdenum ions. They lost 32 of their 42 electrons, leaving 10, the same number as in a neutral neon atom. Non-thermal electrons from electron beams knocked bound electrons out of the ions’ second-lowest orbital, the L shell. Electrons from the next higher orbital, the M shell, moved down and replaced their dislodged counterparts, emitting distinctive X-rays that the electron beam energy and quantum effects polarized.

The team was thrilled to see that the spectropolarimeter had detected polarized X-rays from a high-atomic-number ion — and more of them than anticipated. “It represented some of the first comprehensive polarization measurements that were achieved in a pulsed-power Z-pinch plasma,” Childers says.

Apart from his research on polarized X-rays, Childers analyzed experiments designed to see if decreasing the wire angles aligned with Zebra’s current could yield favorable results. Before Childers joined the group, researchers had done X-pinch shots of stainless-steel wires at angles reduced from the usual 62.5 degrees to 31 degrees. Childers used computer models to examine the experimental results from stainless steel’s main components — iron, chromium and nickel.
He was beginning to flex the computational muscles he would need for his Ph.D. research and for his proposal to the DOE NNSA LRGF. He was approved to work on the theoretical side of experiments, already completed, to explore a new angle on X-pinches.

The polarized L-shell X-rays of his master’s work are driven by non-thermal electrons, which are also responsible for generating K-shell X-rays, including those labeled K-alpha. These X-rays are abundant in X-pinched plasmas because a wide range of ions and, even neutral atoms, can produce them and because non-thermal electrons induce X-ray emission more efficiently than thermal ones.

Other X-rays of interest include ones from particular ion types. For example, ions stripped down to just two electrons, making them helium-like, produce helium-alpha X-rays. Instead of responding to electron collisions, these ions emit X-rays when thermal energy makes their electrons jump up and down between inner orbitals. Rather than trying to eliminate K-alpha X-rays in favor of the other types, “the idea was, how can we maximize the production of both?” Childers says.

Childers’ analysis confirmed that the narrower X-pinched angle produced smaller, more intense hot spots that emitted more radiation, including the desired non-K-alpha X-rays and gave enhanced data on formation of the desired electron beams.

For future research, Childers may draw on work begun during his residencies at Sandia-New Mexico, where he collaborated with Stephanie Hansen and David Ampleford to analyze plasma experiments on the Z machine, which features its own K-shell emission. “Now, instead of being driven by hot, non-thermal electrons, it’s driven by photoionization from basically an ICF plasma,” Childers says.

Many Z machine experiments investigate magnetized liner inertial fusion, or MagLIF, a more complex Z-pinched style. This approach to magneto-inertial fusion uses the machine’s 20 million-ampere current to implode beryllium cylinders that are filled with fusion fuel, placed in an external magnetic field, and preheated via laser. MagLIF targets produce fusion neutrons and bright X-rays.

Childers wrote a new computational code to model MagLIF, including radiation transport in the experiments. “Ryan was an incredibly enthusiastic and energetic collaborator,” says Hansen. She notes that his work helped Sandia researchers understand the spatial origins of key emissions from their ICF targets. “His work will help refine future diagnostics.”

Safronova appreciates the impact that Childers’ work on the MagLIF code had on his growth as a scientist, saying it “provided an invaluable experience for Ryan and his future career. He has great plans on how to continue using and modifying it.”

The next step in Childers’ plans involves finding a place to continue his studies. He’s applied for research posts at the Naval Research Laboratory and at Lawrence Livermore National Laboratory, where he was a finalist for the Harold Brown Postdoctoral Fellowship. At the same time, he’s watching for opportunities at Sandia and at Los Alamos National Laboratory.

Whichever doors open, he has a path in mind: “My essential goal is to continue active research as a staff scientist at one of the national labs.”

A photo from an experimental setup of an X pinch wire-load in an anode-cathode electrode gap. Ryan Childers.
OUTGOING FELLOWS DESCRIBE THEIR RESEARCH EXPERIENCES.

**THIN SKINS PEERING INTO PLASMA**

For his Massachusetts Institute of Technology Ph.D., Patrick Adrian studied plasma’s stopping power, or how other charged particles absorb or release energy as they move through this ionized milieu. First, though, he needed tools to characterize the plasmas themselves — their density, temperature and composition.

Lacking an ideal method, the SSGF recipient developed diagnostics to use at the University of Rochester’s OMEGA laser facility. Adrian built an imaging technique that Livermore scientist Benjamin Bachmann devised for the National Ignition Facility, or NIF. The advance allowed them to observe the plasma’s density as it reached its critical temperature.

At first Adrian focused on testing the diagnostic’s many use cases, he says, but since then the project has grown to collaborations with other researchers and institutions, including Princeton Plasma Physics Laboratory and LANL. “I can really provide something for them and their experiments, and that was pretty fulfilling.”

He used the technique to assess how hydrodynamic simulation codes typically model plasmas. The work showed that among five theories that guide plasma modeling, three do a much better job than the other two. He is now applying that work to simulate inertial confinement fusion (ICF) implosions. Adrian has become an expert on charged-particle transport; he’s among the authors on several NIF-experiment papers, including the work describing fusion ignition.

For his Livermore practicum with Bachmann, Adrian looked at how an ICF shock wave rebounds from the implosion’s center. They used X-ray and other diagnostics to uncover the physics behind this dense, star-like matter. Their results refined plasma-experiment simulations.

**OVERCOMING FLASHOVER**

William Brooks is a dedicated experimentalist. The Texas Tech University doctoral candidate even has an electronics test bench at home. “I couldn’t live without one.”

Brooks, an LRGF recipient, probes the fundamental mechanisms of vacuum surface flashover, a discharge that can afflict pulsed-power devices DOE labs and other institutions use to study materials, fusion and other subjects. The machines deliver pulses of up to millions of joules in less than a millionth of a second, each crossing several insulators between the charge-storing capacitors and the vacuum surrounding the target. Flashover, Brooks says, is like “shoving a wire between two wires you’re trying to keep separate. Your power is not going where you want it.”

Stopping flashover depends on better understanding the phenomenon’s roots, particularly at the anode, the positively charged electrode. With Andreas Neuber, Brooks builds devices to recreate and measure anode-initiated flashover. The devices also were part of a collaboration with Matthew Hopkins of Sandia National Laboratories in New Mexico, where Brooks did his residencies.

On his 2020 placement, Brooks worked with Mark Savage on preparations to upgrade Sandia’s Saturn pulsed-power machine, helping deploy diagnostics for its initial performance. “I got some very hands-on experience” with setting up and calibrating instruments — “all the minutia of running an experiment that you only get” when it’s done.

In 2022, Brooks worked on a Sandia experiment similar to his Texas Tech tabletop test apparatus to produce flashover and capture data on it via high-speed photography and other diagnostics. With Adam Steiner, he processed and analyzed preliminary experimental data, helping quantify new insulators and improve the device’s design.

Brooks says the experience will help him analyze his Texas Tech experiments, which the team has tweaked to force flashover in a specific, repeatable location, enabling precise measurements and producing “almost absolute evidence that the anode is what’s breaking down.”

**BETWEEN THE LAYERS**

Metals are both strong and deformable, but at the nanoscale, materials scientists observe tradeoffs. The smaller the grains, the stronger the metals, but they’re often less ductile and more likely to crack when stretched.

To address this problem, SSGF recipient Justin Cheng uses a model material, copper-niobium nanolaminates, alternating these metals in layers tens of nanometers thick. Cheng built microscopic pillars of the metal alloys and then observed how certain interface structures simultaneously boosted the material’s strength and deformability.
Cheng’s work has used in situ microscopy techniques. That allows him to observe how physical forces alter the materials’ structure in real time. In his Ph.D. research with Nathan Mara at the University of Minnesota, he used in situ scanning electron microscopy, which resolves how micron-scale structures deform and fail when stressed.

During his Sandia practicums with Khalid Hattar, he zoomed in to the atomic scale, using in situ transmission electron microscopy to study how stress and heat induced changes in copper-niobium nanolaminates. His experience broadened his team-building and collaboration skills; he also worked with LANL’s Center for Integrated Nanotechnologies to prepare and test samples. Cheng showed that the materials’ internal structure can enhance thermal stability. Such high-temperature behavior is not common among metals with nanoscale grains. The project launched a continuing collaboration between Minnesota and Sandia.

Outside the laboratory, Cheng enjoys practicing Filipino stick-based martial arts, bouldering and film photography.

WHERE RULES DON’T APPLY

Materials at the extremes fascinate David “Alex” Chin. The SSGF recipient uses a potent laser at the University of Rochester, where he studies physics, to squeeze tiny samples of materials, particularly iron compounds. Over nanoseconds the substances reach pressures millions and billions of times that of our atmosphere.

“We’re starting to understand how things work at these extreme conditions,” where rules governing atoms and their components fail. “That’s what I find the most interesting: the breaking down of our standard understanding, what you learn in undergrad. It’s all wrong at these conditions.”

Chin bombards pressurized samples with X-rays and measures the spectrum — which wavelengths the material absorbs and which it transmits. At Rochester, he designed and built an X-ray spectrometer specially optimized for iron experiments. The device’s high resolution has produced insights into how extreme pressures distort electron orbitals, electronic structure, and crystal configurations. Now Chin is working to calculate the samples’ temperature, a historically inaccessible parameter at these extreme conditions.

“Our goal is to understand what’s happening with these systems and then how it impacts planetary evolution,” Chin says.

Chin interpreted spectrometry data on his 2021 practicum with Sandia’s Eric Harding. The researchers use spectrometers on the lab’s MagLIF experiments, in which powerful magnetic fields crush hydrogen, fusing its nuclei and releasing energy. The researchers know what magnetic field they apply to the targets. Chin’s task was determining the field strength at implosion. To extract the magnetic field data, Chin ran algorithms that fit the experimental spectral data to spectra simulated under varying temperatures and densities.

MESOSCOPIC DISLOCATIONS

Lauren Fey fell for materials science during a high school engineering camp at the University of Illinois at Urbana-Champaign. But the computer science courses she took while earning her undergraduate degree there sealed her interest in modeling new substances.

At the University of California, Santa Barbara, the SSGF recipient works with Irene Beyerlein to study multiprincipal element alloys (MPEAs). Steel and other common alloys have a dominant element, such as iron, combined with smaller amounts of other elements, but MPEAs have no principal component. Their multiple elements in a disordered atomic structure can produce desirable properties. For example, the refractory MPEAs (RMPEAs) Fey studies have high melting points, so they’re useful for high-temperature applications.

Fey uses phase field dislocation dynamics (PFDD) to model MPEAs. The code tracks dislocations — defects that move through materials — at the mesoscale, a step larger than atoms.

PFDD is currently developed at Los Alamos National Laboratory, where Beyerlein worked before joining academia. Fey served her 2021 virtual practicum at the lab with Abigail Hunter, implementing a code capability: incorporating interstitial atoms, such as oxygen or carbon, which can “diffuse around your system and wreak havoc on your dislocations.”

Fey did a similar project in 2020 during a LANL virtual summer, extending PFDD to include cross slip, or when a dislocation glide switches from one plane to another. She uses the tool for her UCSB research.

For a 2022 paper, Fey and colleagues from UCSB and the University of California, San Diego, modeled two RMPEAs. They found that greater short-range order — when atoms have a repeating pattern among nearest neighbors but are random overall — strengthened one alloy, molybdenum-niobium-titanium.

The team hopes the material can be processed to control short-range order. “So even with the same alloy we can tune the properties to what we need,” Fey says.
UNFURLED URANIUM
As a Rowan University undergraduate, Sylvia Hanna attended an American Chemical Society conference lecture about metal-organic frameworks (MOFs), Tinkertoy-like molecules whose carbon-based cages encircle metal-ion hubs. The speaker was Northwestern University’s Omar Farha, who described the use of such materials for detoxifying chemical weapons. “This is really amazing,” Hanna thought at the time. “I really want to learn more about these materials.”

For her Ph.D. research with Farha, Hanna, an SSGF recipient, has studied uranium-based MOFs. These molecules’ uranium atoms can be isolated from each other, helping researchers study their individual behavior. Hanna discovered de-interpenetration: the transition between a densely packed, entangled uranium MOF system to a more open structure. Linking the structural and energetic changes as these molecules unfurl can help with stockpile stewardship applications. One unexpected finding: Large, negatively charged uranium ions can magnetize and repel each other, behavior that’s wildly different from zirconium and other MOF metals. She’s also examined MOF structures’ stability when exposed to gamma radiation, findings that could help researchers modernize the stockpile and design strategies to capture nuclear waste.

Hanna completed a practicum at Sandia in New Mexico and has presented her research at conferences in New Zealand, Germany and around the United States. Those travel opportunities, supported by the SSGF, have shaped her career, she says, “and have honestly been one of the most fun parts of my Ph.D.” Since finishing that degree, she’s worked in the coatings division of Dow Chemical Company in Pennsylvania.

Sylvia Hanna

For the complete listings of current fellows and alumni, please visit the fellowship websites.


For more information, contact program coordinator Kris Moran, kmoran@krellinst.org, (515) 956-3696.
ON THE WATCH

A close-up view of plans for WATCHMAN, an antineutrino detector with the potential to monitor distant nuclear reactors. Learn more about a DOE NNSA SSGF recipient’s work on the project in “Sifting Rare Signatures,” starting on page 15.