Los Alamos Science and Technology Magazine | March 2016

1663

3D-printed explosives
Fine-tuning microbial metabolism
New tamper-evident seals tell all
Breaking bacterial defenses

ATOMTRONICS SURGES FORWARD

Los Alamos NATIONAL LABORATORY EST. 1943

Penguins were on the welcoming committee when members of the Los Alamos Field Instrument Deployments and Operations (FIDO) team arrived in Antarctica in November of 2015. The FIDO team supports the Department of Energy's Atmospheric Radiation Measurement (ARM) program by setting up and operating atmospheric monitoring equipment at various sites around the world for improved climate modeling. To learn more about the Los Alamos role in the ARM program, read "Sampling Sky" in the August 2014 issue of *1663*.

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1663

LOS ALAMOS SCIENCE AND TECHNOLOGY MAGAZINE

About the Cover:

For about two decades, physicists have struggled to invent a new kind of circuit in which ultracold atoms flow along controlled paths and interact in controlled ways. For some applications, including advanced sensor systems and quantum information processing (plus possible future applications that haven't been developed yet), "atomtronic" circuits represent a vast improvement over existing optical and electronic circuits. However, routing atoms through specific paths—the way light is routed through fiber-optic cables and electrons are routed through conducting wires—has proven frustratingly difficult in practice. Now, two Los Alamos scientists have successfully pioneered a reliable new approach. They constructed a tabletop system to guide coherent atoms on "wires" made of laser light that can be instantly and continuously reconfigured to trace out any circuit path—possibly ushering in a new era of atomtronic technology in the process.

About Our Name:

During World War II, all that the outside world knew of Los Alamos and its top-secret laboratory was the mailing address—P. O. Box 1663, Santa Fe, New Mexico. That box number, still part of our address, symbolizes our historic role in the nation's service.

About the LDRD Logo:

Laboratory Directed Research and Development (LDRD) is a competitive, internal program by which Los Alamos National Laboratory is authorized by Congress to invest in research and development that is both highly innovative and vital to our national interests. Whenever *1663* reports on research that received support from LDRD, this logo appears at the end of the article.

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EXPLOSIV

3D printing could revolutionize the high-

THREE-DIMENSIONAL PRINTING IS BLOWING UP. From the obvious—hand tools and chess pieces—to the less obvious—body parts and shelf-stable food—just about every item imaginable is being subjected to the two-step process of digitization and fabrication that is 3D printing.

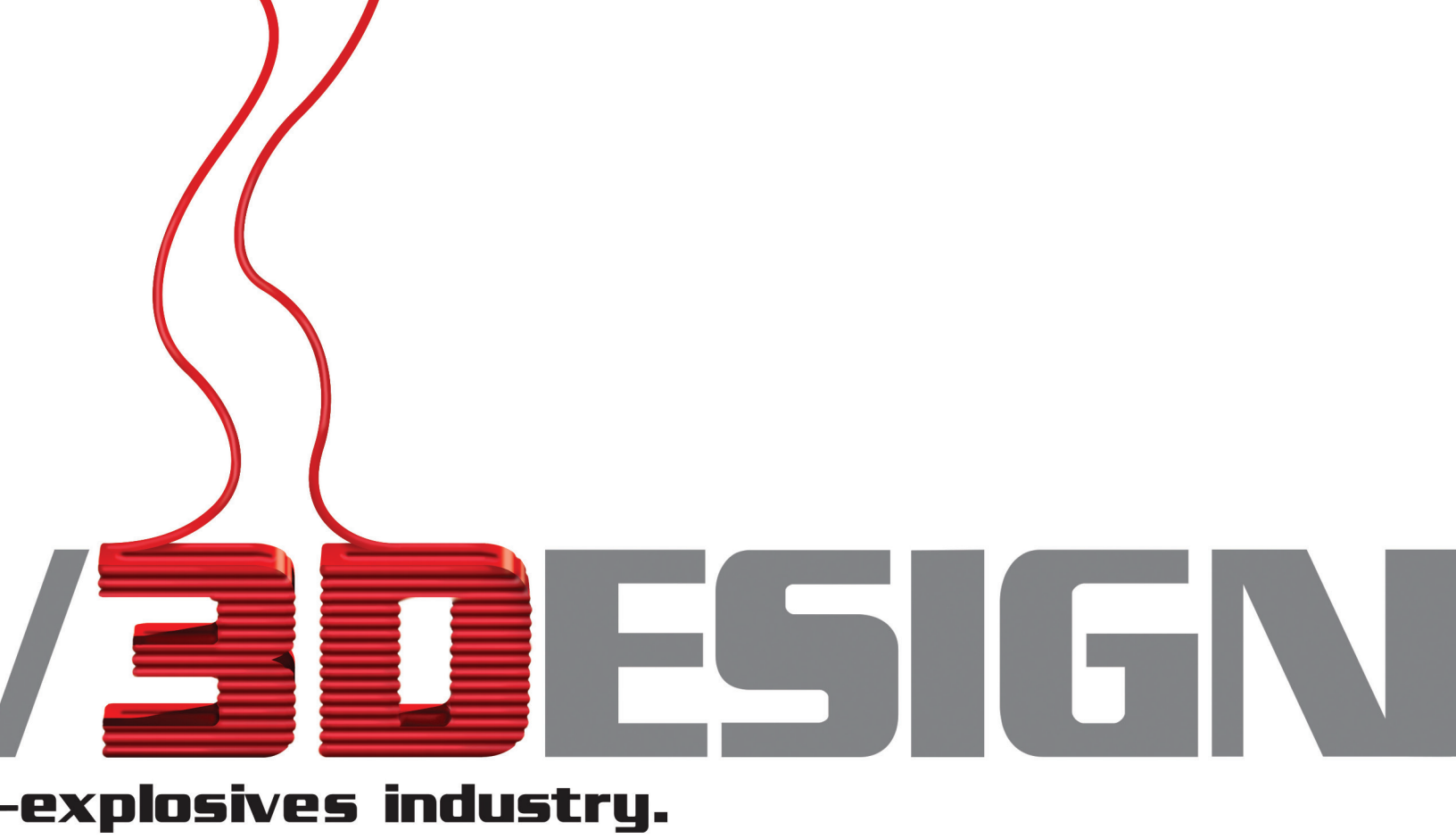
One of the factors fueling the excitement is the ease with which 3D printing can be used to build items with hollow internal spaces—that is, to build something around nothing. This task is always hard and often impossible by conventional manufacturing methods, which usually involve creating an item by removing material from a larger mass and so are referred to as subtractive manufacturing methods. A hollow ball, for example, might be crafted in one of two subtractive ways: by making a hole in a solid sphere and reaching inside to scrape out the center, then covering the hole; or by casting two separate hemispheres, sticking the halves together, and obscuring the seam. A 3D printer, on the other hand, manufactures additively by stacking thin layers on top of one another until a 3D object is formed. So it could whip out a hollow ball in no time without hidden holes or seams.

Los Alamos chemist Alex Mueller leads a team that is using 3D printing to create next-generation high explosives. Since the First World War, scientists have known that the behavior of trinitrotoluene (TNT) can be altered by the addition of certain materials, such as detergent or sand. Infusing TNT with bubbles or grains rendered it more sensitive and easier to detonate—but no one knew why, so TNT was (and still is) difficult to control. The Los Alamos team is working to understand not only what goes on inside an explosive during detonation but also how to control and tailor it through manipulation of its internal hollow spaces and microstructures. And a 3D printer is the ideal tool for the job.

One thing making 3D printing so popular is its ability to build items with hollow internal spaces.

Hot spots and not spots

Explosives are categorized as either low or high, depending on whether they burn (low) or detonate (high). Detonation involves an explosive shock front traveling through the material faster than sound can travel through it, while burning is entirely subsonic. In a conventional high explosive (CHE), such as TNT, the chemical reactions and supersonic shock front are relatively easy to initiate, and therefore CHEs are not immune to accidental detonation. Indeed, fires, accidents, or other munitions can cause a CHE to detonate



unintentionally. To reduce the risk of accidental detonation, Los Alamos supports the development of insensitive high explosives (IHEs), which are insensitive to incidental detonation. An IHE can be dropped, run over, hit with a hammer, or engulfed in flames, and it won't detonate—but it is also more difficult to detonate intentionally and can lack the power of a CHE.

So the choice would seem to be between the efficacy of CHEs and the safety of IHEs. But there might be a way to have both. The approach the Los Alamos team is taking is a sophisticated step-up from mixing soap into TNT. When inclusions such as air bubbles are introduced into a material, that material can either allow the bubbles to escape upon compression (like a sponge), or it can trap the air inside (like neoprene). High explosives can do the latter. So when the material is subjected to a shock wave, the voids (bubbles) inside collapse, which causes a rapid heating of the explosive material due to its uneven flow into or around the voids, and results in tiny points of intense heat referred to as hot spots. Up until now, high-explosive shock sensitivity—the intensity of shock required to initiate detonation—has been largely a matter of how hot spots interact at microscopic scales. These interactions can make a high explosive either very easy or very difficult to detonate. But the Los Alamos team is after something more than crude control of an on-off switch. It wants the best of both worlds: a tailorable explosive with a sophisticated arrangement of hot spots that allows for the energy release to be "tuned" while maintaining insensitivity for safety.

Printing pays off

Mueller came to Los Alamos as a postdoctoral researcher to develop materials for new LEDs (light emitting diodes). Several years ago, he started incorporating 3D printing into his work for a variety of purposes. Then, after brainstorming with some colleagues who were having trouble making off-the-shelf printers do their scientific bidding, they decided to hack one, reprogram it, and adapt it for new types of projects. That's when they began thinking about explosives and the revolution that 3D printing might bring.

"Because it's a new technology, there's this temptation to try and do everything with 3D printing," Mueller explains, "but new technology isn't necessarily always better than the old way. Using a power drill as a hammer, just because it's fancier, isn't going to be better than using a hammer as a hammer. But in this case, the new technology has made the difference from impossible to possible."

Even in the 2D world, before printing comes a lot of theory and design. The team's theoreticians, led by Brad Clements, produce exacting calculations that the experimental team then tests in the lab. Through intense iteration between theory and experimentation, the team has so far zeroed in on some key points.

During detonation, a chemical reaction zone (CRZ) races immediately behind the supersonic shock wave; the shock-compressed voids in the CRZ generate hot spots and in turn

initiate the chemical burn reaction. Because a shock front will move through different materials at different speeds, the type, size, and distribution of hot spots (collectively referred to as the hot-spot profile) can change the size and speed of the CRZ as it travels through the material—this affects the strength of the subsequent blast.

Dana Dattelbaum, a Los Alamos detonation expert, led a series of experiments that tested different ways of seeding hot spots: solid or hollow glass spheres were suspended at different densities in a gel-like liquid explosive. The physical properties of the detonation were measured and compared to reveal how, precisely, different hot-spot profiles affect the shock sensitivity, shock initiation mechanism, and CRZ. This information can help the team determine what hot-spot profile they ought to give their experimental 3D-printed explosive material. "The ability to tailor sensitivity and the resultant energy release in the chemical reaction zone would be a holy grail in detonation-physics research," Dattelbaum says. "Control and manipulation of structures at the microscopic scales through 3D printing is an exciting step toward achieving these goals."

During detonation, a supersonic shock wave races through the explosive.

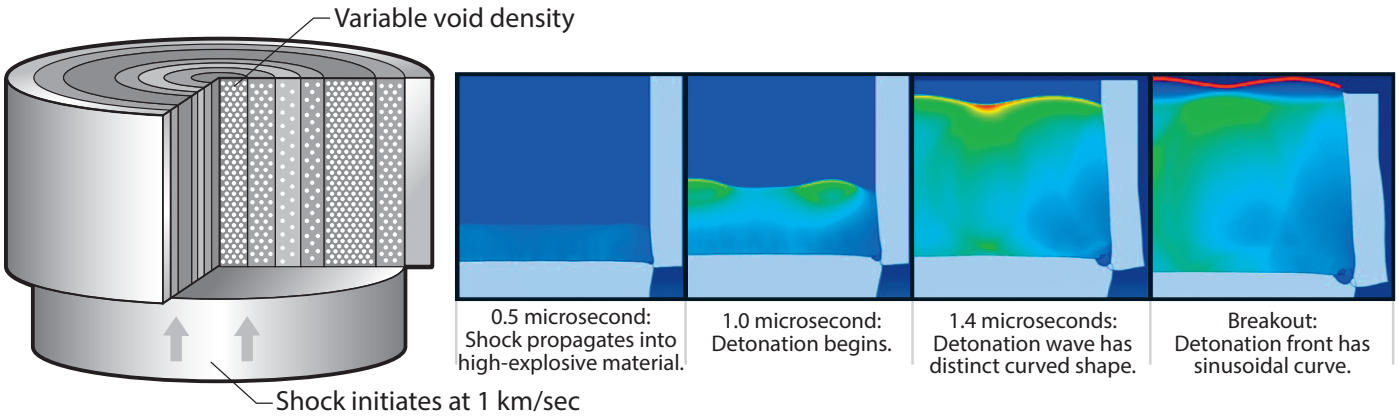
Part of what gives CHEs greater explosive power over IHEs is the way energy is released behind the shock front. In a CHE, the explosive detonates or reacts promptly while in an IHE the energy release is slower, which affects how the detonation propagates. This difference is largely explained at the mesoscale—larger than atomic scale but smaller than what can be seen with the naked eye. With archaic production methods, which usually involve taking a putty-like substance and casting or pressing it into the desired shape, the crystal structure at the mesoscale is a mess. Different discrete mesoscale regions within the material have their atomic structures aligned every which way, with no cohesion or regularity. So each region has to be initiated on its own in a rapid chain reaction. For CHEs, the chain reaction is fast and usually complete—every region initiates and contributes energy to the total explosive output. But for IHEs, each mesoscale region is just as hard as the last to initiate and some just don't go. These regions are called dead zones and are basically wasted material. In short, IHEs are inefficient.

Structures at the mesoscale are highly heterogeneous and famously difficult to manipulate. But thanks to 3D-printing technology, the door to this difficult-to-target, difficult-to-manipulate, difficult-to-measure, nebulous no-man's land has swung open. The Los Alamos team creates each mesoscale layer in a 3D-printed high explosive first by using a fine-featured nozzle to trace out the voids, then a larger-apertured nozzle to fill in the area around the voids. Each layer contains a precise number of voids arranged in the optimal hot-spot profile. No more variable regions means better reliability. No more unpredictability means better safety.

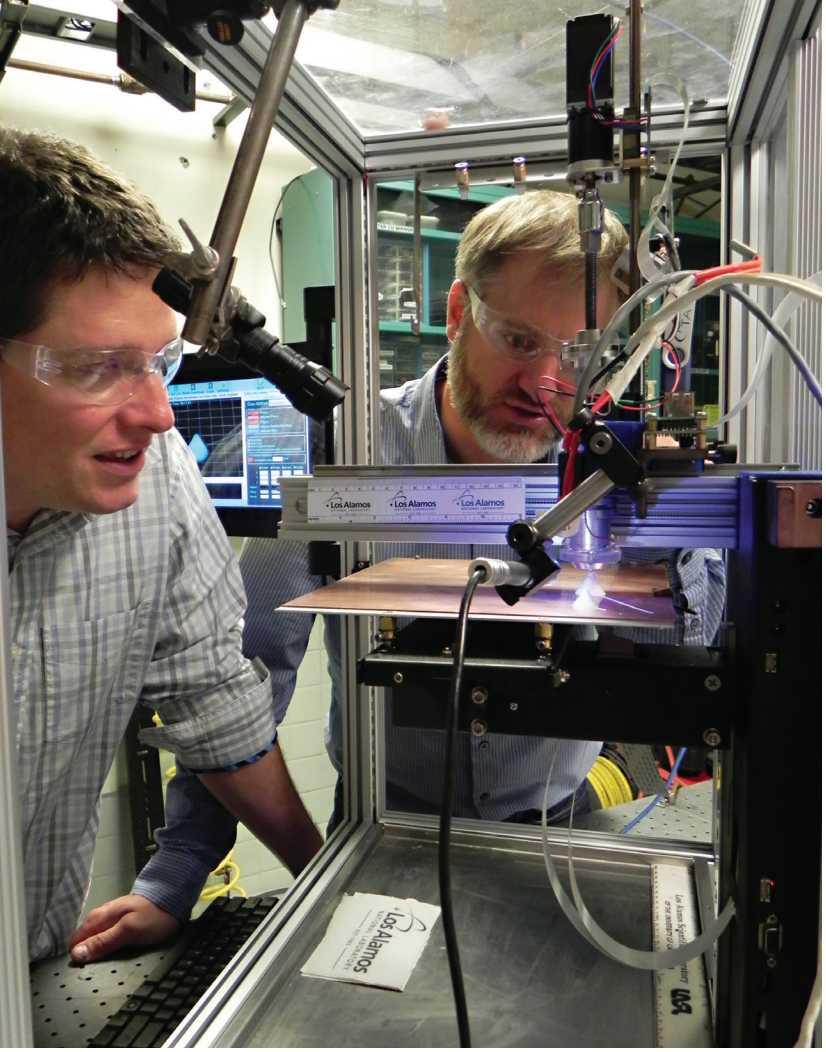
Booming industry

It's not just the manufacturing process that the 3D-printing team is revolutionizing. It's the materials themselves. It might seem that the best way to build a next-generation explosive with high safety and high performance would be to modify an existing material—either increase the safety of a CHE or increase the performance of an IHE. But that's not what these scientists are up to. They are developing entirely new materials. Bryce Tappan, who leads the chemical formulation and synthesis effort on the project, says this is part of what makes their work special. It's not a one-off or an upgrade—it's something brand new. And it's flourishing rapidly.

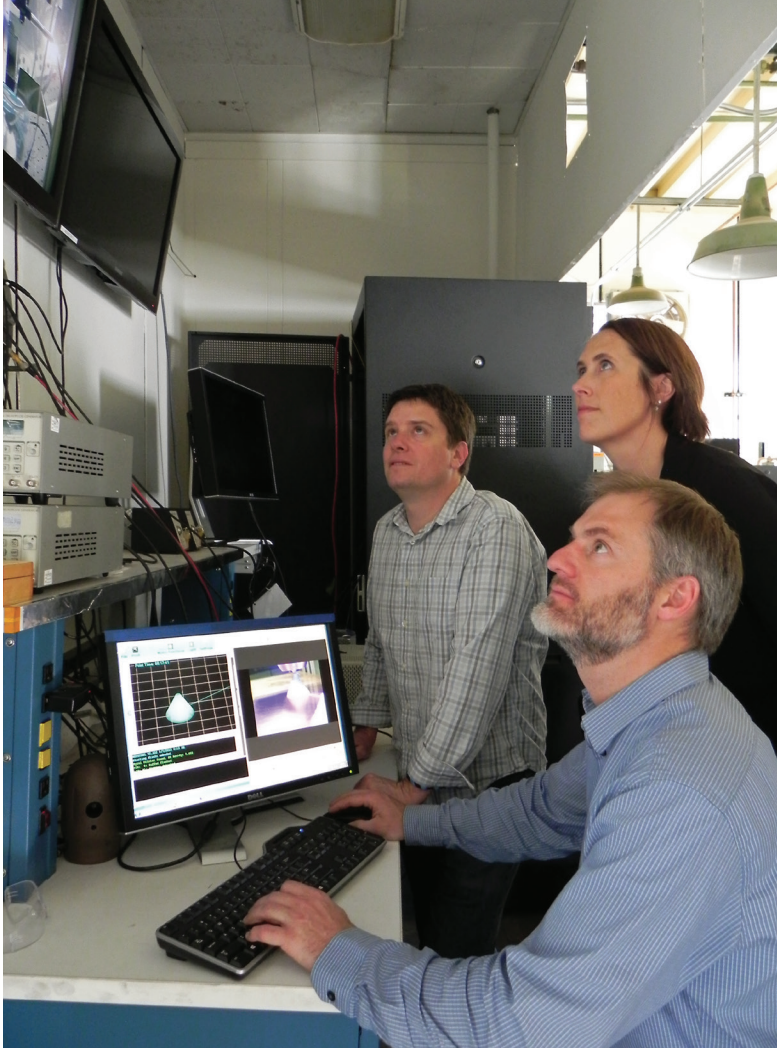
Right now the team is using two kinds of additive manufacturing—both of which can deposit layers at the desired mesoscale size. In fused-deposition modeling, the material is



Los Alamos scientists demonstrated, theoretically, how to exert unprecedented control over the behavior of an explosive by manipulating its microstructure. In this proof-of-concept simulation, they tailored the detonation front at breakout—the point at which an explosive produces an actual blast—by grading the sensitivity of the explosive material. A cylinder of high-explosive material constructed with radially varying void densities was subjected to a shock, initiated by hitting the bottom of the cylinder with a shock plate traveling at one kilometer per second. The higher the void density, the faster the shockwave propagates, and as a result, the detonation front at breakout displayed a distinct sinusoidal shape that confirmed the new level of control.



Los Alamos chemists Bryce Tappan and Alex Mueller watch as their one-of-a-kind 3D printer produces a little cone of mock explosive material. The process allows custom tailoring of internal structures that was not previously possible.



Some of the leaders of the 3D-printed explosives project watch from the safety of a control room as they print a little cone of customized explosive material (left to right: Bryce Tappan, Alex Mueller, and Dana Dattelbaum).

first melted and then extruded in thin layers that solidify upon cooling before the next layer is added, much like a hot glue gun. In optically cured additive manufacturing, ultraviolet light is used to cure each layer as it's deposited, taking it from liquid to solid in mere seconds, just like composite-resin dental fillings.

The team is revolutionizing both the manufacturing process and the explosive materials.

Los Alamos has already developed novel explosives from blended materials, and although the 3D-printing team has the capability in place to work with such mixed materials, the scientists are not yet ready to move on from single materials with air-bubble voids. Mueller is adamant about putting first things first. They're working out the physics, the chemistry, the computation, and the models. But because of the existing knowledge base at the Lab and the readily available resources, facilities, and unparalleled expertise, they are uniquely situated at the forefront of the high-explosive additive manufacturing field.

"Some people think we're just up here building new dangerous and terrifying things," says Mueller, "but really what we're trying to do is make everything a whole lot safer." LDRD

—Eleanor Hutterer

More **mesoscale and explosives research** at Los Alamos

- **Materials at the mesoscale**
  http://www.lanl.gov/discover/publications/1663/2015-january/materials-at-the-mesoscale.php
- **Re-engineering insensitive high explosives**
  http://www.lanl.gov/discover/publications/1663/2015-october/digging-crystal-deep.php

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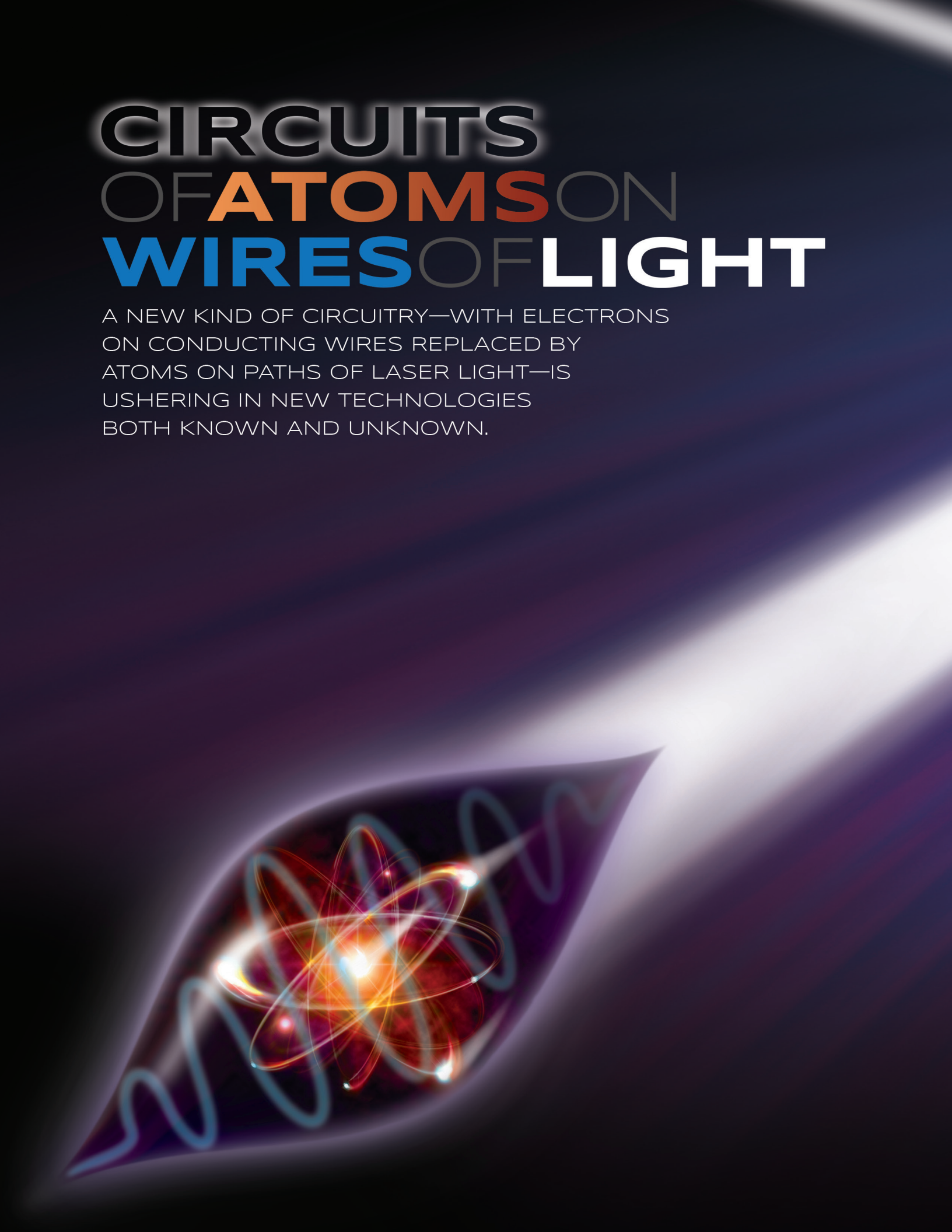
CIRCUITS OF ATOMS ON WIRES OF LIGHT

A NEW KIND OF CIRCUITRY—WITH ELECTRONS ON CONDUCTING WIRES REPLACED BY ATOMS ON PATHS OF LASER LIGHT—IS USHERING IN NEW TECHNOLOGIES BOTH KNOWN AND UNKNOWN.



WHAT ARE THE PRACTICAL APPLICATIONS of your research? For some scientific endeavors, such as controlling nuclear reactions, the answers are immediately evident. In other cases, the full potential of a scientific discovery may not be realized until much later, such as when scientists first studied quantum mechanics without knowing it would lead to the transistor, the basis for all electronic computing technology. But for some research, the practical applications come in both varieties, as is the case for a new "atomtronic" matter-wave circuitry scheme created by Los Alamos physicists Malcolm Boshier and Changhyun Ryu.

"Our matter-wave circuitry can be used for an ultrasensitive navigation system that doesn't rely on GPS, and people are deeply interested in that," Boshier says. "And I'm confident it can be used for an atom-scale lithography system that would assemble tiny devices by delivering atoms to very precise locations, like an 'atom laser pointer.' But this capability is so new, it's like developing the first electronic components and having only the faintest glimpse of what will eventually come from them."

What exactly is a matter-wave circuit? Matter waves are roughly what they sound like: waves borne of matter particles, e.g. atoms, just as electromagnetic waves comprise light. But while light waves can be manipulated with fiber-optic cables and other standard optical components, such as lenses and mirrors, and can be used to construct practical technologies like communications networks, an analogous type of control over matter waves has proven elusive. Until now, that is. And how Boshier and Ryu accomplished it is nothing short of ingenious.

Constructive interference

Every undergraduate physics student learns about the wave-particle duality: different forms of matter and energy have the properties of both waves and particles. Light waves, for example, can be separated into distinct particles called photons and detected one at a time. They have momentum and can push against matter objects (very gently at everyday light levels) just like particles. Similarly, matter particles such as protons and electrons exhibit behaviors specific to waves, such as diffraction and interference, as when water waves pass through narrow openings and cross paths, respectively.

What is actually waving in a matter wave isn't simple to describe, but it produces readily observable outcomes nonetheless. Send matter particles through two narrow slits, and their wave nature emerges: the particles are more likely to appear on the other side of the slits in locations where the waves spreading out from each slit are in phase (say, both waves near their peaks) than in locations where they are out of phase (one near its peak and the other near its trough). For some technologies, such as certain types of high-precision sensors that rely on such wave interactions, matter waves are inherently better than light waves.

In a Sagnac interferometer—the device Boshier cited as a GPS-free navigation instrument—waves sent both directions around a loop interfere at their collision point. The larger the loop, the greater the device's precision. And the degree to which the converging waves are in phase, as evident in the resulting interference pattern, provides information about how the spatial orientation of the loop has been changing. Because the wavelengths of matter waves (or light waves) are mathematically related to the momentum of matter particles

> IT'S LIKE FIBER OPTICS, BUT WITH THE ROLES OF MATTER AND LIGHT REVERSED.

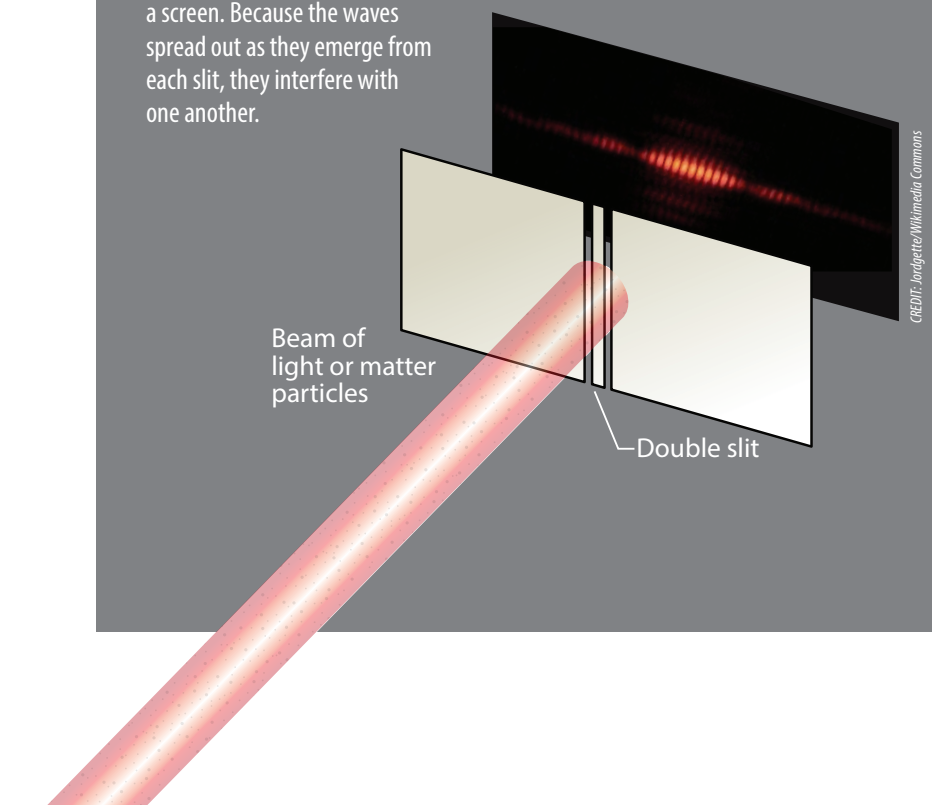
Wave-particle Duality

Matter and energy exhibit a wave-particle duality: particles act like waves and waves act like particles.

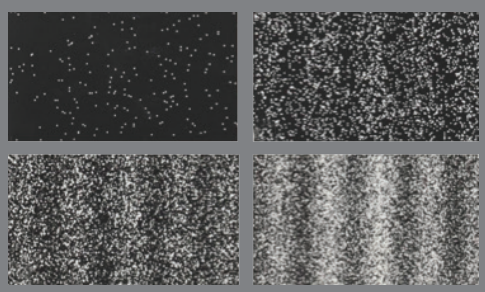
In a double-slit experiment, a beam of either light waves or matter particles passes through two slits and is then imaged on a screen. Because the waves spread out as they emerge from each slit, they interfere with one another.

With light waves, this interference produces a pattern of alternating light and dark patches on the screen.

With matter particles, such as electrons, the impact point for each particle striking the screen is recorded. Even if the particles are fired off one at a time, an interference pattern eventually accumulates, demonstrating the wave nature of particles. Successive frames show what happens as more particle impacts accumulate.



CREDIT: Jordgette/Wikimedia Commons



CREDIT: Dr. Tonomura/Wikimedia Commons

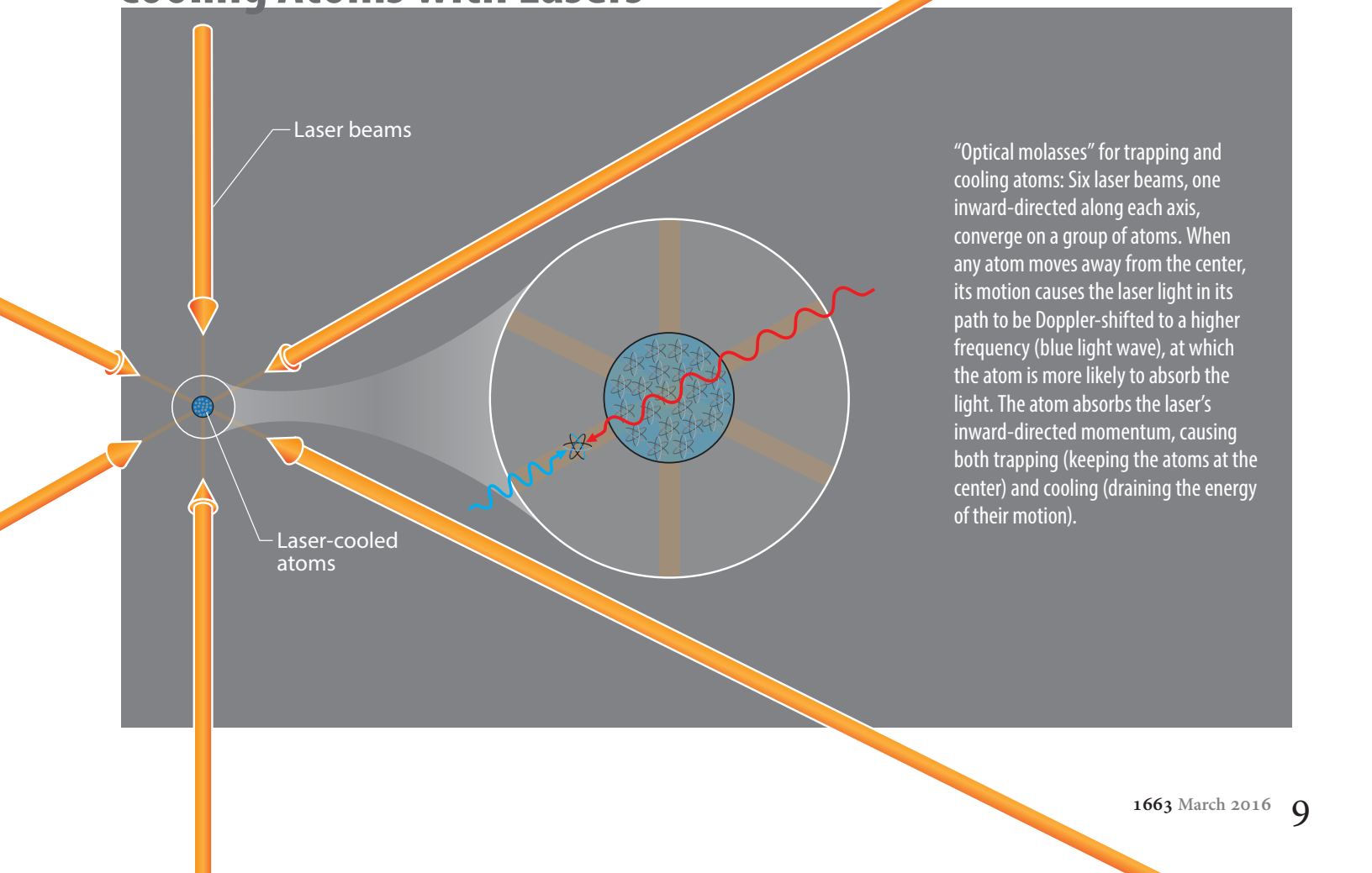
(or photons), the motion of the interferometer itself influences the interference pattern in a traceable way.

Already, Sagnac interferometers based on waves of laser light are used on submarines, essentially acting as high-end gyroscopes to keep track of how the vessel has turned and reoriented since the last time it surfaced for a GPS fix. Similarly, one can imagine special ops personnel tracking their motion through enemy bunkers, or spelunkers tracking their motion through underground caves, out of sight of any GPS satellites, with such an interferometer. There's just one problem: Sagnac interferometers accumulate measurement errors the longer they are used without calibrating off a GPS signal. Yet due to the physics involved, an equivalent Sagnac interferometer using atom-based matter waves instead of light waves would be about ten billion times more sensitive, in principle allowing errors to accumulate for much longer without significantly jeopardizing the accuracy of the readout. In addition, the atom-based version could be made much smaller than its light-based counterpart because a Sagnac interferometer's performance is proportional to the area enclosed by its main loop, and one can afford to sacrifice a little area for greater portability when there's a factor-of-ten-billion performance improvement to play with.

Switching from light waves to matter waves would similarly enhance other key navigational instruments and sensors. Interferometers that split a matter-wave beam in two can later compare the two beams for phase changes that belie wavelength changes and their corresponding momentum changes. For example, if one of the split-beam components is above the other and therefore moves through a slightly different gravitational field, then the resulting interference pattern can be used to infer subtle changes in gravitational-field strength. Such changes might be caused by changes in the underlying earth, such as when passing over a large deposit of heavy metals or a hollowed-out underground facility. And because there is no observable difference between constant acceleration-causing gravity and constant acceleration caused by anything else, the same type of matter-wave interferometer would work equally well as a high-sensitivity gravimeter or accelerometer. The latter could provide precise motion data to complement a Sagnac interferometer's detailed rotation data, for a more complete navigational instrumentation package.

Boshier and Ryu have completed successful proof-of-principle experiments for each of these applications—something people in the field have been trying to do with varying degrees of success for about 15 years. The missing element, now in place, was the ability to confine and control atoms in circuits of any configuration.

Cooling Atoms with Lasers



"Optical molasses" for trapping and cooling atoms: Six laser beams, one inward-directed along each axis, converge on a group of atoms. When any atom moves away from the center, its motion causes the laser light in its path to be Doppler-shifted to a higher frequency (blue light wave), at which the atom is more likely to absorb the light. The atom absorbs the laser's inward-directed momentum, causing both trapping (keeping the atoms at the center) and cooling (draining the energy of their motion).

Canvas of light

Creating useable matter waves relies on two main achievements: establishing a coherent collection of atoms, so that each atom contributes to the same interference pattern without canceling one another out, and steering them along a narrow path akin to a wire. Everyone in the research community seems to agree on how to accomplish the first objective, but the leading approach for the second objective has long been plagued with difficulty. The general idea was to construct nonphysical wires for the matter waves with carefully arranged magnetic fields. But because the magnetic fields would have to be almost perfectly smooth, the surfaces of the metal used to produce them would need to be comparably smooth. And so far it has proven impossible to create conductors with sufficiently smooth surfaces at the nanoscale.

CIRCUITRY MADE OF LIGHT CAN BE INSTANTLY RECONFIGURED TO SUIT ANY NEED ON THE FLY.

Boshier and Ryu decided to go another way entirely. Instead of magnetic fields, they chose to confine, align, and drive rubidium atoms with lasers, the electromagnetic waves of which include electric fields that oscillate back and forth. With each reversal, these electric fields rearrange the atoms' electrons to make them align with the electric field. If the field at a given instant is oriented in such a way as to push electrons in a particular direction, then each atom's electrons slide slightly that direction while still remaining bound to the atom.

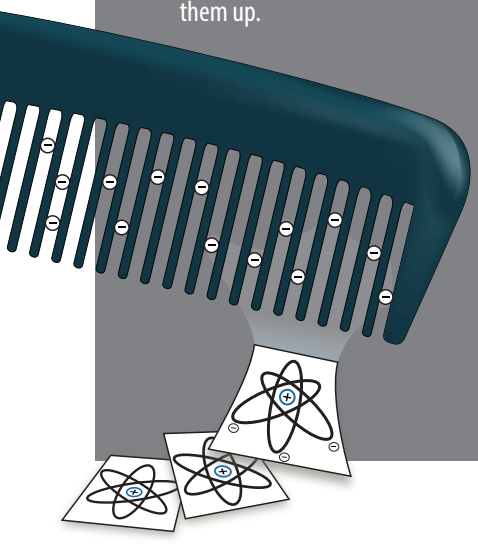
The same thing happens when a plastic comb is negatively charged after dragging electrons off of someone's hair, and then brought close to a shred of paper. The electrons in the paper are pushed away by the negative-negative repulsive force. Then, because the paper's positively charged atomic nuclei are, on average, slightly closer than its electrons to the negatively charged comb, the paper is attracted to the comb.

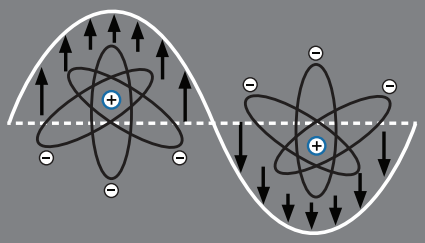
Similarly, Boshier's and Ryu's atoms are attracted to the highest-intensity part of the laser-induced electric field. Therefore the atoms won't drift away from the laser light. And each time the laser's electromagnetic wave reverses direction, the atoms' electrons shift in response, so the atoms continue to be drawn toward wherever the light is most intense. In this way, the lasers trap the atoms. Moreover, the same approach can be used to start the atoms moving along a circuit by creating a laser-intensity gradient to attract them toward the brightest region. Then, because the whole experiment takes place in a vacuum, the atoms maintain their motion even after the gradient is discontinued because there is no friction or air resistance to slow them down.

Controlling Atoms with Lasers

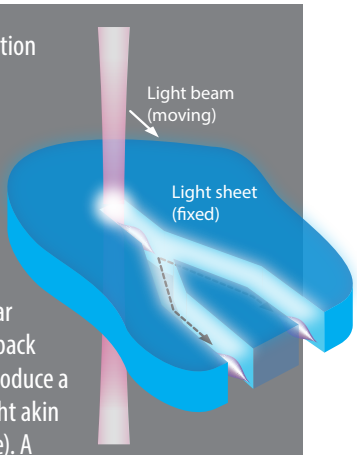
An electric field causes materials to polarize, slightly shifting their positive and negative charges into a configuration that attracts the materials toward the source of the electric field.

A comb strips electrons from hair, giving the comb an overall negative charge, which produces a corresponding electric field. Scraps of paper near the comb become polarized as a result (indicated by the stretched atom on the uppermost scrap), allowing the comb to pick them up.

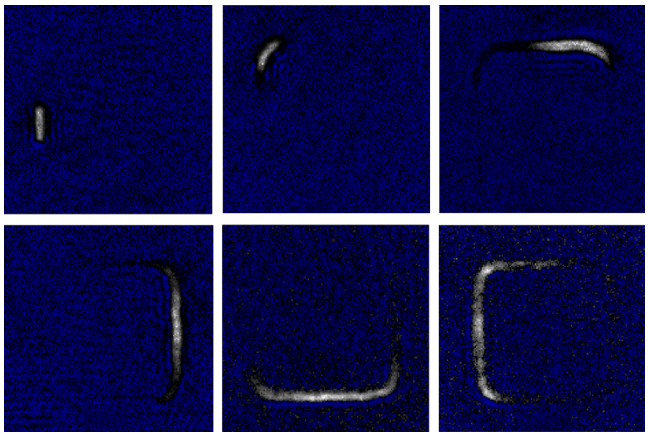


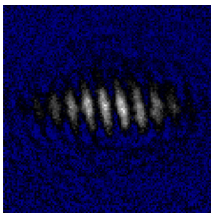


Electric fields intrinsic to laser-light waves have the same effect: nearby atoms become polarized and are therefore drawn into the laser beam and held there. As the laser-light wave oscillates, its electric field reverses direction, but that causes the atoms' polarization to reverse direction too, so the force of attraction between the atoms and the laser beam is unchanged.

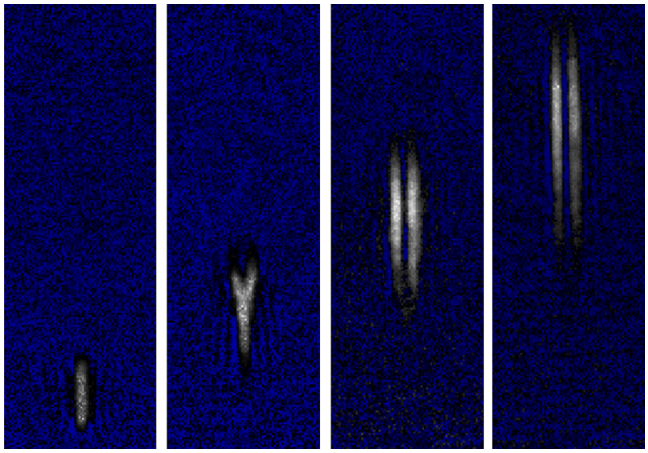


To guide matter waves, electric fields from a laser beam are used to trap atoms and channel them along a particular path. One laser scans back and forth rapidly to produce a horizontal sheet of light akin to a circuit board (blue). A second laser (pink) pierces through the light sheet perpendicularly and scans about rapidly as well, tracing out a circuit pathway on the horizontal light sheet. The second laser is focused so that its most concentrated, most intense part intersects the horizontal light sheet, so the atoms are tethered to the circuit path marked by the intersection of the two beams. The path can do anything; shown here, it forms a Y-junction, one of the forms successfully demonstrated by Los Alamos researchers.





Los Alamos researchers validated key aspects of matter-wave circuits, including bends (upper panels), splits (lower panels), and interference patterns from split beams (right).



Two perpendicular lasers sustain the matter-wave circuitry. The first sweeps from side to side, tracing out a sheet of light to act as the circuit board. The side-to-side motion is too rapid for the trapped atoms to "notice," forming the illusion of a smooth light sheet, in much the same way that individual frames in a 24-frame-per-second animation change too rapidly to notice, forming the illusion of smooth motion. The second laser is oriented vertically and adjusted so that its focus is narrowest (most intense) where it crosses the plane of light from the first laser. This second laser traces out a path, effectively painting a wire on the light-sheet circuit board.

"If we want our atom stream to turn, we paint a bend in the circuit with the vertical laser," Boshier explains. "Our lasers adjust much more quickly than the atoms move, so we can easily change the circuit at any time by painting different lines ahead of the atoms. The result is a lot like fiber optics, but with the roles reversed: it's light guiding matter instead of matter guiding light."

The atoms move along the painted circuits at about 20 millimeters per second. That's much faster than electrons typically "drift," in physics parlance, through a wire. But because the wire is chock full of conduction electrons, even a very slow overall drift can convey a large current of electricity.

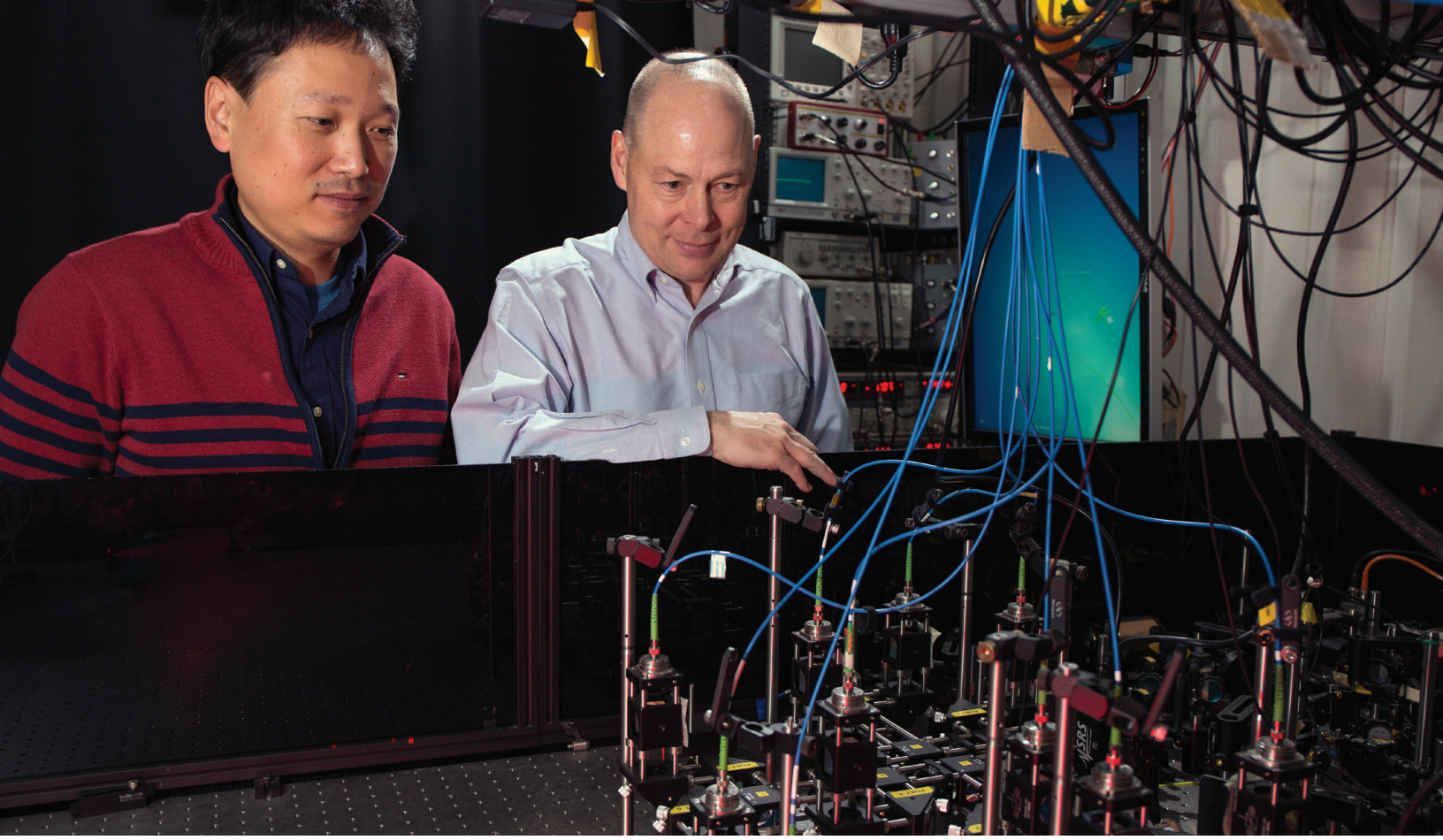
Boshier and Ryu accomplished something similar with matter waves, too—flooding an entire painted circuit with atoms. The result is a superfluid atom circuit, analogous to the superconducting electrical circuit often used in ultrasensitive magnetometers called SQUIDs (superconducting quantum interference devices). The superfluid matter-wave circuits recently proved successful in detecting rotation and might further help to probe new aspects of fundamental physics. But as with matter-wave circuitry in general, their full impact is difficult to predict so early in their existence.

Cold shoulders of giants

Making matter-wave circuits functional depends on getting all the atoms into their lowest-energy, or ground, state and keeping them there. Whether turning, splitting, or interfering, the atoms must remain in the ground state. Such a collection of atoms in the ground state is called a Bose-Einstein condensate (BEC), and maintaining a BEC requires not only very delicate control of the laser-painted circuitry, but also very, very cold atoms to start with.

FOR SOME APPLICATIONS, MATTER WAVES ARE INHERENTLY BETTER THAN LIGHT WAVES.

Just how does one cool a small collection of atoms? With more lasers, of course! In conjunction with a magnetic field to help keep the atoms in place, six laser beams are trained to converge on the atoms from each direction—left and right, ahead and behind, and above and below. The lasers are chosen at a frequency slightly lower than the peak frequency for the atoms to absorb the light. If a particular atom happens to be moving to the left, it will experience higher-frequency light waves coming from the left-side laser and lower-frequency light waves from the right-side laser due to the Doppler effect. (This is the same phenomenon that causes sound waves from a police siren to be higher pitched when the cop car is approaching and lower pitched when receding.) Therefore the leftward-moving

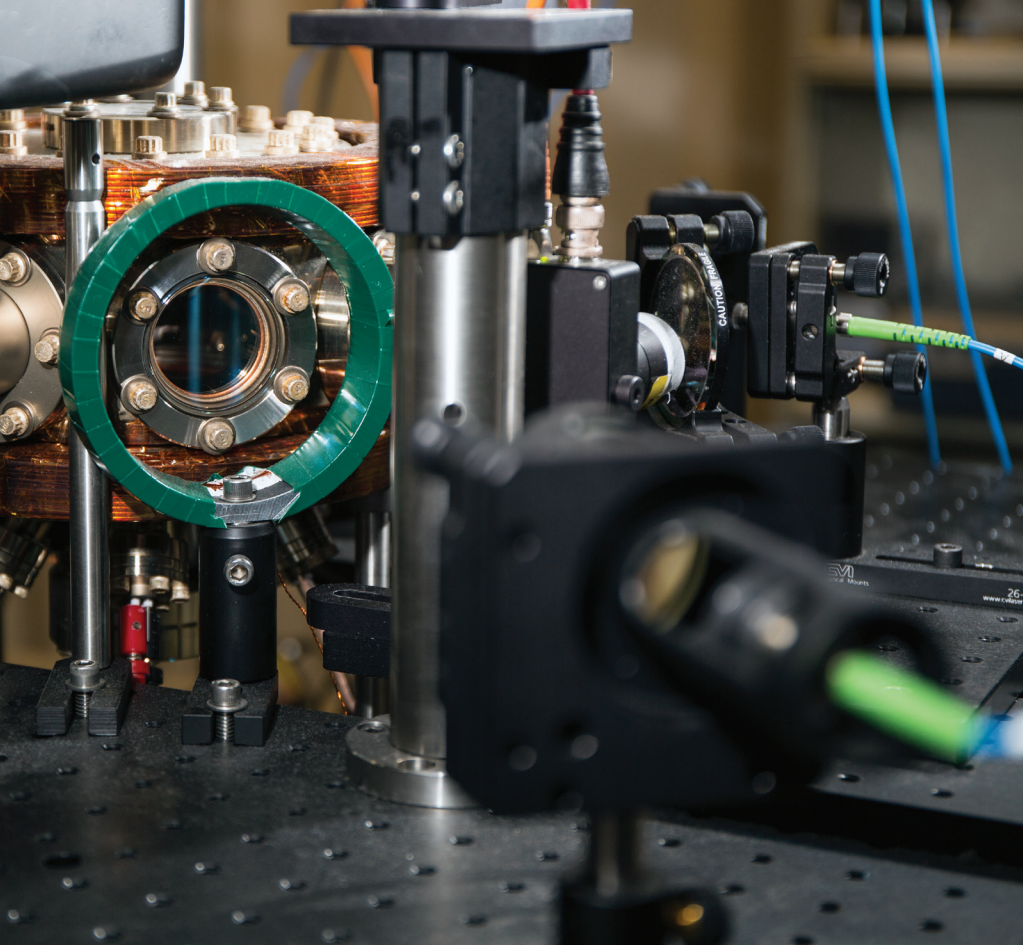


1 Changhyun Ryu (left) and Malcolm Boshier stand by their forest of lasers. Fiber-optic cables (blue) send the laser beams off to the duo's matter-wave circuit experiments.

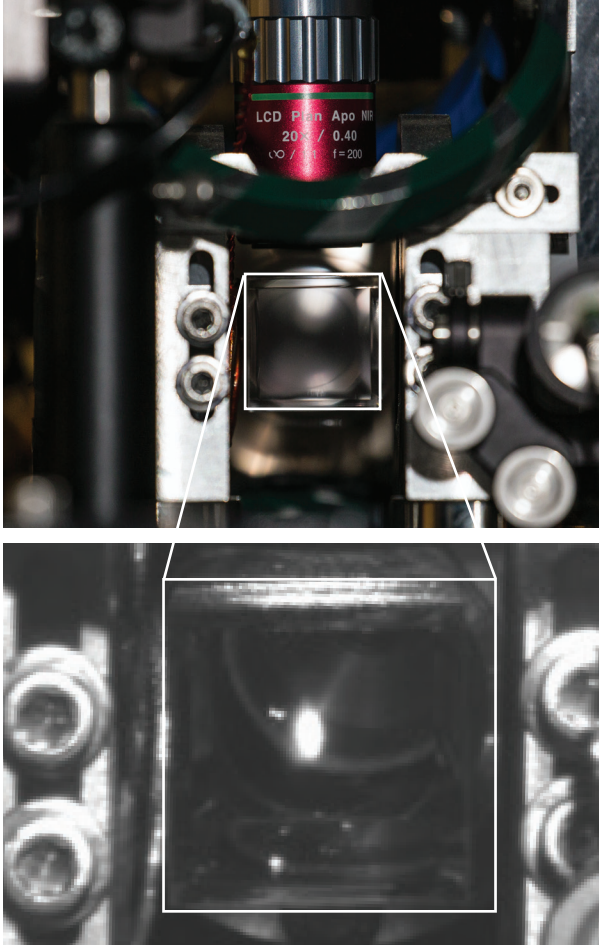
atom is more likely to absorb laser light from the left, the momentum of which pushes the atom to the right. The converse is also true: an atom moving to the right is more likely to be pushed to the left. Therefore these two lasers, together with the others pointing along the forward-backward and up-down axes, sap the atoms' motion—an effect sometimes referred to as "optical molasses." Whatever direction atoms are moving, the combination of lasers slows them down, making them sit relatively still at the center. And even though the atoms gain energy by absorbing laser light, they immediately re-radiate that energy away, so the lasers don't heat the atoms. On the contrary, the lasers produce a profound energy drain by slowing the atoms, cooling them to microkelvin temperatures—millionths of a degree above absolute zero—but still not quite cold enough.

To make coherent matter-wave circuitry, the atoms must be in an even colder BEC at 20 nanokelvins (billionths of a degree). The extra nudge colder happens similarly to the way humans cool by sweating: an evaporation process "boils off" the most energetic atoms from the sample (or the most energetic water molecules from the skin), reducing the average temperature of the ones left behind. After releasing the atoms onto the laser-light sheet upon which the matter-wave circuits are painted, Boshier and Ryu dial down the laser-trapping intensity to allow energetic atoms to evaporate away. The evaporation must be quite pronounced to achieve nanokelvin temperatures in the atoms that remain behind; all but the coldest few atoms out of every hundred thousand are allowed to leave.

Fortunately, while the laser-painted matter-wave circuitry application had to be largely invented from scratch, the technology for achieving a cold BEC didn't. In the past 20 years, trapping atoms with lasers and sustaining a BEC each resulted in a Nobel Prize, and each has become somewhat commoditized since. The former has evolved into an off-the-shelf device called a magneto-optical trap; it's a glass box a few inches across, with six laser entry points, sandwiched between electromagnets. The latter is also manufactured commercially, typically the size of small refrigerator but getting smaller,



2 The lasers (blue cables with green connectors) are directed through windows (inside green ring) into a magneto-optical trap. Four other lasers entering from other directions join the two visible here, converging to both trap and cool a collection of atoms called a Bose-Einstein condensate.



3 (Upper frame) The atoms are then shuttled to a glass box (beneath red cylinder) within a second magneto-optical trap. There, after further cooling, two more lasers create an optical circuit for the atoms to follow. One of these (not visible here) creates a horizontal sheet of light to act like a circuit board, while the other (red cylinder) paints the wires on it. (Lower frame) A monochrome infrared camera reveals a glowing bead of light coming from the trapped atoms as they absorb and re-emit laser light.

with tabletop systems and handheld components undergoing research and development. Even the painting lasers are the same mass-produced kind found in DVD players. It appears eminently possible that matter-wave technology could become both powerful and portable in the years to come.

Call of the wild frontier

Guided ultracold matter waves are the key to an emerging field—one promising enough to have the compelling name atomtronics but so new that most of its potential applications have yet to be demonstrated. Many researchers are interested in atomtronics, believing it will prove useful, maybe even transformative, in a variety of ways. One major application may turn out to be quantum computing. Another seems likely to be advanced signal processing. But whatever the application, it will rely on components analogous to those found in electronic and optical circuits, such as batteries, diodes, and transistors. Many such atomtronic-equivalent components have already been demonstrated by other researchers, and now Boshier and Ryu have added the critical missing link: a reliable, flexible method for joining these components together to make complex atomtronic circuits. They invented a system for launching BEC atoms into the laser-drawn wires and carefully adjusting the action of their lasers to guide matter waves around corners without damaging their ground-state coherence. They successfully created beam splitters and interferometers and used them in proof-of-principle demonstrations of advanced rotation and acceleration sensing systems.

And they have done it all with the ultimate in flexible circuitry: wires made of light that can be instantly reconfigured to suit any need on the fly. LDRD

—Craig Tyler

Resisting Bacterial

Los Alamos scientists are taking an in-depth look at how bacteria defeat death-by-antibiotics.

SOME BACTERIA ARE ESPECIALLY TOUGH. For billions of years, bacteria have evolved numerous mechanisms to protect themselves from toxic chemicals in their environment—some of which we humans now use as antibiotics. Applying their time-tested methods of thwarting chemical threats, these hardy microbes are responsible for nearly two million antibiotic-resistant infections annually in the United States.

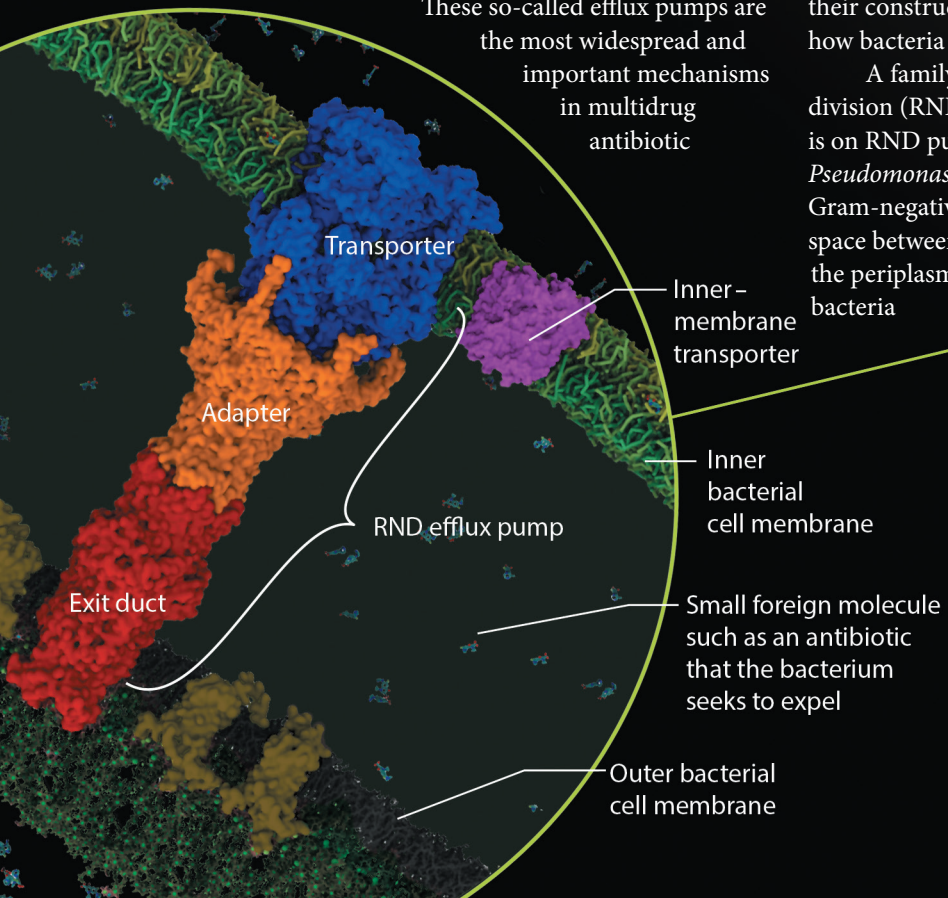
Bacteria have developed many types of defenses. Like layering for winter, some microbes wear complex coatings to serve as physical barriers to the outside world. In addition, bacteria can literally stick together to create an even stronger barrier and communication network, through which they share their defense strategies. Bacteria have even developed mechanisms to spit out any foreign toxins that get through the barriers. But if those toxins are antibiotics, intended to protect a patient against the targeted bacteria, then the patient's ability to conquer the infection might be compromised.

This spitting-out system is made possible by a set of proteins that work together as a molecular machine to pump the antibiotics out of the bacterium. These so-called efflux pumps are the most widespread and important mechanisms in multidrug antibiotic resistance. However, a complete and quantitative picture of efflux-mediated resistance is lacking. And this is a problem because bacteria are becoming resistant to more and more of the available antibiotics, putting humanity on the brink of a public-health crisis.

A multidisciplinary team of Los Alamos scientists is working on a project to understand how efflux pumps work. The researchers' goal is simple: to deactivate the bacteria's efflux pumps, thereby preventing the world's supply of antibiotics from becoming defunct. [*To learn more about the problem of antibiotic resistance, see "The Mold Rush" in the October 2015 issue of* 1663].

Gnana Gnanakaran, a theoretical biologist at Los Alamos, is the lead for the project targeting bacterial efflux pumps. Gnanakaran has gathered together a world-class collection of scientists connected by the Laboratory but widely diverse in their expertise. The group includes nearly 20 researchers, divided into teams: mathematicians and computational modelers, molecular and cell biologists, and structural biologists. Their task is to dissect all aspects of efflux pumps—their construction, how they pump out noxious molecules, and how bacteria regulate their production and use.

A family of efflux pumps called resistance-nodulation-division (RND) is the target of the team's research. The focus is on RND pumps from two types of gram-negative bacteria, *Pseudomonas aeruginosa* and *Burkholderia pseudomallei.* Gram-negative bacteria have two membranes, with a space between the membranes called the periplasm. These bacteria



Bacterial efflux pumps are molecular mechanisms for removing toxins—including antibiotics. Learning to thwart their operation by understanding how the pumps work, how they are regulated, and their role in bacterial communities is key to defeating a major type of antibiotic resistance.

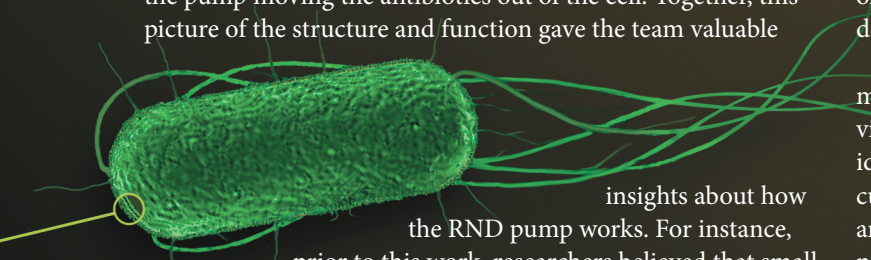
Resistance

also have many types of efflux pumps—some that span just one membrane and others, such as the RND, that span both. Together, these characteristics make gram-negative bacteria seemingly indestructible.

"We want to learn more about the assembly of these pumps and how they are utilized so that we can disable them to ensure antibiotics stay inside the bacteria," Gnanakaran says. Furthermore, a few compounds already manage to clog efflux pumps, so the researchers want to know more about those inhibitory mechanisms so more effective drugs can be designed.

Structural biologist Tom Terwilliger and his team approached understanding RND pumps by first looking at models of protein structures other researchers had made using various protein visualization techniques. RND pumps are made up of three proteins that work together to span the two membranes of the bacterium—a transporter stuck in the inner membrane, an adapter that holds the whole thing together in the periplasm, and an exit duct stuck in the outer membrane.

Using this information about the RND structure, Gnanakaran and other theorists used computer simulations to suggest how the proteins might fit into the inner and outer membranes. They identified channels through the pump where the antibiotics might enter and developed an atom-scale computer model to demonstrate the function of the pump moving the antibiotics out of the cell. Together, this picture of the structure and function gave the team valuable insights about how the RND pump works. For instance, prior to this work, researchers believed that small and large molecules entered the RND pump differently, but the Los Alamos model suggests that antibiotics of all sizes are first pushed into the periplasm by a separate type of inner-membrane transporter and then move into the RND pump to exit the cell.



"We hope to visualize this mechanism directly by determining the three-dimensional structure of RND pumps from *Burkholderia pseudomallei* with antibiotics bound to them," says Terwilliger. His team has obtained crystals of these proteins (bound with antibiotics) and plans to use x-ray diffraction to visualize the proteins in these crystals.

However, Gnanakaran's vision is to understand more than just the structure and function of the proteins; by investigating the genetic regulation of the RND pump and bacterial cells' interactions with each other, he hopes to elucidate more about the pump's overall use. Cell biologists Goutam Gupta and Kumkum Ganguly and their team carried out this portion of the project by using a knockout strain—one that does not have the gene to produce an RND pump. The knockout allows the researchers to study what happens when antibiotics accumulate within an organism that cannot make an RND pump. By sequencing the genes that the knocked-out bacteria turned on at specific points in time, the scientists inferred which proteins were being made—and found an overexpression of other types of efflux pumps.

"This is a really important observation," says Gnanakaran. "This means the bacteria can compensate for the loss of one pump by producing others."

But that's not all. Bacteria live in tight-knit communities and use specific molecules to communicate with each other. These molecules can signal the need to create a biofilm—a network of protein, DNA, and sugar that helps bacteria stick together as a barrier against intruders—by stimulating specific gene networks. When the Los Alamos team studied an over-expresser strain of bacteria, one that has a much higher number of pumps at work, it found there was also an increase in the formation of biofilms and the production of virulence factors, which are molecules that make a microbe more pathogenic. This further demonstrates that when foreign molecules, such as antibiotics, are prevalent, bacteria create more pumps to get rid of the molecules and tell their neighbors to stick together and do the same.

Now, the team has developed models to describe mathematically the interconnections among bacterial metabolism, virulence, biofilm formation, and antibiotic resistance to identify novel treatment strategies. These models go beyond the current conventional models in describing the accumulation of antibiotics inside bacteria. They illustrate how these interconnections define cellular states and can vary between pathogens.

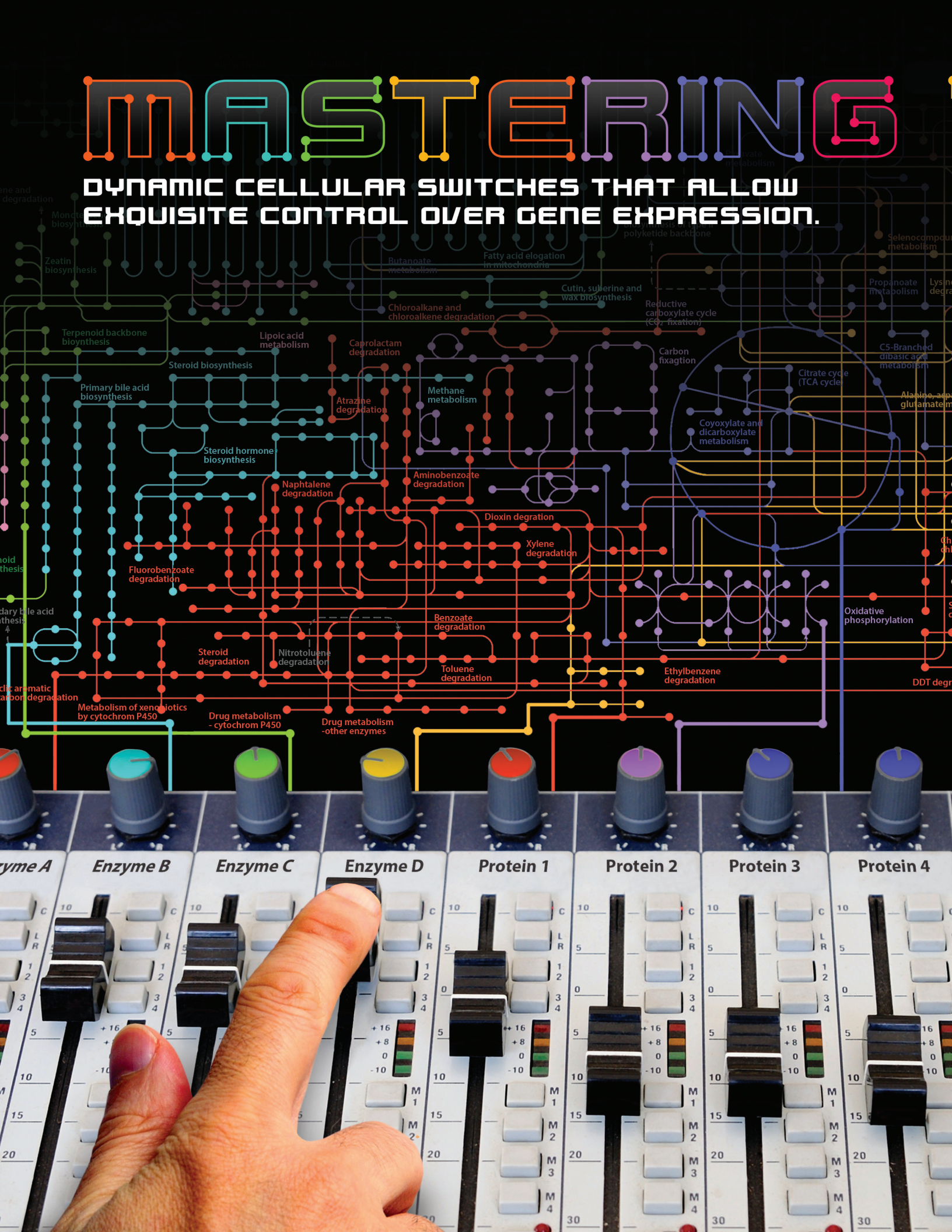
This type of approach that examines different systems—such as how proteins work together as a machine, the genetic codes that control these machines, and the relationships between individual bacteria—is often referred to as systems biology. By evaluating these integrated models, the research team hopes to identify drugs that can simultaneously avoid multiple pumps.

With such highly evolved resistance strategies, humans face an all-out war against bacteria that will do anything they can to survive. Although there are many factors contributing to the looming antibiotic-resistance crisis—including the overuse of antibiotics and a deficit in developing new ones—a comprehensive understanding of how bacteria defy drugs in the first place is an invaluable piece of the puzzle. LDRD

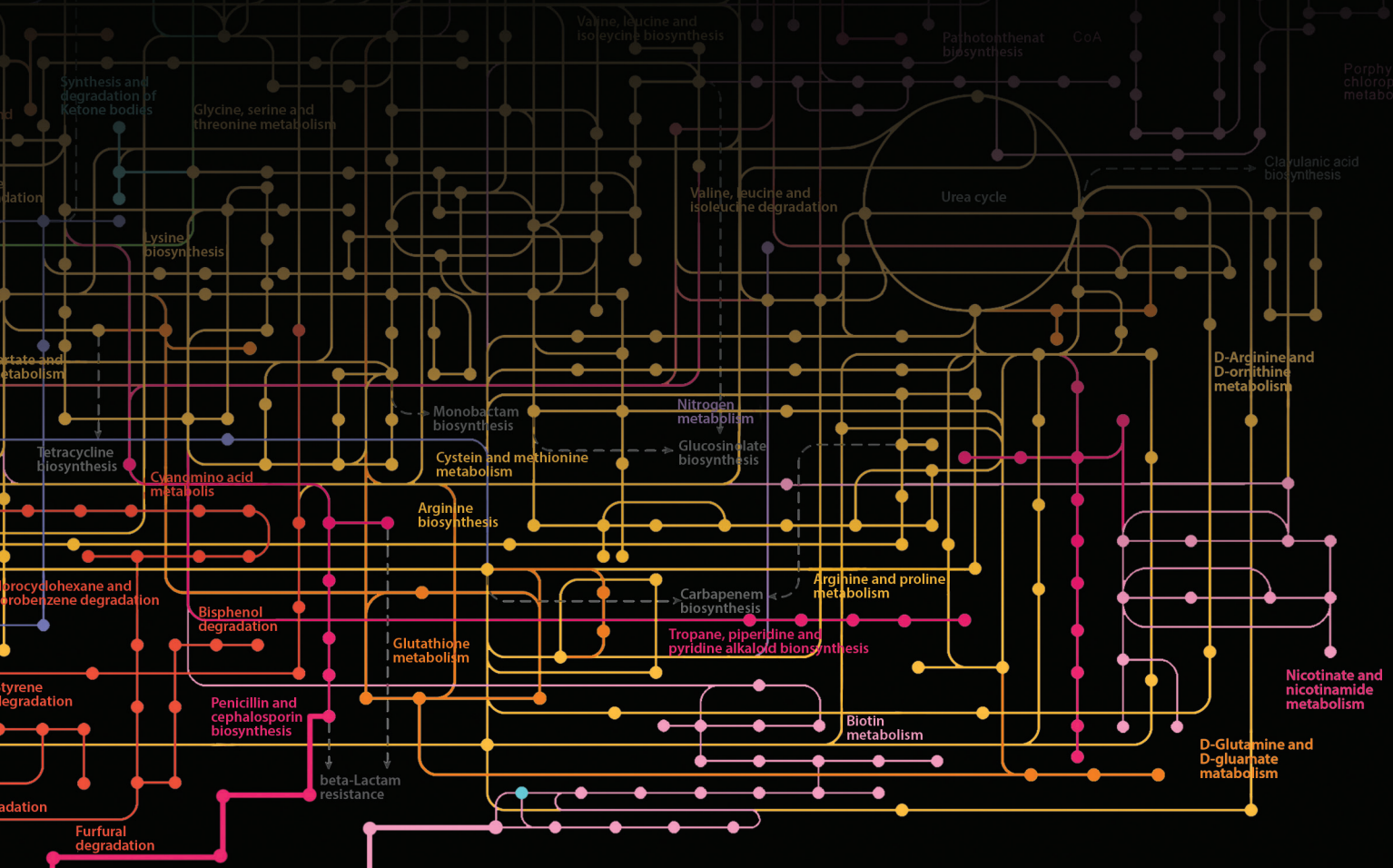
—Rebecca McDonald

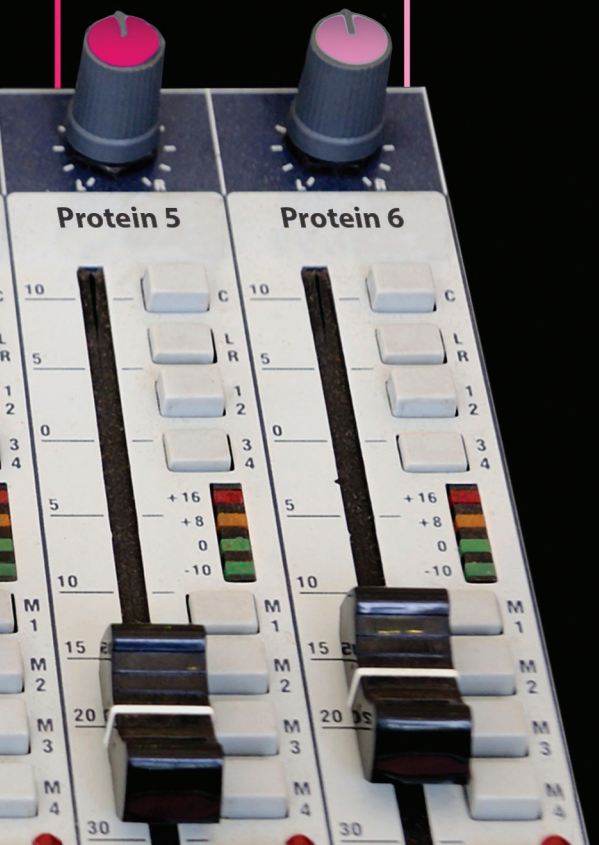
MASTERING

DYNAMIC CELLULAR SWITCHES THAT ALLOW EXQUISITE CONTROL OVER GENE EXPRESSION.



THE MIX





THE STUFF OF LIFE is widely agreed to be deoxyribonucleic acid, or DNA. The stalwart double helix has become iconic as the molecule that encodes and ensures a living thing's genetic stock. But add two atoms—an oxygen and a hydrogen—and instead of DNA you get its wily sibling, ribonucleic acid, or RNA. Arguably the more charismatic of the two nucleic acids, RNA is less familiar than DNA outside of scientific circles.

Established dogma simplifies RNA to the intermediary between DNA and protein—the gofer that shuttles protein production instructions from a cell's nucleus to its outlying and scattered protein production factories. But RNA is far more involved than that. Yes, the messenger that carries instructions from the nucleus is made of RNA. But so is the message itself, the protein production machine receiving the message, and also the handler molecules that wrangle protein building blocks from the cellular ephemera and deliver them into that machine. Many viruses use only RNA to encode their genomes, and RNA regulates gene expression in higher organisms at just about every step along the way from mitosis to apoptosis—that is, from a cell's creation to its destruction.

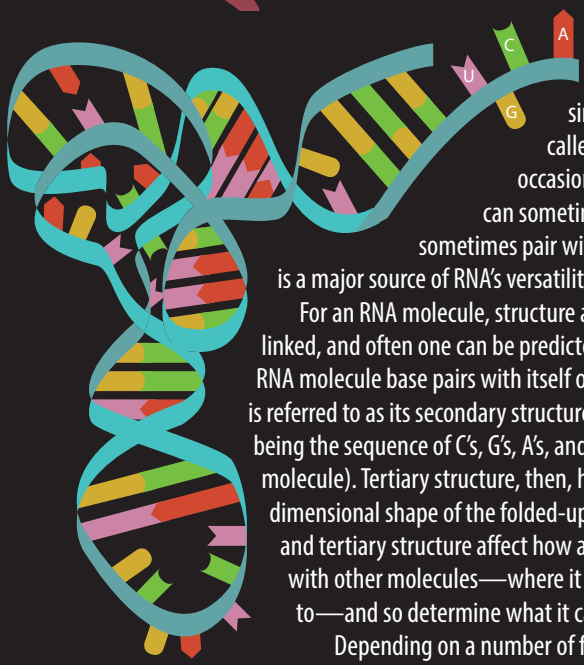
Because RNA is such a central player to the processes of life, it is the subject of much study. But it's very complex—far more complex than DNA. Whereas DNA usually takes a single shape, the double helix, RNA takes all sorts of different shapes, and its functionality comes from the shape it takes. Predicting an RNA

A tale of two nucleic acids

In the utility drawer of cellular machinery, DNA is like a spoon: stable, predictable, the absolute right tool for a very specific job. RNA is like a Swiss army knife: versatile, delicate, taking myriad forms to tackle numerous jobs. Whereas DNA is usually a double-stranded helix, with each complementary strand twisting around the other to provide strength, structure, and reliability, RNA is typically single stranded. But, biochemically, it still "wants" to pair up. So with no sister strand to bind to, it kinks and twirls back on itself forming elaborate loops, bulges, hairpins, and helices.

DNA and RNA both participate in base pairing, a process in which the nitrogenous bases on one strand share hydrogen atoms with the bases of another strand, forming hydrogen bonds that bridge the gap and hold the two strands together. Generally speaking, the four bases of RNA follow the rule that cytosine (C) pairs with guanine (G) and adenine (A) pairs with uracil (U) (in DNA base pairing, adenine pairs with thymine (T)). But there's some flexibility to that rule.

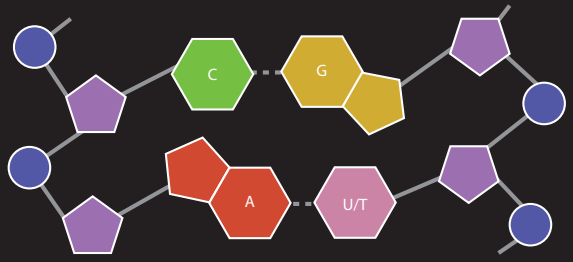
Because G and A are similar to each other in size and shape (belonging to a class of double-ringed molecules called purines), and C and U are similar to each other (belonging to a class of single-ringed molecules called pyrimidines), they can occasionally swap partners. So G can sometimes pair with U and C can sometimes pair with A. This flexible base pairing is a major source of RNA's versatility.



For an RNA molecule, structure and function are inextricably linked, and often one can be predicted from the other. How an RNA molecule base pairs with itself or with other RNA molecules is referred to as its secondary structure (the primary structure being the sequence of C's, G's, A's, and U's that make up the RNA molecule). Tertiary structure, then, has to do with the three-dimensional shape of the folded-up RNA molecule. Secondary and tertiary structure affect how an RNA molecule can interact with other molecules—where it can fit and what it can bind to—and so determine what it can do.

Depending on a number of factors, the same primary structure can result in different secondary and tertiary structures, which impart different functions. Both regulatory mechanisms being studied by the Los Alamos group, riboswitches and riboregulators, capitalize on this interchange to control gene expression.

The two strands of a DNA molecule (pink) pair with and bind to each other. The single strand of an RNA molecule (blue) pairs with and binds to itself, forming elaborate structures that impart the molecule's many functions.



Both DNA and RNA undergo base pairing, wherein a purine (A or G) hydrogen bonds with an opposing pyrimidine (C or U/T). Usually C pairs with G and A pairs with U/T, but partner swapping can occur and contributes to RNA's versatility.

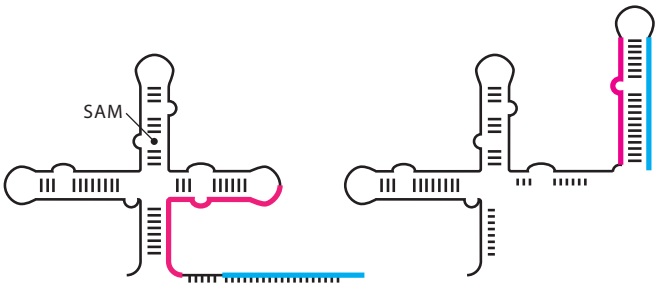
molecule's 3D shape, the way it folds and loops and coils, is notoriously difficult. But by using its genetic sequence (primary structure) as a starting point, scientists are getting better at mathematically predicting these complex secondary and tertiary structures through computer simulation.

IN THE CELLULAR UTILITY DRAWER, DNA IS LIKE A SPOON, AND RNA IS LIKE A SWISS ARMY KNIFE.

Taking a combinational approach—mathematical simulation and biochemical experimentation—Los Alamos researchers are capitalizing on RNA's versatility to adjust bacterial metabolism for a variety of far-reaching goals, such as the design of new drugs, environmental clean up, and even energy production. Through the discovery of natural tricks and invention of new tactics, they are harnessing the power of RNA to help dial in and fine tune the right metabolic mix.

Natural tricks

Theoretical biologist Karissa Sanbonmatsu models RNA molecules and their mechanisms to better understand how they work. Having built a previous successful career in plasma physics, Sanbonmatsu was drawn to biology in general, and RNA modeling in particular, by the enigmatic ribosome. Made mostly of intricately folded RNA, ribosomes are the molecular machines that assemble proteins based on RNA instructions called transcripts. Much of the work in Sanbonmatsu's lab is focused on ribosomes, and the group is a world leader in ribosome modeling. But lately, the group has also been



The mechanism of a riboswitch from the hot-springs-dwelling species of bacteria *Thermoanaerobacter tengcongensis*. Through variable base pairing, the same RNA molecule can change shape in order to regulate gene transcription. (Left) When the ligand molecule SAM (black dot) is bound to the riboswitch, the RNA takes a form (pink not paired with blue) that prevents gene transcription. (Right) When the ligand molecule is not present, the riboswitch takes a different conformation (pink paired with blue) that allows gene transcription. The two structures have the exact same genetic sequence, but the binding of the ligand favors one conformation over the other.

working on a different class of RNA machines, subcellular stoplights called riboswitches.

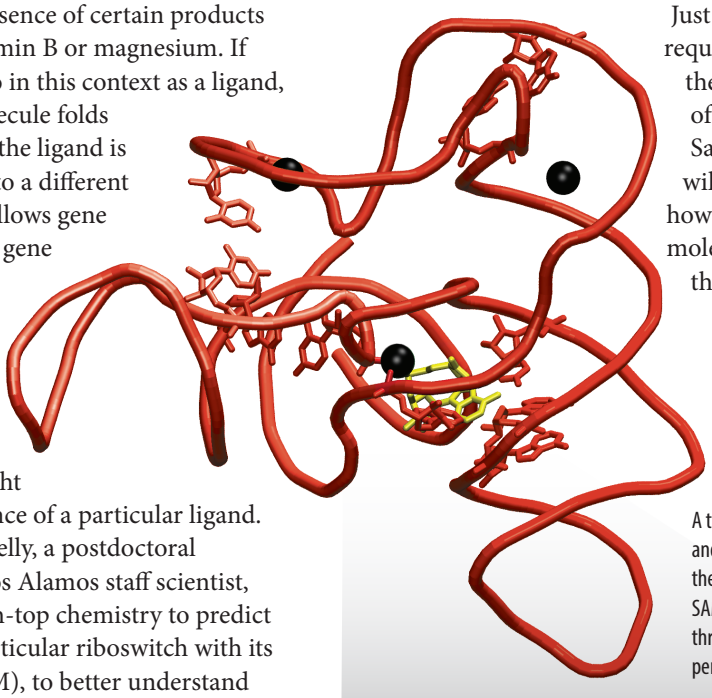
Naturally occurring in bacteria, riboswitches are small RNAs that are controlled by the presence of certain products of normal metabolism, such as vitamin B or magnesium. If the metabolism product, referred to in this context as a ligand, is bound to the RNA, the RNA molecule folds into one shape, or conformation; if the ligand is not present, the same RNA folds into a different conformation. One conformation allows gene transcription—the first step toward gene expression, wherein a transcript, or copy, of the DNA gene is constructed from RNA—and the other conformation blocks gene transcription. So the riboswitch is essentially a regulator of gene expression, giving a green or red light depending on the presence or absence of a particular ligand.

Sanbonmatsu and Scott Hennelly, a postdoctoral researcher at the time and now a Los Alamos staff scientist, used computer modeling and bench-top chemistry to predict and validate the interaction of a particular riboswitch with its ligand, S-adenosylmethionine (SAM), to better understand how riboswitches work. SAM regulates sulfur metabolism, participates in gene regulation, and directs its own production via riboswitch. The SAM riboswitch operates by competitive mutual exclusion: through flexible base pairing, a portion of its sequence (the C's, G's, A's and U's) can pair with either of two nearby regions of the same RNA molecule. Which one it pairs with determines whether the switch is in the on or off position. When concentrations of the ligand SAM are high, SAM binds to the riboswitch, which prevents the transcription of the gene encoding SAM synthetase (the enzyme responsible for activating SAM), so the switch is off and no more SAM gets made. When the concentration of SAM is low, the SAM-less riboswitch takes a conformation that permits the transcription of the SAM synthetase gene, thus flipping the switch on and allowing for the production of more SAM.

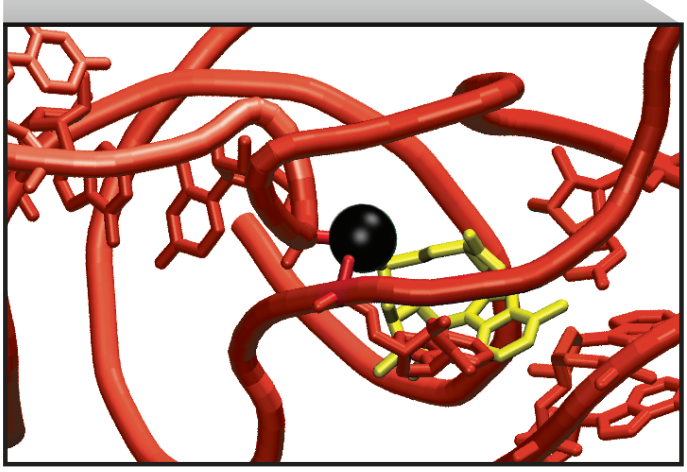
And if that's not convoluted enough, it gets better—because RNA structures often require the presence of certain ions for correct formation. Sanbonmatsu and Hennelly found that in addition to SAM binding, the transcription-blocking conformation of the SAM riboswitch depends on the presence of divalent magnesium (Mg^{2+}). The "transcription-off" position requires SAM and three molecules of Mg^{2+} bound to three specific locations on the RNA. But puzzlingly, very high concentrations of Mg^{2+} can induce the riboswitch to the "transcription-on" position despite SAM being bound to the RNA. Additional experiments show that modifying any of these three sites so that Mg^{2+} can't bind also made SAM less able to bind, thereby destabilizing the "transcription-off" conformation. Sanbonmatsu and Hennelly conclude that there must be a cooperation between SAM and Mg^{2+} where SAM magnifies its ability to control the structure of the riboswitch by recruiting Mg^{2+}.

"We think SAM acts like a crowbar to pry open certain sites so that Mg^{2+} can bind, and at physiological concentrations, this shuts down transcription," Hennelly explains.

Just knowing that Mg^{2+} is required, though, isn't the end of the story. In fact it's kind of a new beginning. Next, Sanbonmatsu and her team will plunge into figuring out how Mg^{2+} and SAM cooperate molecularly and exactly what they do inside the SAM riboswitch. How does the presence or absence of



A three-dimensional view of the SAM and Mg^{2+} binding sites on a portion of the SAM riboswitch. The ligand molecule SAM (yellow) is in the center, and the three magnesium ions (black) are on the periphery.



Mg^{2+} determine how well SAM can bind? What about free-floating Mg^{2+} ions—do they have any influence? And just how is it that excessive quantities of Mg^{2+} can override SAM? In collaboration with researchers at Rice University, the team is working on faster new models and fancier new algorithms that will start to answer some of these questions.

"While we know for the most part what RNA does," says Sanbonmatsu, "we have a long way to go to understand how it does it. Understanding the 'how' is going to be the key to some blockbuster new discoveries."

New tactics

Bacteria evolved the riboswitch mechanism of RNA-based gene regulation all on their own. But Los Alamos biochemist Cliff Unkefer, along with Sanbonmatsu, Hennelly, and a team of others, is taking the idea that RNA makes a good control switch to a whole new level.

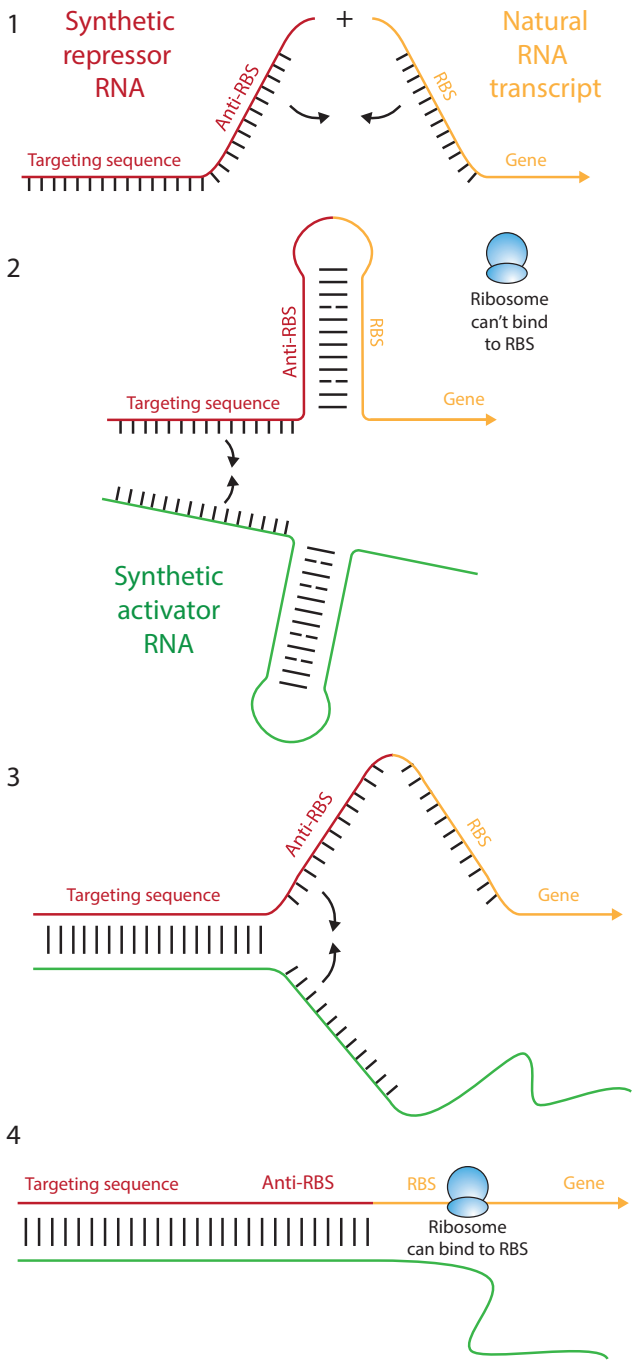
WE'RE TRYING TO AFFECT ONE PATHWAY IN THE MIDDLE OF A SEA OF PATHWAYS.

"The idea," Unkefer says, "is to bypass billions of years of evolution and engineer entire bacterial metabolic pathways to a particular end." That end could be either the production or consumption of particular products that we humans either want more of (e.g. fuels) or less of (e.g. toxins).

Consider a generic metabolic pathway that is mediated by a series of enzymes: Enzyme-A performs some sort of action on chemical-A, typically adding something or taking something away, yielding a product that is a new chemical, which gets modified next by enzyme-B. Enzyme-B converts the chemical into something that gets modified next by enzyme-C and so on in a cascade of sequential reactions. Unkefer and his team want to engineer that whole thing. With that goal in mind, the team has pioneered the development of a new class of artificial regulatory RNA molecules, which it calls riboregulators, and which are entirely separate from innate riboswitches.

Whereas riboswitches modulate gene expression by allowing or disallowing the production of a gene transcript, riboregulators operate by allowing or disallowing translation of gene transcripts into protein by ribosomes. In order for a ribosome to translate a gene transcript into a protein, the ribosome needs to attach itself to the transcript. But it can't just clamp on any old place; it has to find and clamp on at a very particular sequence, conveniently called a ribosome-binding site (RBS), which usually reads AGGAGG and is located just before the gene on the transcript. So it stands to reason that if ribosomes can't find the RBS, they can't clamp on, and the protein can't get made. That's the strategy the Los Alamos riboregulator team tried, and it worked.

First, the scientists synthesized a short sequence of RNA that contains, among other things, a segment mostly complementary to the RBS, having maybe five perfect matches and one flexible match to the AGGAGG of the RBS. Next, they attached the synthetic RNA like a tail to an actual gene transcript right next to the RBS. This put the anti-RBS sequence and the RBS near one another on the same strand of RNA, allowing them



How a riboregulator uses the ribosome binding sequence (RBS) of a gene transcript (yellow) to regulate ribosome access and consequent protein production: (1) The Los Alamos team attaches a synthetic piece of RNA (red) containing a targeting sequence and an anti-RBS sequence to the RBS at the end of the gene transcript. The anti-RBS sequence binds to the RBS, making ribosomes unable to attach and preventing protein production. (2) Next, they add a synthetic activator RNA (green) to bind to the targeting sequence of the repressor RNA and maneuver a neighboring segment, which is a better match to the anti-RBS sequence, into proximity to the anti-RBS. (3) The anti-RBS breaks bonds with the RBS and forms new bonds with the better-matched segment (green pairs with red), making the RBS (4) available for ribosome attachment to produce a protein. The amount of activator added allows researchers to fine-tune how much protein gets made.

A trio of Los Alamos riboregulators: (left to right) Cliff Unkefer, Karissa Sanbonmatsu, and Scott Hennelly.

to pair with each other, which prevents roaming ribosomes from clamping on. That's the repressor function: production of the protein encoded on that transcript has been repressed. But there's also an activator function that can be dialed up or down, making the system tunable, which is why it's a ribo*regulator* and not a ribo*switch*.

The activator function comes from a second synthetic RNA that competes for the anti-RBS of the repressor, repressing the repressor and resulting in activation. The RNA tail that was attached to the transcript to repress it also contained a segment called a targeting sequence, which acts like a trap to attract and anchor the activator RNA. The activator is free-floating and not attached to anything, but it has a segment that is a perfect match to the targeting sequence of the repressor RNA, so the two strands eventually pair up. Now that the activator is bound to the repressor, a segment of the activator that is a perfect match to the anti-RBS is brought into proximity to the anti-RBS. Because the anti-RBS was a pretty good match to the RBS but not a perfect match, when the perfect match sequence on the activator comes along, the anti-RBS breaks bonds with the RBS and pairs up with the better-matched sequence on the activator RNA. Now the RBS is available, and ribosomes can come at will to crank out protein molecules.

LIKE WITH A SOUND MIXING BOARD, YOU CAN'T JUST TURN EVERYTHING ON FULL BLAST AND HAVE IT SOUND GOOD.

How much activator RNA is around determines how much protein gets made, and how much protein gets made affects all the downstream steps of the metabolic pathway. In the previous generic enzyme cascade, where enzyme-A turns chemical-A into chemical-B and so on, riboregulators could be used to tweak and adjust each step in that cascade. So far, the team has successfully managed to riboregulate two genes in the same cell. But as Hennelly points out, "If there are ten achievable levels of expression for each of five different proteins, that's 100,000 different unique combinations. That's the tunability we're talking about. That's what's new and what I'm excited about."

So the riboregulator team's vision of engineering entire metabolic pathways isn't too far out. Now they're working out the details of combination. "It's kind of like a sound mixing board," Hennelly says, "you can't just turn everything on full blast and expect it to sound good. There are a lot of controls. Sometimes when you turn one up you have to turn another one down."

It's a ribo world

So far, the riboregulators have worked exactly as the team had hoped. But beyond the scientific satisfaction of one's theories and hard work panning out, riboswitches and riboregulators have tangible gains to offer as well. Both mechanisms are powerful tools for synthetic biology applications. One example is bioremediation: making bacteria metabolize chemicals that they ordinarily wouldn't consume in order to clean up environmental messes. Another example is bioenergy—engineering bacteria to produce fuels or help remove carbon dioxide from the atmosphere.

Riboswitches are also promising targets for new antibiotics. Because they are in bacterial cells but not in human cells, a riboswitch-targeting drug would be handy in fighting infection. And the high specificity of riboswitches for their particular ligands would make the drugs easily targeted to the bacterial gene of choice.

The regulation of gene expression is outrageously complex and frequently relies on the unique characteristics and abilities of RNA. So although DNA is the handsome figurehead of genes and genetics, RNA is the unsung hero. Scrappy and resourceful, RNA acts as field crew, moving team, courier service, fact checker, and gatekeeper. And in the hustling and bustling metropolis of a living cell, that truly is the stuff of life. LDRD

—Eleanor Hutterer

More **RNA research** at Los Alamos

- **Ribosomes: the smartest living nanomachine**
  http://www.lanl.gov/discover/publications/1663/issues-archive/august2008.pdf
- **Counting RNA molecules to monitor bacteria**
  http://www.lanl.gov/discover/news-stories-archive/2013/June/disease-causing-organisms.php

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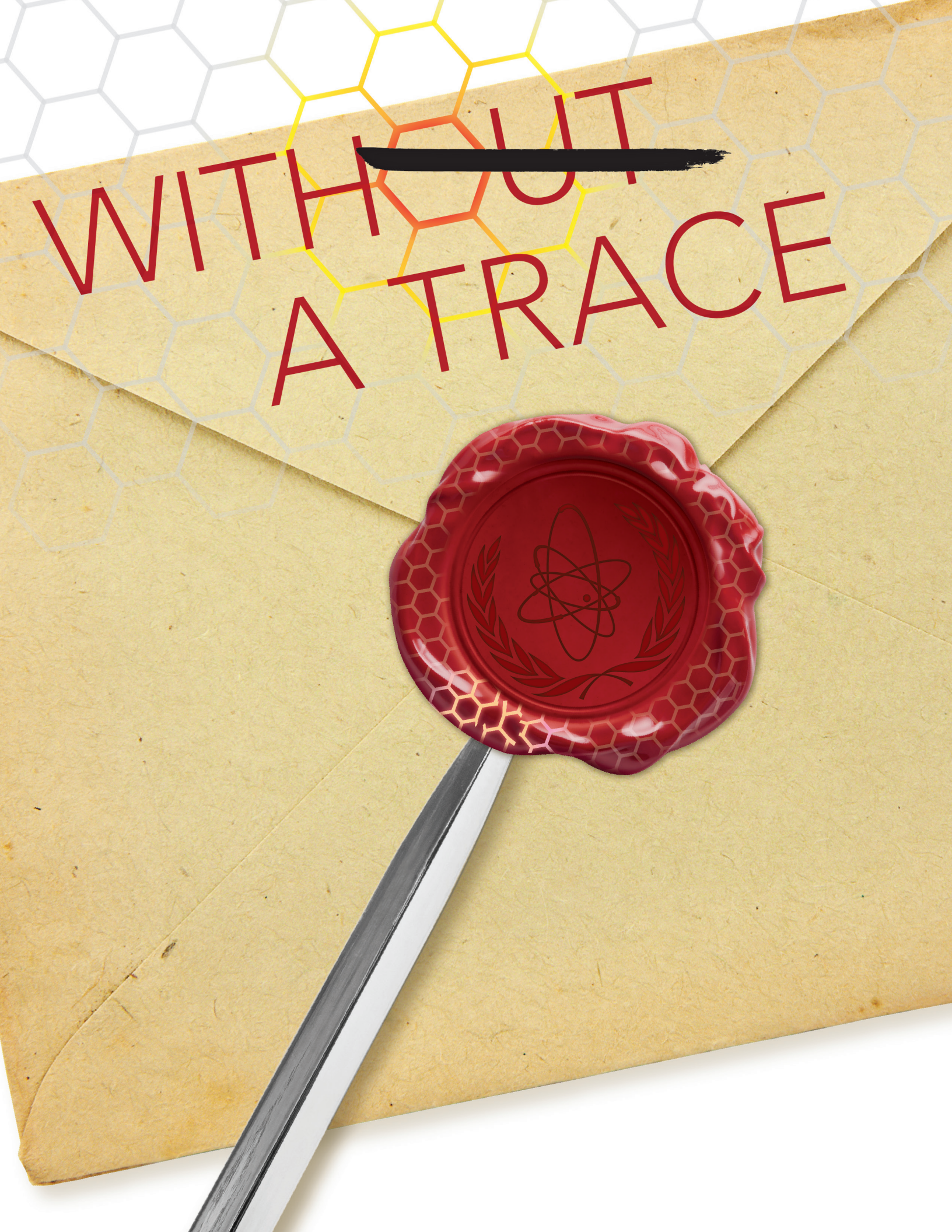

WITHOUT
A TRACE

SOME PACKAGES ARE SO VALUABLE THAT THEY REQUIRE A WAY TO UNEQUIVOCALLY REVEAL IF ANYONE HAS TRIED TO GET IN.

A WAX SEAL ON CORRESPONDENCE among royalty in the 16th century had a very specific purpose. It did not lock the envelope—anyone could surely get in and reveal the confidential contents. However, the security breach would be known. The unique stamp imprinted in the wax would be permanently damaged and the receiver of the message would be the wiser. The practice of safeguarding parcels continues today as tamper-evident seals are added to a variety of consumer products for this very reason: to let people know if someone has tried to get in. For instance, a simple plastic wrap tears if a medicine bottle is opened, and a vacuum makes the lid pop upon opening a jar of spaghetti sauce.

When it comes to special nuclear material, however, the stakes are much higher, and plastic wrap won't suffice. Anyone who would tamper with this kind of cargo would likely have a sophisticated method in hopes of evading detection. And although tamper-evident materials have come a long way since the sealing wax of the 16th century, there is still room for improvement. Paving the way for a new era of verification technologies, a team at the Los Alamos Engineering Institute is developing a novel tamper-evident seal that is both remotely readable and self-authenticating.

Continuity of knowledge

In 1957, the International Atomic Energy Agency (IAEA) was created to ensure the peaceful use of nuclear technology after President Eisenhower's "Atoms for Peace" speech to the United Nations General Assembly. As part of its safeguards mandate under the Nuclear Nonproliferation Treaty, the IAEA regularly conducts inspections of nuclear sites worldwide. This includes monitoring facilities for enriching uranium and fabricating fuel for nuclear reactors to verify that nuclear material hasn't been diverted from peaceful activities.

The IAEA uses seals to maintain continuity of knowledge on nuclear material in storage, or in transit between facilities, and even on monitoring equipment, such as surveillance cameras. The seals play an important role in reducing the inspectors' efforts spent on materials not currently in use, freeing up precious time for the IAEA to pursue other tasks. By verifying a seal on the outside of a storage container (typically applied at the interface where normal access occurs), the inspectors can quickly inventory the material by counting it as a single item—without having to remeasure the individual contents.

Ideally, a tamper-evident seal must fulfill certain requirements. First, it must be robust against the common mechanisms someone might use to defeat it. For instance, if the seal is stuck onto a drum with an adhesive, an adversary might use steam or solvents to lift it, or even simple mechanical action to pry it off. However, if the seal has characteristics that make such techniques obvious, the adversary's actions would be known. For instance, the seal material could have properties that make it break into pieces rather than deform elastically as a single object, so that it crumbles when an attempt is made to remove it. Conversely, the seal must also be robust against environmental changes (such as elevated humidity or high radiation fields) so that it doesn't give a false positive for

Single pristine graphene sheet

tampering whenever such conditions change. Tamper-evident seals should be authentic—devices the IAEA inspectors can recognize as their own—and they should be difficult to counterfeit. Finally, seals must be inexpensive and efficiently monitored, since the IAEA typically deploys more than 30,000 of them per year.

Currently, seals are created via many sophisticated methods. Some have barcodes or labels that change upon tampering, while others use etchings or crimping patterns that require manual examination to verify. Unfortunately, many of the seals currently in use require a lot of the inspectors' time for verification.

THE MATERIAL IS THE CIRCUIT, THAT'S THE KEY.

Karen Miller is a scientist in the Nuclear Engineering and Nonproliferation Division at Los Alamos who works on technology development for nuclear safeguards. A few years ago, she was participating as a mentor in the Advanced Studies Institute at the Los Alamos Engineering Institute, and she had an idea for streamlining the inspectors' verification process.

"I was excited to learn of the high detection sensitivity the Institute scientists were able to achieve using certain materials and advanced sensing for structural-health monitoring," Miller says. "I realized that what I was seeing could be useful for tamper-evident seals." Miller posed a challenge to the multidisciplinary group of doctoral students and postdoctoral researchers she was mentoring: she asked them to develop a novel tamper-evident technology.

The team first developed a solution that was based on a cable consisting of multiple elements with different resistance properties. The concept developed by the students was to look at changes in the resistance of the cable to determine whether or not tampering had occurred. At the completion of this program, David Mascareñas, one of the scientists at the Engineering Institute, began to think more deeply about the challenge of tamper-evident seals. As a result, he and postdoctoral researcher Alessandro Cattaneo decided to combine two scientific hot topics: a material called graphene and a signal-processing scheme called compressive sensing.

Strong, yet sensitive

Graphene is a one-atom-thick hexagonal sheet of carbon—basically a single layer of graphite from a pencil. Isolation of single-layer graphene was realized in 2004, earning its discoverers a Nobel Prize in 2010, and has since been the center of a great deal of excitement due to its strength, flexibility, and ability to efficiently conduct electricity. During this time, much work has been done to produce graphene, or graphene-like materials, in more efficient ways.

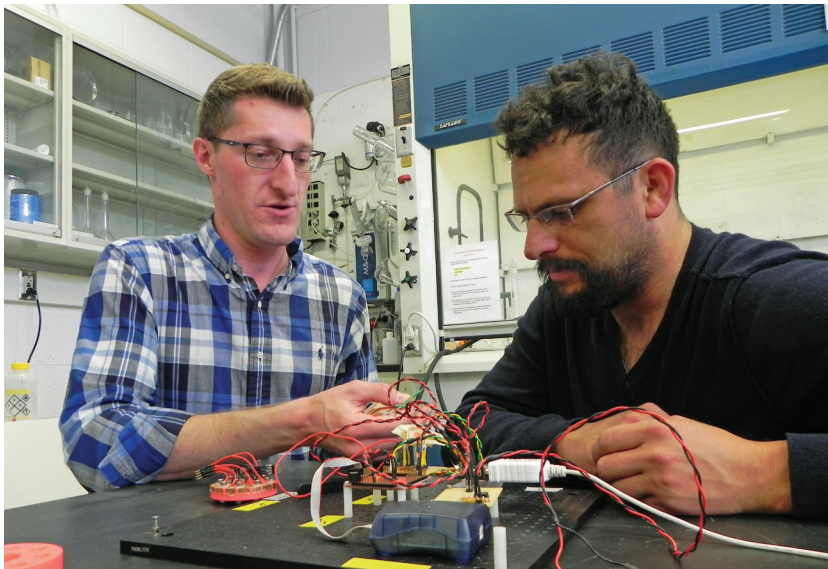
The first production of graphene was made by repeatedly pulling sheets of graphene off of graphite using sticky tape. Scientists have since been able to exfoliate graphite by adding acid and high temperatures to oxidize and break up the layers. Then, this graphite oxide (GO) solution can be vacuum filtered, creating a thin, paper-like film that can be selectively reduced via temperature or laser engraving to remove the oxygen atoms, resulting in reduced graphene oxide (rGO) on the top few layers of the GO film. The GO-reduction process leaves holes in the honeycomb-shaped lattice of carbon atoms, making the resulting graphene less conductive but maintaining most of the desired graphene characteristics in a more efficient production process.

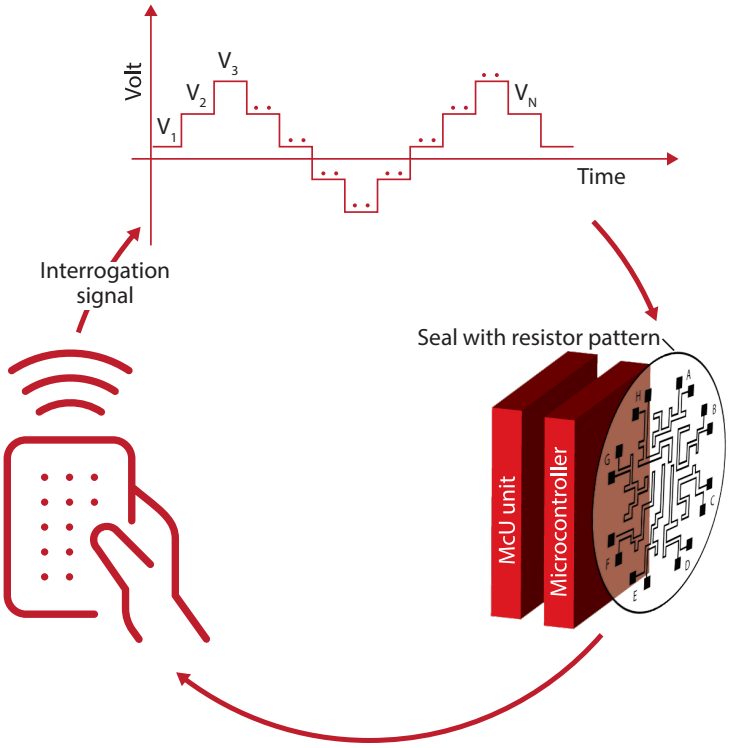
Mascareñas and Cattaneo hypothesized that the paper-like mixture of GO and rGO could be used as a tamper-evident seal with an integrated electrical fingerprint—a unique signature created by printing or embedding a circuit on the film. The paper-like material can be bent and manipulated to

The International Atomic Energy Agency deploys approximately 30,000 tamper-evident seals per year to barrels and other containers of special nuclear material. The seals are used to help ensure that none of the material is diverted from peaceful activities.

CREDIT: International Atomic Energy Agency

Alessandro Cattaneo (left) and David Mascareñas adjust the electronics connected to their prototype tamper-evident seal. Once optimized, they will be able to miniaturize the micro-controller unit so that it can be easily hidden behind the seal.





How the seal works: First, a remote reader sends an interrogation signal of voltage samples (V_1, V_2, V_3…V_n) through the rGO resistors in a random sequence (D, C, A, A, F...). This process is repeated many times using different random resistor sequences. The output that is sent back to the reader is a series of compressed samples in a linear combination of the initial interrogation signal—a sparse data set used to verify that the whole resistor circuit is intact.

use as a seal, but once in place, its delicate lattice of carbon atoms is easily disrupted to indicate foul play.

"The material *is* the circuit," Mascareñas says. "That's the key."

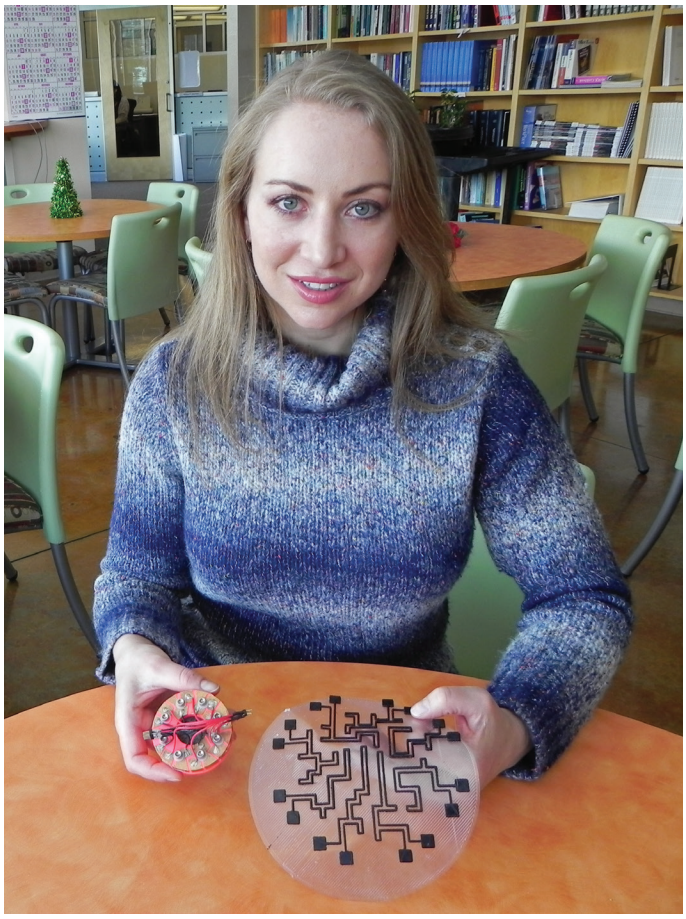
To make the seal, Mascareñas and Cattaneo pulled together a team of materials science and engineering experts, including colleagues at the Los Alamos Center for Integrated Nanotechnologies. Using a laser, team members engraved onto the GO paper seal an rGO-based pattern of eight resistors, each of which is characterized by a unique resistance value. Knowing that the conductivity of graphene is highly sensitive to humidity, temperature, and breakage, they felt any tampering would damage the circuit pattern. But they still needed a way to detect the change.

Critical minimum

Since coming to Los Alamos, Cattaneo has worked closely with Mascareñas on advanced sensing. In particular, he has become an expert in a relatively new method of signal processing called compressive sensing (CS), which has proven to be a key aspect of the team's tamper-evident seal.

Widely used since 2004, CS relies on the idea that high-resolution data actually contain a lot of redundant information. Take the example of a high-resolution photo. When the image is compressed, the redundant information is thrown out—posing the question: why not *only* collect the most important data in the first place?

Adapting this concept to the tamper-evident seal, CS is used to both encrypt and decrypt a sparse interrogation signal used to authenticate the



In her right hand, Alexandria Marchi holds the first prototype of the team's tamper-evident seal. Encased in a protective container (orange ring), the rGO and GO film is visible as a dark circle in the middle. In her other hand, she holds a 3D-printed version using an off-the-shelf conductive material printed on a polyurethane sheet, making the whole seal much thinner and more flexible. Ultimately, she plans to integrate graphene-based materials into polymers to make the seal 3D-printable.

seal and verify its integrity. To achieve this, the seal is equipped with a microcontroller that routes the interrogation signal through a series of resistors in the seal in a random sequence known only to the receiver. By repeating this operation multiple times using different random sequences, a set of compressed samples is collected—a random linear combination of the interrogation signal's values after their amplitudes have been modified by the rGO resistors. A modification in the circuit structure of the seal caused by a tampering attack will irreversibly compromise the encryption and decryption mechanism, thus enabling tampering detection. Integrating these electronics into the seal provides a low-power verification scheme that is both self-authenticating and adaptable to small environmental changes.

This data can be gathered remotely—so if an inspector walks into a warehouse with 1000 containers, the signal can be sent out to the seals without requiring the inspector to walk up

Reduced graphene oxide

to each individual container. Extra security layers can be added by enabling the inspector's reader to change both the interrogation signal and the switching sequence used to route the signal through the resistors. Ultimately, using the CS technique, the reader can recreate the circuit architecture, confirming the integrity of the seal.

The Engineering Institute team tested its seal against a number of tampering scenarios, performing 100 simulations on each scenario. Their initial results were promising—the error rates were within reason, and the seal proved to be robust against small perturbations in the environment that could otherwise cause false positives.

"The seal is designed to provide irreversible evidence that someone has tried to contact the item or location," Cattaneo says.

Can you print that?

Now that they have a successful first prototype, members of the team are focusing on seals that can be made faster, more cheaply, and with greater stability. (Simulations showed that if the material stability were improved, false positives could be eliminated entirely.) Seaborg Institute Postdoctoral Fellow Alexandria Marchi joined the team in 2014 and began to look for a way to speed up the manufacturing process of the GO-rGO film.

"Right now, the material takes time to make—about three weeks," Marchi says. "In order to make these seals on a larger scale, we need them to be made in minutes."

Marchi decided to try printing the seal using a standard commercial inkjet printer. First, she experimented with adding different polymers to the GO material in order to increase its stability, facilitate the breakdown of the layers, and control viscosity and particle size to make the material flow easily through a printer. Then, to further adapt the process for printing, she added a solvent. But Marchi still wasn't satisfied with the result and has turned to 3D printing as a possible solution.

Using a 3D printer, Marchi could eliminate the need for the GO paper and laser engraving the circuit by building the seal with a graphene-embedded, 3D-printable filament. Her first attempt resulted in a seemingly more robust seal, which was created in a fraction of the time (see photo on page 25). After that will be a round of tests to evaluate its performance.

One challenge Marchi anticipates is how to attach the seal to a container. An ideal solution would be to integrate the adhesive properties into the seal material itself. Or better yet, if the 3D-printing process is optimized, Marchi suggests that an entire container could be printed using a modified graphene-based printable material.

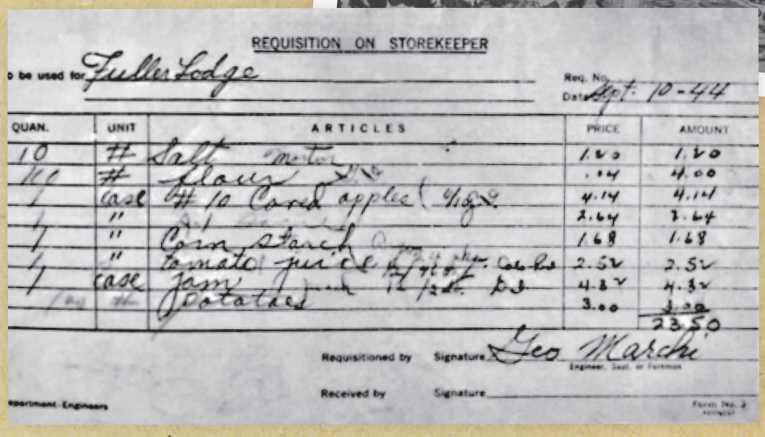
"We could make the whole container into a sensor," Marchi says. This way, any attempt to access the container—not just at the standard opening—would be known. Surely that would be the best tamper-evident seal of all. LDRD

—Rebecca McDonald

A Manhattan Story

The rich history of Los Alamos and its role in the Manhattan Project has long been inspiration for books, movies, and a television series. But for some in Los Alamos, it is a very personal history, as their families have lived and worked here for generations. Alexandria Marchi, a postdoctoral researcher working on tamper-evident seals, has one of those personal histories; for four generations, her family has been a part of Los Alamos. Marchi's great-grandfather, George B. Marchi Sr. (photo at right), was the chef at Los Alamos's Fuller Lodge from 1943–1960. (A surviving requisition order of his reminds us that a case of tomato juice cost only $2.52 in 1944.) Her grandfather, George Marchi Jr., was the Lab's Chemical Warehouse Group Leader, and her grandmother, Rita, was a Lab typist.

Alexandria Marchi's father spent his early years growing up in Los Alamos, but she grew up in Albuquerque. Her path back to Los Alamos began with an undergraduate cooperative-education position in the Lab's Gas Transfer Systems Group while she attended the New Mexico Institute of Mining and Technology. After receiving her Ph.D. in biomedical engineering from Duke University, she decided to return to Los Alamos in the Engineering Institute, where she currently holds a Seaborg Institute Postdoctoral Fellowship. In addition to her work on tamper-evident seals, Marchi is investigating high-accuracy density measurements and fluid compatibility of plutonium. She is currently working with her alma mater (New Mexico Tech) to encourage more students to enhance their education through student jobs at the Lab. Marchi hasn't forgotten her roots and believes strongly in "educating students here in New Mexico and keeping them here."



REQUISITION ON STOREKEEPER

To be used for Fuller Lodge Req. No. Date Sept. 10-44

QUAN.	UNIT	ARTICLES	PRICE	AMOUNT
10	#	Salt meat	1.20	1.20
100	#	flour	.04	4.00
1	case	#10 Corn apples 6/gal.	4.14	4.14
1	"	Pie	2.64	2.64
1	"	Corn starch	1.68	1.68
1	"	tomato juice 6/#10 cans	2.52	2.52
1	case	Jam	4.80	4.80
		potatoes	3.00	3.00
				23.50

Requisitioned by Signature Geo Marchi

Received by Signature

spotlights

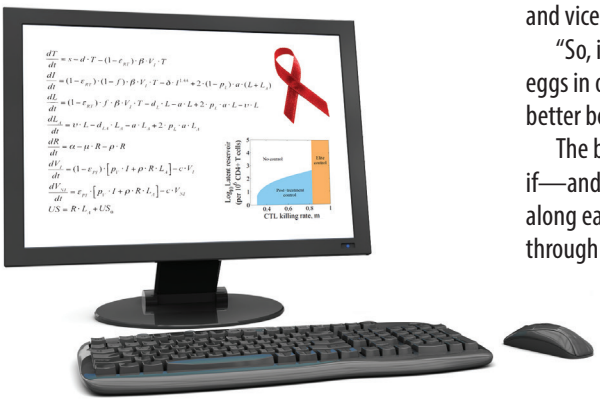
Fit for a Cure

In his work toward understanding the infection dynamics of HIV, the Laboratory's Alan Perelson works exclusively with model patients. Literally. He builds computer models of HIV infection to help make sense of puzzling clinical data.

When asked whether he is a virologist or a mathematician, Perelson quips, "Yes." Pressed for more, he clarifies, "I am a mathematical modeler of viral systems and immune processes."

Experimental and clinical studies provide the numbers, such as the number of HIV-susceptible cells in a volume of blood or the average number of viruses circulating in the blood. Perelson takes those numbers and devises complex mathematical equations to describe their relationships to one another, then fits his model to the data. If it's a good fit, he can illuminate portions of the virus-host relationship that are otherwise murky. And during the past year, his team has made some compelling new discoveries.

When a French study reported that a dozen or so patients had quit antiviral drug therapy yet maintained undetectable virus levels—representing a functional cure to an incurable disease—Perelson wanted to know why. If researchers can understand how that happened, then clinicians might be able to help more patients achieve a functional cure. Perelson and postdoctoral researcher Jessica Conway hatched a theory that these patients, who had each been diagnosed and treated very soon after infection, had in so doing given their immune systems a leg up, which kept down the number of viruses in their blood.



By including immune cells in their model, Perelson and Conway determined that an early diagnosis and prompt initiation of treatment can lead to a smaller "latent reservoir"—a hidden population of infected cells. These cells, as long as they aren't producing more viruses, are invisible to the immune system. But they can become active later and suddenly begin producing viruses. The more cells there are in the latent reservoir, the harder it is for the immune response to contain them once they start producing viruses. Very early treatment for the study patients capped their virus numbers at low levels, keeping their latent reservoirs small, thus allowing their immune systems a chance to get ahead of the infection.

The next question Perelson wanted to answer had to do with the nature of the immune response. Certain types of antibodies, called broad neutralizing antibodies (BnAbs), are effective at preventing the spread of infection from one cell to the next. But because BnAbs only appear years into an HIV infection, their utility is usually handily overwhelmed by the virus. Perelson wanted to find a way to make BnAbs appear early in the infection, when they can do the most good.

To do this, he and postdoctoral researcher Shishi Luo built a model of virus-antibody coevolution. HIV mutates liberally to evade neutralization by antibodies. Similarly, the immune system uses mutation to produce a spectrum of antibodies in hopes that some of them will be strongly matched to the virus. The result is an evolutionary arms race with both sides trying to stay nimble while casting a wide net. The model revealed that antibody production is a zero-sum game, with BnAbs coming at a cost to other types of antibodies and vice versa.

"So, if you're going to put all your antibody eggs in one basket," Perelson says, "it had better be the right basket."

The best antibody basket is indeed BnAbs if—and it's a big "if"—the BnAbs come along early enough. The way to do that is through viral genetic diversity. More variation early on—say, from an intentionally diverse vaccine preparation—leads to more BnAbs sooner, shifting the infection dynamic in favor of the host.

But Perelson isn't concentrating solely on the host response. Recently he and postdoctoral researcher Ruian Ke, along with several external collaborators, have been exploring ways of working the other side of the arms race: the latent reservoir, that sleeper cell of sleeper cells. A popular strategy, dramatically called "shock and kill," attempts to first stimulate latently infected cells into becoming productive and then target them for destruction. Recent clinical results from a latency-reversing agent (LRA) called Vorinostat were inconsistent, with varying extents and durations of activation. Perelson's task was again to suss out why such variation occurred and also to quantify the impact of Vorinostat. The model that fit the clinical data put LRA-activated cells into a different category than ordinary virus-producing cells and also allowed them to return to latency after a period of time, which makes Vorinostat less an agent of "shock and kill" and more one of "surprise and confuse."

So Vorinostat turns out to be a lackluster LRA. But when new, better LRAs come along, Perelson and his models will be set to crunch the numbers. Since drug discovery and clinical trials take years, it's a relief to know that, for model patients at least, a cure may be just a few clicks away.

—Eleanor Hutterer

Nuclear War Against Cancer

Exposure to nuclear radiation causes cancer—and sometimes cures it. But radiation, like chemotherapy, can be an indiscriminate killer, attacking cancerous and healthy cells alike. The damage to healthy cells can be quite widespread, which is why the prospect of cancer treatment often generates apprehension nearly on par with the cancer itself.

However, a treatment called radioimmunotherapy (RIT) delivers specialized, radioactive isotopes, or radioisotopes, directly to cancerous tumors within a patient's body. There, cell-killing radiation from the radioisotope bombards cancer cells while minimizing damage to the surrounding healthy tissue.

The key to success is multi-pronged, requiring the ideal radioisotope to obliterate the tumor, a biological delivery system to get it there, and a specialized molecule that holds the radioisotope tightly within the delivery system.

RIT targets cancer cells that express a distinctive antigen on their outer surfaces. An antibody specific to that antigen is attached to the radioisotope, and when the antibody encounters its antigen, that means the medicine has reached the tumor, even if tumors are scattered all over the body. Not all cancers produce a distinctive antigen for targeting, and therefore not all cancers can be treated with RIT, but those that do include heavy hitters such as prostate cancer, colorectal cancer, melanoma (skin), leukemia (bone marrow), and non-Hodgkins lymphoma (blood). Finding suitable antibodies to deliver the radioisotopes is a major challenge, and it is likely that better antigens to target have yet to be discovered, but several successful antibodies have already been demonstrated.

Eva Birnbaum runs the Los Alamos program for isotope production and applications, and Kevin John leads the national tri-lab isotope effort, which engages the Los Alamos, Oak Ridge, and Brookhaven national laboratories to produce RIT isotopes. While other researchers work to refine the antibodies, Birnbaum and John focus on finding and demonstrating the most effective radioisotope for treatment—and then making a lot of it.

"The optimal radioisotope needs to do two almost contradictory things," John explains. "It has to deliver a powerful dose of radiation to kill the tumor completely—without damaging healthy tissue in the immediate vicinity of the tumor and without lingering too long in the patient's system. It has to show up, do its job, and then go away."

Birnbaum and John believe the tri-lab team has found its winner with the isotope actinium-225, which undergoes radioactive decay by emitting an alpha particle. Being far more massive than the particles produced by any other form of radioactivity, alpha particles are released with high energy and relatively slow speed. As a result, they deliver a powerful punch in a short distance—typically only a few cell diameters—thereby affecting the tumor cells but not many of the surrounding healthy cells.

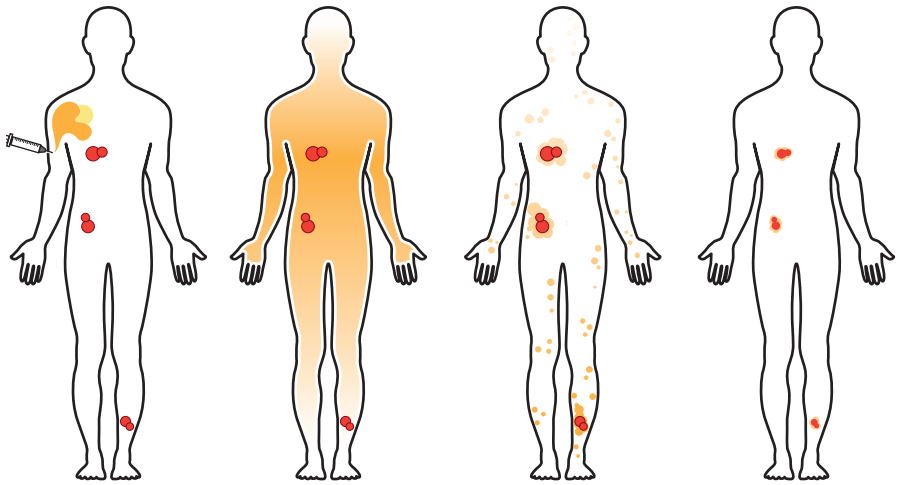
Actinium-225 also has the benefit that, after its nucleus decays by expelling an alpha particle, what's left behind is no longer actinium-225 but francium-221, which is also an alpha emitter. So, too, are the next two decay products—four alpha particles for every atom of actinium-225. So a little goes a long way. "The four alphas are especially important," Birnbaum says. "It's like repeated hammer blows in the same spot. After the initial hit, each successive impact multiplies the damage."

Additionally, actinium-225 has a half-life of just ten days—long enough that most of the administered dose has time to reach the tumor before decaying but short enough that very little of it lingers in a patient's body in the months following treatment. (Francium and its decay products have a half-life of only minutes or seconds.) The short timescale in which the isotope's powerful four-alpha radiation dose is concentrated and its subsequent radiological inertness are what make actinium-225 such an ideal nuclear weapon against cancer.

Because of its brief half-life, actinium-225 cannot be found in nature and must be made in a laboratory. Los Alamos and Brookhaven are doing so with their powerful proton-accelerator beams trained on a thorium target, resulting in a variety of radioisotopes, including actinium-225. Scientists then apply a series of chemistry-based purification methods to isolate the actinium from the other elements produced. It might sound straightforward, but the details matter. The targets have to be designed to withstand irradiation conditions that could otherwise melt them, and the chemistry process has to isolate highly pure actinium-225 from approximately 400 other isotopes.

RIT with actinium-225 can only become a reliable cancer-treatment option if the isotope's production can be scaled up to meet the increasing medical demand. Indeed, actinium-225 was originally developed for clinical research at Oak Ridge around 15 years ago, but practical applications remained limited by an insufficient supply. Fortunately, tri-lab scientists have successfully demonstrated the first major steps toward a large-scale, economically viable supply of the needed isotope. They estimate that once the full production pipeline is established—an investment of 5–10 years—it will take only a few days of beam time to match the present global annual production of actinium-225. Thereafter, accelerators at Los Alamos and Brookhaven, and chemical-processing capabilities at Oak Ridge, are planning to keep pace with the growing medical need.

So will it cure, or at least treat, different cancers? To find out, the tri-lab team has been collaborating with international clinical research leaders, building on years of research using the original Oak Ridge supply of actinium-225 on cancer-cell cultures and cancer-afflicted mice. In addition, human clinical trials performed to date show great effectiveness with a variety of actinium-225-



1. The patient receives an injection of the targeted radioisotope.

2. As the radioisotope circulates throughout the body, its attached antibody searches for a specific antigen found only on cancerous cells.

3. The radioisotope collects around cancerous cells and delivers radiation to those cells while minimizing damage to the body's healthy tissues.

4. Over time, the radioisotope decays, eliminating the radiation sources from the patient's body.

based drugs. One such drug under development to treat acute myeloid leukemia (AML), for example, has been tested on 18 patients at varying dosages and every time showed significant anti-leukemic activity with no toxicity to the patient. An expanded clinical trial is currently seeking additional AML patients to further assess the drug's effectiveness, and several others drugs based on actinium-225 are in the development pipeline as well.

"It looks really promising right now," Birnbaum says. "If FDA-approved clinical trials continue to pan out, then doctors can establish guidelines for actinium-225 treatments, what dosages to use, and so on. It's a real opportunity to deliver life-saving medicine in quantities that can have a tremendous impact."

"Through nuclear physics and chemistry," adds John. LDRD

—Craig Tyler

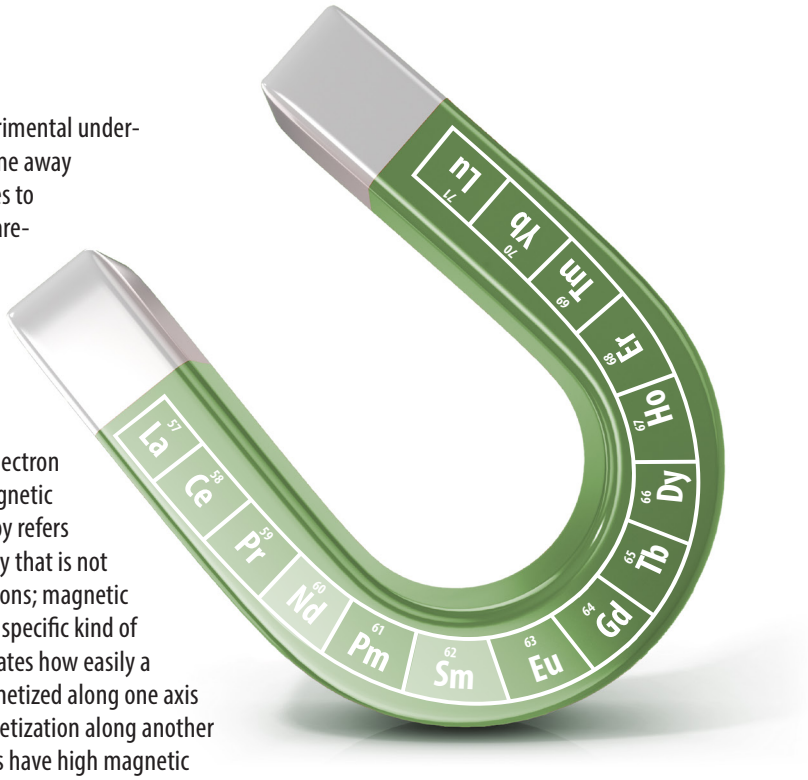
Mineral Magnetism

In addition to holding holiday cards to refrigerators well into the new year, magnets are also used in everyday items such as cell phones, children's toys, and shower curtains. Certain magnets garner the grandiose status of "strong magnets," and although the computing, medical imaging, and manufacturing industries all rely on strong magnets, by far the largest consumers of strong magnets are green technologies like wind energy and electric vehicles.

Strong magnets draw their defining strength from rare-earth minerals, such as neodymium and samarium. While these aren't exactly rare in nature, there is a scarcity in the United States stemming from limits on foreign sources, and each year, rare-earth minerals get harder to come by. Hence, the Laboratory is making a concerted effort to create rare-earth-free strong magnets.

A Los Alamos team led by materials physicist Joe Thompson wants to delineate what the crucial microscopic properties are that make a material magnetic. If the team can parse those out, it might be able to create new strongly magnetic materials without rare-earth elements.

To tackle this many-faceted problem, the team devised a two-pronged approach that combines quick computation with in-depth theoretical and experimental understanding. What it came away with was a set of rules to guide its search for rare-earth-free, strongly magnetic materials. The rules are very specific and have to do with ideal crystal structure, electron-electron interactions, and magnetic anisotropy. Anisotropy refers to a physical property that is not identical in all directions; magnetic anisotropy, then, is a specific kind of anisotropy that indicates how easily a material can be magnetized along one axis while resisting magnetization along another axis. Strong magnets have high magnetic anisotropy. Armed with the set of rules they devised, the scientists set about making and measuring materials they thought might pass muster.



To explore a material's physical properties, it is best to work with a single crystal of the material, in which the constituent atoms are arranged in a single ordered lattice. Synthesis of candidate magnetic materials in the necessary single-crystal solids proved time and cost restrictive. But the team quickly devised a workaround: because the materials were magnetic, they could be synthesized as polycrystals (much easier and faster to produce than single crystals), ground into a fine powder, then aligned by magnetic field while being glued back together into a single-crystal-like solid. This aligned-powder approach shaved months off of the time for initial analysis and helped whittle down the pool of candidates for further examination.

The material yttrium pentacobalt (YCo_5) is magnetic and free of rare-earth minerals, but it falls just short of the strength requirement to be classified as "very strong." However, YCo_5 is still a decent proxy for what the Los Alamos team is after. So, in concert with the aligned-powder effort, the team conducted a series of calculations and experiments aimed at a microscopic understanding of YCo_5's magnetism. By studying YCo_5 in depth, the team achieved two things: first, it proved the validity of its design-guiding rules, and second, it established a benchmark to which it could compare new candidate materials.

Out of hundreds of candidates, a single compound containing iron, germanium, and tellurium emerged as the front runner. Now, the time and cost to synthesize a true single crystal was easily justified. And that crystal has withstood ever-more rigorous probing of its magnetic nature.

But the new material is not quite ready for the mainstream. Since it becomes a strong magnet only at subzero temperatures, its immediate applications would be quite limited. Thompson is confident, however, that with further experiments and calculations, and by examining closely related compounds, there is promise for raising the temperature while maintaining the magnetism.

"The project was motivated by the need to replace rare-earth magnets in green technologies like wind turbines and electric cars," says Thompson. "We don't want dependence on those minerals to impede progress." Considering that a popular model of hybrid car uses more than two pounds of neodymium in each motor and that a typical wind turbine uses more than 100 pounds of it, the United States is consuming millions of pounds of neodymium per year. With green technologies gaining serious traction, the timing is perfect to find an alternative to endangered rare-earth magnets, allowing their use to go the way of whale oil and fade back into obscurity. LDRD

—Eleanor Hutterer

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