LDRD Quarterly Highlights

Mission Agility · Technical Vitality · Workforce Development

IN THIS ISSUE

SDRD SITE-DIRECTED RESEARCH & DEVELOPMENT

HIGHLIGHTS

Valet unmanned aircraft system significantly extends small drone range

In October 2021, the Nevada National Security Site (NNSS) successfully performed an aerial drop of a small unmanned aircraft system (UAS) from a larger UAS in a flight at Jean, NV, in cooperation with subcontractor Unmanned Systems, Inc. (USI). NNSS and USI used an all-electric Harris Aerial H6 hexacopter aircraft and NNSS sensors on a 3DR quadcopter. The goal was to demonstrate successful data gathering by launching a small UAS with limited range from a larger UAS with longer flight endurance and range. Using a robust UAS as a valet to drop a small, mission-specific payload in dangerous or inaccessible environments could serve multiple missions, including emergency response. The need for this development arose from the Fukushima Daiichi nuclear power plant reactor core meltdown, when radiological measurements were needed in areas too dangerous for humans.

The H6 carrying the 3DR drone. (Image credit: NNSS)

The NNSS demonstration was funded by the Site-Directed Research and Development (SDRD) Program. The multidiscipline SDRD team, led by Andrew Davies and composed of members from the Special Technologies Laboratory and the Remote Sensing Laboratories, included Rusty Trainham, Manny Manard, Cameron Priest, Ed Bravo, Paul Guss, and Kurt Rempe, and Hovig Yaralian from USI.

SDRD team members placing the valet and payload drones for takeoff. (Image credit: NNSS)

The 3DR UAS with NNSS sensors, flying independently. (Image credit: NNSS)

The team performed tests of graduated difficulty, investigating deadweight drops of increasing mass, sensors, controls swapping, and power draws. In all, there were 12 flights performed in an air launch series, and 6 in a ground control system switching test series. The hexacopter UAS flew well, as did the smaller 3DR launched from it, and all test objectives were met.

NNSS produced a video that documents some of the challenges the NNSS team encountered and offers a close look at the drone delivery process. *(DOE/NV/03624--1259)*

NNSS develops micro ion traps for real-time chemical analysis in harsh environments

Researchers at NNSS have been funded by the SDRD Program to develop a diagnostic for real-time, specific chemical analysis in harsh environments. The NNSS technology will include an ionization source, a printed circuit board (PCB) containing an array of Paul-type micro ion traps, and an ion detector. This important work bridges the gap between nonspecific in-field chemical analysis and traditional, delayed lab-based techniques, helping to align response priorities with timely, accurate ground truth in a variety of challenging settings. The three-year project is in its final year of development.

Currently, remote real-time chemical analysis is possible, but the sensors used are nonspecific. They are capable of sensing a family of compounds, such as volatile organics, but are not able to identify the actual chemicals being analyzed. It is also possible to capture the chemical in an adsorption trap or sampling bag and return it to the base of operations for analysis with laboratory techniques, such as gas chromatography-mass spectrometry, at a later time.

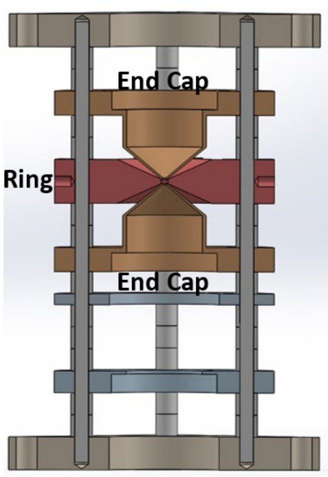
A device capable of providing analytical specificity in the field and transmitting the data back to the operator would bridge this gap and be a significant improvement for operational scenarios where chemical analysis is required.

The team is using inexpensive, off-the-shelf materials to create a small mass spectrometer for in-field analysis of specific chemical materials (volatile organic compounds, chemical weapon agents, toxic industrial materials, etc.). To maintain as small a footprint for the system as possible, the team has designed the unit to have trapping regions measuring hundreds of microns. In contrast, typical ion traps have trapping regions measuring several centimeters. The unit is being designed to be small and lightweight for remote operation, such as on UAS platforms, with the potential of making measurements in harsh environments. The system is being engineered to use relatively inexpensive components that are lightweight and low power, with the goal of being smaller and lighter than any portable mass spectrometer that is currently commercially available.

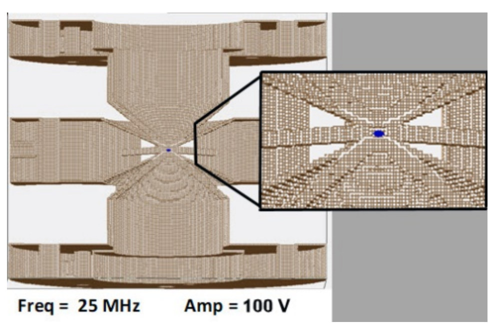
A Paul-type ion trap functions by confining ions in a region of space between three electrodes using a combination of direct current (DC) and radio frequency (RF) electric fields. The DC component of the field is applied to the two end cap electrodes, confining ions axially, and the RF is applied to the ring electrode. A mass spectrum of the ions is obtained as the trapping field is altered in a way that destabilizes the trajectories of the ions according to their mass-to-charge ratio (m/z). Ions are then sequentially ejected from the trap and are detected.

During the first year of development, the team performed ion trajectory simulations (SIMION v8.0) to determine the feasibility of confining ions on a submillimeter size scale and the parameters this would require. These simulations suggest efficient ion confinement can be obtained for trapping regions measuring 250 microns from the center of the trap to either end cap (z_0). To maintain trapping efficiency at these sizes, an RF of approximately 25 MHz must be applied to the ring electrode. This result is consistent with observations made as part of their previous efforts and with those reported in the literature. RF amplitudes required to confine ions in a micro trap are similar to those applied to a standard trap (25–100 V_P). Simulations also indicate that trapping can be performed at elevated pressures of up to 100 Torr. Operating in this pressure regime provides the benefit of greatly reducing the system's vacuum requirements.

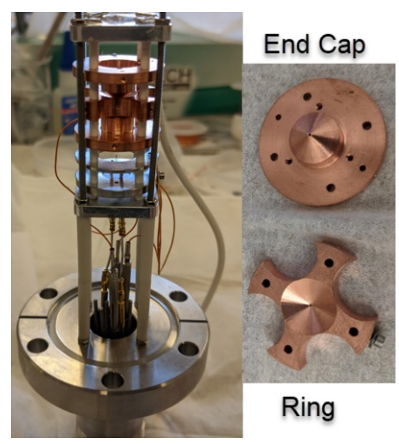
The team used results obtained in Year 1 to design a prototype of the micro ion trap, with z_0 = 250, during Year 2. The team input the SolidWorks model directly into SIMION v8.0 to verify that the geometry of the trapping region of the prototype was capable of efficient ion confinement. A SolidWorks model of the prototype and the results of the simulations are shown below. The team had these parts machined in-house and assembled the unit. A photograph of the assembled unit is provided below.



SolidWorks model of micro trap (Z_0 = 250 µm)

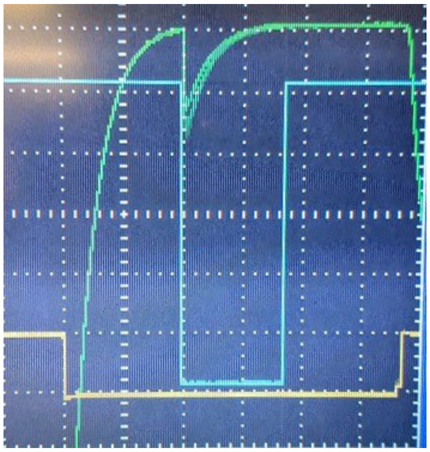


Simulation using SolidWorks geometry at 100 Torr, with 3x zoom of trap volume



Micro ion trap prototype

While testing the prototype, the team acquired data that demonstrated ion confinement in the micro trap. These data were acquired with an RF of 25 MHz and amplitude of 40 V_P. Here, ions held in the trap are extracted by application of a negative voltage pulse to the end cap nearest the ion detector. This causes all ions to be drawn out of the trap and detected.

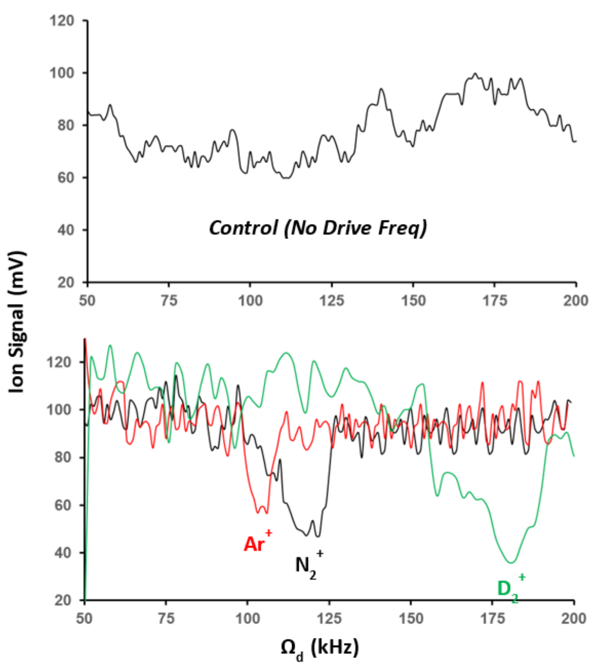


Results of a prototype test showing improved trapping efficiency and signal-to-noise ratio. Ions held in the trap are extracted by application of a negative voltage pulse to the end cap nearest the ion detector (blue trace). This causes all ions to be drawn out of the trap and detected (green trace).

After achieving ion confinement, the team set out to acquire data that illustrated mass-selective ejection from the trap. A second RF was applied to one end cap electrode. The team used the second RF to drive ion motion inside the trap, destabilizing ion trajectories and ejection from the trap. The specific frequency leading to ejection from trap is inversely proportional to m/z of the confined ions. By scanning the drive frequency (Ω_d), the team obtained mass analysis of ions in the trap.

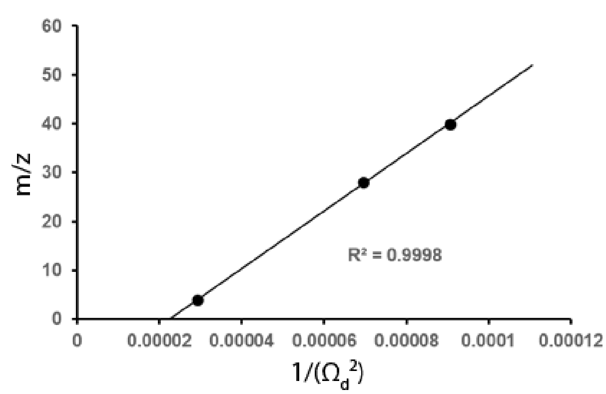
A graph showing mass-selective ion ejection is provided below. The team acquired these data by applying Ω_d to the trap while ions were confined inside and then using the negative voltage pulse to probe the trap for the presence of ions within. If Ω_d forced ions out of the trap, no signal will be measured when the pulse voltage is applied. Ω_d is then stepped and the process repeated for a range of frequencies. Three test gases, D_2^+ (m/z = 4), N_2^+ (m/z = 28), and Ar^+ (m/z = 40), were used to establish if mass-selective ejection was occurring. The valleys in ion signal are observed at different values of Ω_d for the three molecular ions. Ion ejection is achieved at Ω_d values of approximately 185, 120, and 105 kHz for m/z = 4, 28, and 40, respectively. From the Mathieu equation, we know that the m/z ratio of the ion ejected from the trap should be inversely proportional to square of Ω_d:

$$\frac{m}{z} \propto \frac{1}{(\Omega_d)^2}.$$



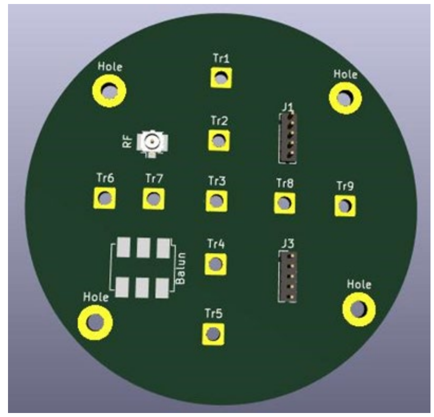
Mass-selective ejection from the trap (mass spactra)

A plot of m/z versus ($1/\Omega^2$) is shown below. The plot is linear, with an $R^2 = 0.9998$. These data strongly indicate that mass-selective ejection is occurring with the system.



A plot of m/z (D_2, N_2, and Ar) versus ($1/\Omega_d^2$) resulting in ejection from the ion trap

Finally, a PCB that contains an array of nine micro ion traps was designed. The PCB is 1 inch in diameter and 0.125 inches thick. The array will mitigate the reduction in sensitivity resulting from the reduced size of the trap caused by Coulomb repulsion (smaller traps necessarily hold fewer ions). This simplifies the design of the system, leading to a device that could potentially be produced quickly and inexpensively. All circuitry needed to provide the electric fields to the various component of the device is provided as part of the PCB layout.



The micro ion trap array (z_0 = 250 µm) PCB contains an array of nine micro ion traps (Tr1–Tr9, shown in yellow).

The development of small, field-portable systems for chemical detection and identification is of interest to multiple government agencies. Inexpensive instruments capable of providing real-time chemical analysis with reasonable sensitivity and selectivity in remote and/or harsh environments, such as on a UAS, is desired. A device capable of providing analytical specificity in the field and transmitting the data back to the operator would be a significant improvement for certain operational scenarios. Additionally, a design concept that eliminates the need for costly components would lead to a potentially disposable instrument, if chemical analysis is needed in situations where the system could not be recovered.

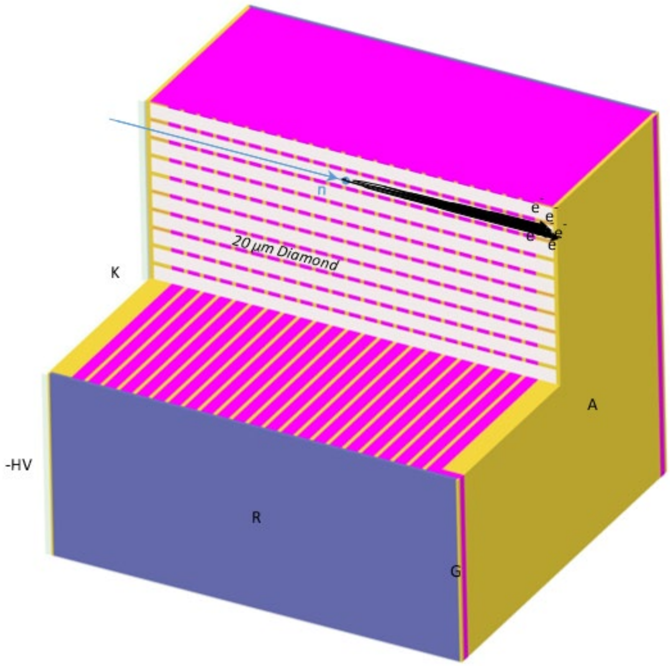
All photos and illustrations courtesy of Manuel Manard and the SDRD micro ion trap development team. *(DOE/NV/03624--1260)*

NNSS team develops a multilayered avalanche diamond detector for fast neutron applications

Researchers funded by the SDRD Program are developing a multilayered avalanche diamond (MAD) detector suitable for radiation detection applications. Initial MAD detector work has resulted in an article in SPIE Optical Engineering + Applications, which summarizes why diamond is ideal for this detector work: "The atomic and electrical properties of scCVD [single-crystal chemical vapor deposition] diamond…make this material attractive and suitable for use in radiation detection applications. Diamond has been acknowledged to have high radiation hardness and thus superior long-term stability. Due to its high atomic density and low atomic number, diamond has a high neutron detection efficiency per unit volume and limits gamma ray interaction probability." This work is important to the success of high-flux neutron source experiments across the DOE complex, including Neutron Diagnosed Subcritical Experiments at NNSS.

This work is novel because it uses thin crystalline layers wherein a large electric field (10–100 V/µm) can be applied for avalanche secondary electron gain. It cannot happen in thicker, bulk crystals as the presence of charge self-screens the applied field. Stacking of thin diamond layers or sections of one layer allows the high-field application while increasing the overall thickness and sensitivity of the diamond detector for better signal-to-noise quality. Higher gain with good signal-to-noise ratio allows the detector to be useful in a variety of scenarios less proximate to the source.

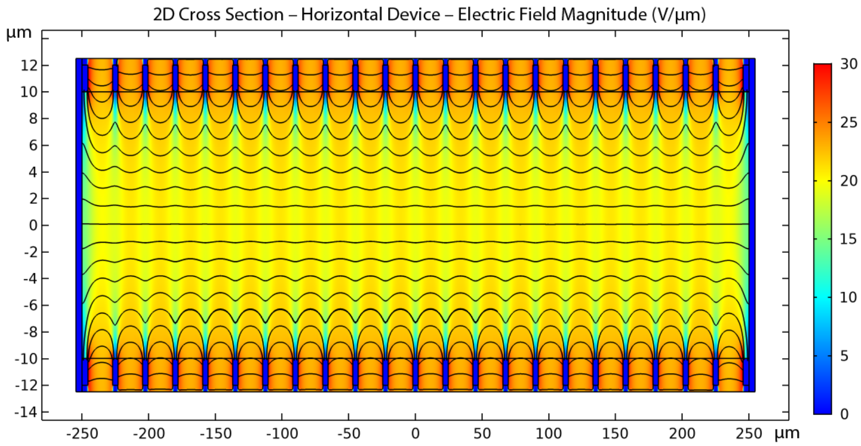
NNSS researchers are exploring two concepts for the high-field application: "horizontal" and "vertical" transport geometries. In either scenario, the metallization on thin diamond layers acts something like the dynodes in a photomultiplier tube (PMT). Unlike the PMT, however, the gain occurs within the intervening space, and the dynodes merely apply the field for transported gain. The following pictured one is somewhat experimental, but is the most straightforward. It is a horizontal geometry wherein the electrons transport internally from one (left) end of the diamond chip to the other (right) end, acquiring a saturation velocity and multiple secondaries per initial electron. The hybrid stack of multiple layers act in parallel for increasing the net current signal.



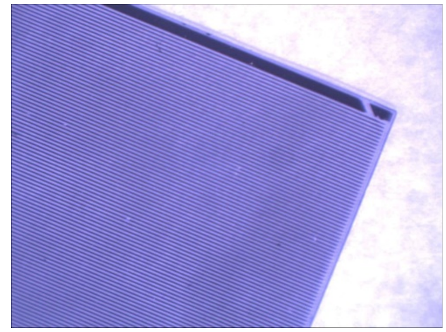
MAD detector horizontal concept device, hybrid stack with cutaway view, ~10x vertical scale. Hybrid stack is ~400 µm thick × 4 mm × 4 mm with twenty 20 µm scCVD diamond wafers (white). Each layer includes fine graded metallization (gold) encapsulated with Si_3N_4 passivation (magenta). The assembled stack includes a fired ceramic thick-film resistor (R) in contact with the graded fine metallization, and thicker endcaps, ground (G), and biased cathode (K). Anode (A) is segmented with passivation to separate bias current from signal current.

In the horizontal device, the full width of the diamond (~4 mm) is used as an accelerator for electrons to reach saturation velocity and keep producing secondaries until they strike the anode. However, unlike a large monolithic block of amorphous diamond, the proximate internal electrodes in this case maintain a high accelerating field in the presence of charge without intercepting the electrons. Unlike a multilayered ceramic chip capacitor, this hybrid construction is grown as single-crystal "plates," cut to size, and lithographically processed with metal and passivation patterns. The vertical scale is ~10x, and the cutaway view reveals several ~20 µm thick diamond wafers laid together and bonded. Each has thin Cr/Au metallization ~5 µm spaced by ~20 µm, and passivated overall (magenta). Following processing, they are stacked and bonded to form this macro block, and thick-film resistor paste coated and fired to form the graded potential distribution similar to a PMT. The fine metal between layers maintains the applied field in the presence of charge. The height is ultimately limited by the number and appropriate thickness of wafers. Twenty are illustrated, although twelve are estimated to produce an acceptable neutron sensitivity volume, and will be used in the first full-up demonstration.

The CVD diamond can be grown to a thickness appropriate to the charge density that can be mitigated with applied field, and we maintain a pitch-to-height aspect ratio $\lesssim 1$. The figure on the next page shows the field distribution for a 0.5 mm width, which can accommodate 20 V/µm with a dual-polarity scheme, ±5 kV at anode and cathode (requiring a +5kV bias tee on the anode). This smaller subdivision would be replicated eight times on a single 4 mm wafer, and even smaller subdivisions for greater electric field. However, patterning of such replicated sections requires more intricate masking steps, which will be pursued after a simpler two-layer stack demonstration. We expect to see that the horizontal concept preserves secondaries much better than a vertical device and does not require so strong an electric field, which will then determine the amount of integration necessary. The microscope photo on the next page shows the actual metallization to be used on this first multilayered prototype, consisting of 10 µm fine lines and gaps, the best that modest lithography to achieve.

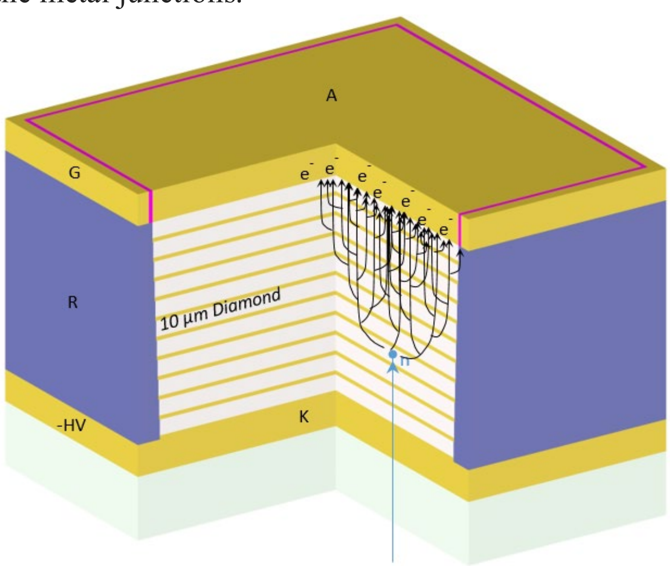


Edge-on cross-sectional view (~10x vertical scale) of a 20 µm × 500 µm horizontal device showing all electrodes (blue) and the calculated electric field (green, yellow, orange) within the diamond volume at ±5 kV bias. Black contours illustrate lines of force electrons will experience being transported toward the anode at right. The proximate inter-metal potentials along top and bottom maintain localized field within the volume at around 20 V/µm.



Microscope photo of a horizontal device scCVD diamond layer Cr/Au metallization (double-sided, symmetrical). The thicker band along the top edge is anode and (smaller) ground electrode. These are embedded within silicon nitride passivation in a multilayer stack and biased from the outer edges.

In the alternative vertical concept shown below, diamond chips are simply stacked, with anode at the top of the stack, and cathode at the bottom, with each layer biased via an ultrathin (~10 nm) metal interface. The whole area of the diamond chips act in parallel for increased net signal, and we are presently limited to 4 mm × 4 mm in scCVD diamond. We have demonstrated the fusion bonding of two such layers, and so having multiple avalanche layers is a proven fabrication capability. Multiplicative gain (of order 2^N for N-layers) is achieved by high-field transport through the thin, permeable intermetal dynode interfaces and continue being accelerated, into/through successive diamond layers. We would expect ~30 such layers for single neutron detection. However, loss is expected for any electrons born too close to the metal interfaces. These will not achieve enough energy to pass through and should be reclaimed at the metal junctions.



MAD detector vertical compression-bonded stack, 125 µm × 4 mm × 4 mm shown at 32x vertical scale. Cutaway reveals several ~10 µm thick internal diamond multilayers with ~10 nm ultrathin metallization (gold). Negative potential of ~20 V/µm is applied to the bottom cathode K with ground ring G and center anode A at the top. The internal metal is biased via a thick-film resistor R coating the side walls of the stack and adequately distributes the electric field despite the presence of internal charge. Resistance is designed for stiff current ~500 µA. Neutron, n of typically 14 MeV, can generate ~100 primary electrons.

CVD diamond (not necessarily single-crystal) could be grown on ultrathin metal for repeating monolithic diamond layers and is best grown with cathode down for graded edges, which favor increasing field density in the direction of flow. Then it is flip mounted onto a circuit card and original substrate laser cut from the top (initial) diamond layer, and finally outer metal deposited. Optional passivation barrier (magenta) helps isolate bias current from anode. High internal capacitance supplies the needed impulse charge.

When horizontal and vertical stacked devices were first proposed, the goal seemed very challenging, but NNSS is finding success in concert with Applied Diamond, Inc., which has successfully developed proposed methods for compression bonds, fine metallization, passivation, and thick film resistor processes. In both cases, the difficulty lies in the specific steps of processing the assemblies, and the vertical challenges are first being addressed in the horizontal two-layer device. Either design has some trade-off in potential losses. As design and process integration improves, variations on tighter interweaving of repeated electrode configurations are likely to leverage smaller overall bias for the same field patterns. If field trials prove successful, such detectors will find use as neutron time-of-flight spectrometers in support of Stockpile Stewardship, High Energy Density Physics, and Global Security missions at NNSS.

All illustrations courtesy of Amber Guckes and the SDRD MAD detector team. *(DOE/NV/03624--1262)*

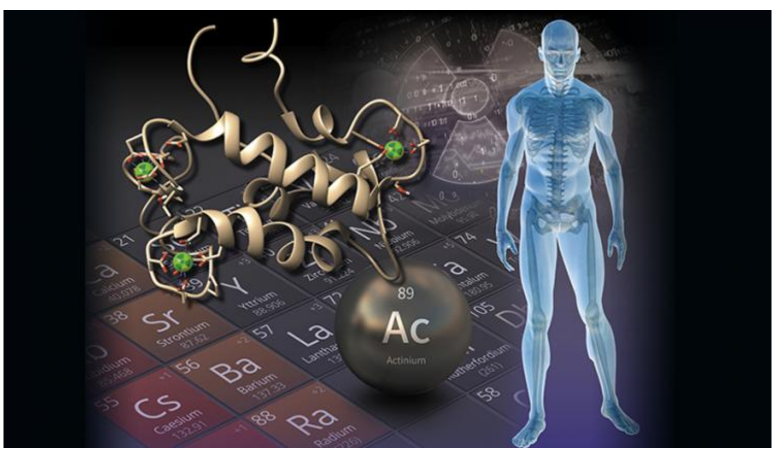
Lawrence Livermore National Laboratory

HIGHLIGHTS

Livermore and Penn State researchers demonstrate how a newly discovered protein helps cancer therapies and nuclear material detection

Livermore National Laboratory (LLNL) and Penn State scientists have demonstrated how a protein called lanmodulin can be used to recover and purify radioactive metals like actinium, an element that could be beneficial for both next-generation drugs used in cancer therapies and the detection of nuclear activities.

Radioactive metals hold unique and essential places in a variety of medical imaging and therapeutic applications, but they require lengthy separation processes to purify them as well as synthetic and costly chelators (molecules tailored to bind the radioactive metal ions) that must form exceptionally stable complexes in the patient to minimize toxicity. Actinium-based therapies could revolutionize cancer medicine, with treatment efficacy hundreds of times higher than current drugs. However, they remain out of reach because of difficulties throughout the actinium supply chain, from producing isotopes to studying the element's chemistry, and developing of robust chelators.



Actinium is a radioactive element that could revolutionize cancer medicine, but its chemistry has thus far remained elusive. LLNL and Penn State researchers developed a new approach to study, capture and purify medical isotopes, including actinium. Their strategy leverages a natural protein that can tightly bind to medical isotopes without interacting with process impurities like radium and strontium.
(Artwork by Thomas Reason/LLNL)

The LDRD-funded team showed how lanmodulin can be used to bind, recover, and purify actinium to at least 99.5% purity obtained in a single step. They did the same for another medically relevant radioisotope, yttrium-90, which is used for cancer therapy and diagnostics. The unprecedented efficiency and simplicity of the protein-based approach also allows the preparation of actinium at much lower cost and the probing of its chemistry more conveniently. The process also is likely extendable to many other radioactive isotopes used in radiation therapy and imaging.

"Our approach, which combines lanmodulin's tight and specific binding with inexpensive filtration devices, allowed us to easily access minute quantities of radiometals, as low as a few attograms, where traditional technologies based on synthetic chelators fail," said LLNL scientist Gauthier Deblonde, lead author of a paper appearing in *Science Advances*. "What we accomplished here was simply unfathomable a few years ago."

Find more information about this process on the LLNL website. *(LLNL-WEB-45845)*

Livermore analyst constrains magnitude of the 2020 Beirut explosion

On August 4, 2020, one of the largest non-nuclear explosions in history pulverized a Beirut port and damaged more than half the city. The explosion resulted from the detonation of tons of ammonium nitrate, a combustible chemical compound commonly used in agriculture as a high-nitrate fertilizer, but which can also be used to manufacture explosives. Since that time, explosive yield estimates have varied widely, and in some cases, were inconsistent with what would be expected based on the amount of ammonium nitrate stored at the Beirut harbor. In addition, the crater size, seismic magnitude, and mushroom cloud height seemed to be inconsistent.

Before and after images of the Beirut explosion on August 4, 2020.

LLNL physicist Peter Goldstein has studied how water saturation of the explosive, ground, and possibly water and debris from the near-source environment can help reconcile differences in the yield estimates obtained using these different measurements. Goldstein's LDRD-funded research, which appears in *Countering WMD Journal*, analyzes the crater dimensions, seismic magnitude estimates, and the cloud height of the explosion. He shows that all the data are consistent with a yield of around a kiloton when water/saturation is accounted for.

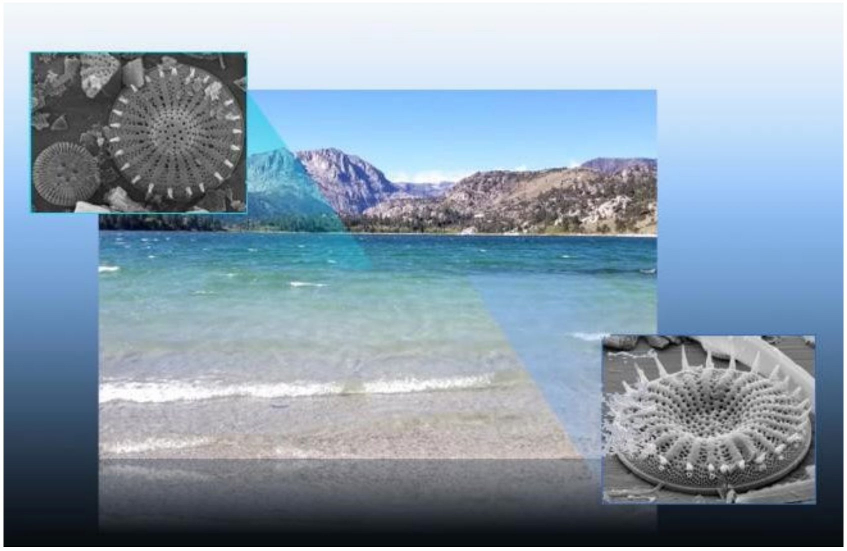
He reports that the "evidence suggests that the relatively large crater radius is due to a high degree of saturation of the ground beneath the explosion. It is likely that this saturation increased coupling of shock wave energy to the surrounding material and reduced the effective stress/strength of the material.". He also found that yield estimates based on seismic body-wave magnitude, the maximum debris cloud height and the observed crater depth corroborated the estimates based on crater radius.

Find more information about Goldstein's analysis on the LLNL website. *(LLNL-WEB-45845)*

Climate change in the Sierra Nevada has profoundly altered its lake ecosystems

Climate change has significantly impacted the natural systems of the Sierra Nevada, including the mountain lakes that are an iconic part of California's natural beauty. New LDRD-funded research from an LLNL scientist and colleagues from the University of Kentucky and Indiana State University shows that lake-sediment cores from a subalpine lake in the eastern Sierra Nevada record significant, sometimes abrupt, changes to lake conditions and ecology over the last three millennia. The new study reveals just how dramatically climate change has already impacted aquatic ecosystems in the Sierra

Nevada, highlighting the need for action to protect them. The research appears in the journal *Global Change Biology*.



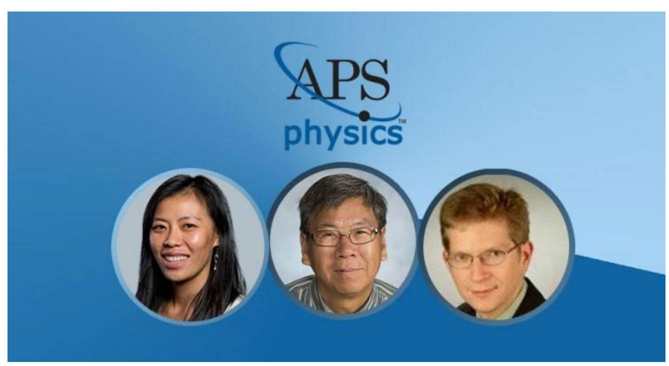
June Lake beach in the Sierra Nevada of California. Climate change is disrupting the water cycle in the Sierra Nevada in ways that are challenging to predict, which lowers society's resilience by limiting water resources. Photo by Mike McGlue/University of Kentucky. Insets: Diatom fossils from June Lake sediments under scanning electron microscope. (Photo by Jeffrey Stone/Indiana State)

Lake-sediment records allowed the team to reconstruct the region's climate history over the past 3,000 years. To do this, the team, led by LLNL physicist Susan Zimmerman, studied diatoms, a type of algae that leave behind tiny silica fossils that are preserved in lake sediments. The diatoms revealed a detailed history of the lake and its response to changing seasonality, including in the Late Holocene Dry Period and the Medieval Climate Anomaly, which are well-known periods of ancient drought in the region. But the most striking feature of the fossil record was the uniqueness of the 1840–2016 period. The team detected the most dramatic changes to the June Lake ecosystem at that time, with the fossils suggesting low water levels, low nutrient concentrations, and strong water column stratification. The data suggest that "hot droughts" of the Industrial Era altered the lake state to conditions unseen in the last three millennia, showing that changes attributable to anthropogenic climate change began as early as the mid 19th century.

Find more information about Sierra Nevada climate change on the LLNL website. *(LLNL-WEB-45845)*

Three LLNL scientists honored as American Physical Society fellows

Three LLNL physicists with strong ties to LLNL's LDRD program have been selected as 2021 fellows of the American Physical Society. The new fellows, who are all former LDRD principal investigators, represent a range of physics expertise, including intense laser–matter interactions and inertial fusion energy science, modeling of magnetically confined fusion, and warm dense matter experimental science. Tilo Doeppner, a physicist in the High Energy Density Division of the National Ignition Facility and Photon Science (NIF&PS) Directorate, was chosen for "pioneering new regimes of warm dense matter experimental science from Mbar to Gbar pressures on high-energy lasers and light sources, relevant to understanding brown dwarf and white dwarf interiors and inertial confinement fusion science."



From left: Tammy Ma, Xueqiao Xu, and Tilo Doeppner

Tammy Ma, a physicist in the High Energy Density Division of the NIF&PS, was selected for "outstanding scientific contributions and leadership in the field of intense laser-matter interactions and inertial fusion energy science."

Xueqiao Xu, a physicist in the Physics Division of the Physical and Life Sciences Directorate, was cited for "wide-ranging contributions to the understanding of the tokamak edge, including edge pedestal stability and the onset and evolution of edge localized modes and for leading the development of edge simulation models and codes."

More information about LLNL's American Physical Society fellows can be found on the LLNL website. *(LLNL-WEB-458451)*

Los Alamos NATIONAL LABORATORY

HIGHLIGHTS

LANL LDRD researchers are working to make plants more drought resistant

Los Alamos National Laboratory (LANL) LDRD researcher Sanna Sevanto, in the Laboratory's Earth System Observations group, and her team are researching how microbial adjustments in soil can alter a plant's physiology. Could a plant be made to require less water by adding microbes? That's the question Sevanto is trying to answer. The team is currently studying the efficacy of two different microbiomes: one from the Crops Research Laboratory in Fort Collins, Colo., and the second from Los Alamos.

In the natural environment, a plant is part of a rich ecosystem that includes microorganisms. These microbes include bacteria and fungi that are paramount to a plant's growth and performance. But in northern and central New Mexico, the soil tends to be thick and clay-like, lacking in diverse microorganisms, and one of the reasons rain water infiltrates the soil so poorly. (If you've tried planting flowers in this type of soil, you've no doubt watched the flower quickly wilt.) This is one reason why it's critical to develop methods to improve soil and drought tolerance of plants.

Sevanto and her team are introducing new microbes into a plant's ecosystem to determine whether a plant's physiology can be altered to become more drought resistant. Their research so far has shown it is possible; the LANL-based microbes made the plant grow bigger while requiring less water. Their research will continue into seeing whether a plant can be made to withstand a moderate or severe drought. With more drought resistance, plants would be better able to flourish in drier conditions, securing the food chain for years to come.

Sanna Sevanto in the Earth Systems Observations greenhouse at TA-51. (Image credit: LANL)

Find more information about this research on the LANL website.

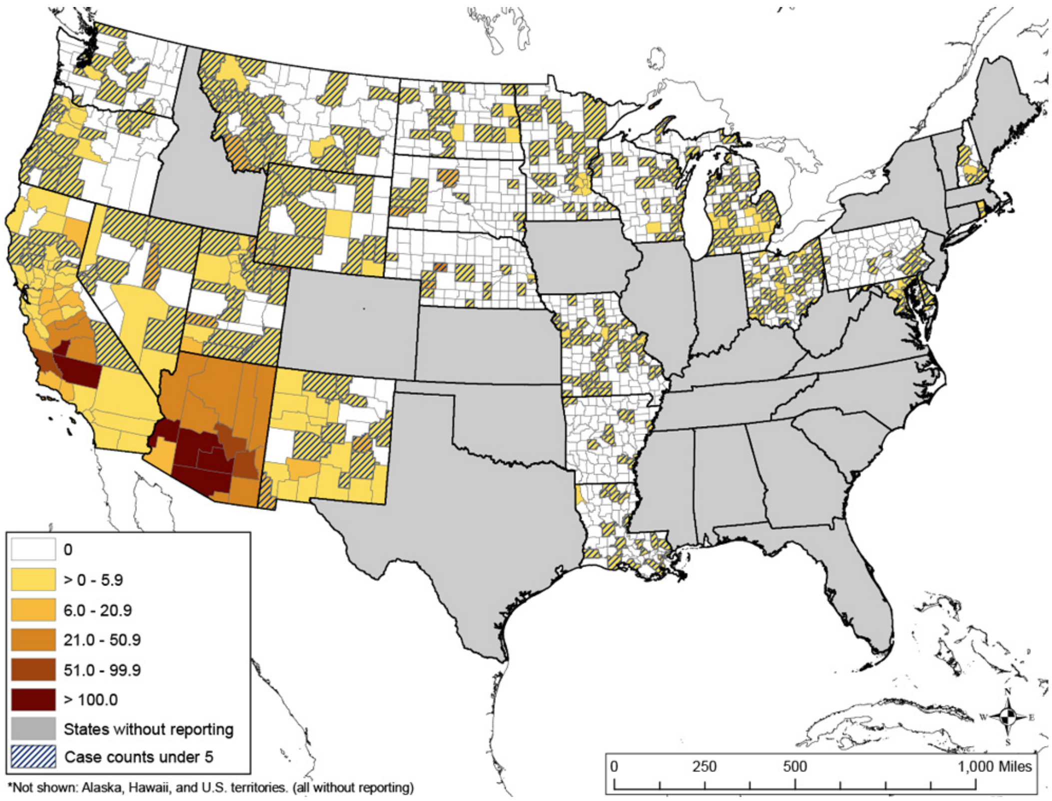
Work supported by the LDRD program was funded via project 20200109DR, "Directed Plant-Microbiome Evolution for Food and Biofuel Security." *(LA-UR-21-29088)*

LANL LDRD Researchers discover the fungus among us – Valley fever

A 2019 study by a LANL researcher and a team of other researchers at the University of California, Irvine documented the expansion of Valley fever, projecting that the fungal infection's range will likely more than double in the United States, with the list of affected states jumping from 12 to 17, and the number of individual Valley fever cases predicted to grow by 50% by the year 2100. The same research offers a few tools for tamping down the disease's impact.

The fungus itself finds its way into human lungs when rainfall soaks the ground, allowing the fungus to grow, and then a dry spell triggers it to form spores, which are easily stirred up in dust. Whether gardening, landscaping, doing construction, or merely driving a dusty road, humans (and their trail-following canine companions) can breathe in the microscopic spores.

Within the lungs, the tiny spores expand into ball-like packets called spherules, which divide internally to fill with even smaller endospores. Eventually, in the warm, welcoming environment of the lung, the spherules rupture and release their payload to spread through the body's surrounding tissue.



[This map](#) from the Centers for Disease Control and Prevention shows the average incidence of Valley fever per 100,000 that was reported by county from 2011–2017.

What this means for an exposed person is a bout of flu-like symptoms, with coughing, fever, headache, muscle aches, joint pain and fatigue, all of which can look familiar enough to be either ignored or misdiagnosed. In mild cases, two weeks or more will be required to recover. But the U.S. Centers for Disease Control reports that as many as 40% of people infected with it will need hospitalization. Beyond the flu-like version of Valley fever, for some people the disease morphs into a serious pneumonia and it can spread into other parts of the body, even the brain, and into serious skin lesions. At LANL, research is underway to explore how potential climate conditions could affect predictions of the number of monthly Valley fever cases in the two highly endemic regions for this disease—the San Joaquin Valley of California and south-central Arizona. Researchers are also working to create a high-resolution risk map of where the fungus is likely growing in the soil, based on climate and soil conditions. This will help disease mitigation by informing the community where extra precautions may be needed to prevent dust exposure.

In New Mexico, for example, only 31% of clinicians considered Valley fever when they had a patient that showed signs of a severe respiratory infection. For these reasons, the research team considers that Valley fever cases in New Mexico have been very likely underreported. An increase in cases in 2019 could be a result of higher disease awareness and better reporting. But, overall, increasing both clinician and patient awareness of Valley fever could decrease the time to patient diagnosis, saving both health and cost burdens from this disease.

Read the original article in the *Albuquerque Journal*.

Work supported by LDRD was funded via project 20200682PRD1 "Forecasting Valley Fever Disease Risk Using Machine Learning." *(LA-UR-21-28023)*

LANL LDRD researchers discover relatively new cryptographic protocol proving the authenticity of digital information without revealing the information itself

The easiest way to cheat on your math homework is to find the answers somewhere, such as the internet or an answer key. The best way for a teacher to prevent this kind of cheating is to issue the widely dreaded requirement to "show your work."

Showing the work usually reveals whether that work is legitimate and original, but it's a burden: the teacher must now review every student's every line of work. This may be a burden some teachers are willing to accept, but what if, instead of the answer to a math problem, one were trying to prove the veracity of satellite imagery (which could have been intercepted and faked)? Or the proper manufacture and assembly of parts for a nuclear weapon (which could have been subtly sabotaged)? Or the output from a computer network that controls critical infrastructure (which could have been hacked)? Or the accuracy of scientific experiments, data, and analysis (which could have been biased)?

In such cases, evidence of tampering, or some other manner of inauthenticity, may be expertly hidden in one small corner of the greater whole. And even if a "show your work" approach were sufficient in theory, finding one incongruous detail in the endless terabytes needed to prove the validity of such complex information would be a nearly hopeless task. Moreover, it would require actually showing—sharing, transmitting, publishing—"your work," thus putting sensitive information at even greater risk.

The solution to this rather esoteric challenge is something called a "zero-knowledge proof" (ZKP). It's a technique that cryptographically encodes a small, robust, random sample of what "showing your work" would entail—evidence of a spot check, of sorts, but without including any of the actual work—together with a clever mathematical manipulation designed to ensure that any data tampering, no matter how small or well hidden, is overwhelmingly likely to get picked up. "The math of it has already been worked out," says Michael Dixon, a scientist in LANL's Advanced Research in Cyber Systems group.

A proof could take the form of an entire "show your work" explanation. But this extra information is undesirable. It requires the transmission and examination of large amounts of data or back-and-forth interaction.

A better solution is based on an important result in computational complexity theory known as the PCP theorem ("probabilistically checkable proof"). The theorem essentially states that if you have a mathematical proof of a particular length, it is possible to reconfigure that proof into a longer one that can be verified, with great accuracy, using only a random sampling of a very small subset of that longer-form proof. That's the spot check. The resulting cryptographic proof is something called a zk-SNARK: a zero-knowledge succinct non-interactive argument of knowledge. Here, the terms "succinct" and "non-interactive" eliminate the cumbersome varieties of ZKP.

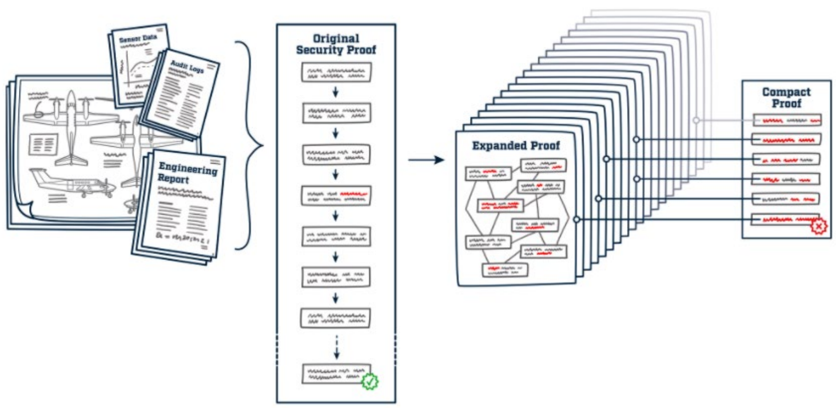
With zk-SNARKs, a complicated data product can be passed along between numerous parties—even explicitly distrusted parties—before it reaches its final recipient, and yet that recipient can be assured of the data's veracity in the end. Dixon refers to this as a "chain of provenance": at each stage of working with a data product, a new zk-SNARK combines the verification associated with the current stage with the previous zk-SNARK, which verified all prior stages, confirming that the information was processed properly by all the appropriate computational procedures and not touched by anything else.

Private information, public security

From a national security perspective, ZKPs have immediate value. The U.S. military, for example, needs to verify that the complex defense systems it purchases from large numbers of private-sector contractors and subcontractors have been built precisely according to approved specifications. They must have properly sourced parts and be correctly assembled, carefully transported, and faithfully deployed—all succinctly and convincingly verified at every step of the way without having to take the whole thing apart or, in the case of nuclear weapons, perform a weapons test, which is prohibited by international treaty. (Similarly, complex civilian products involving foreign or domestic private-sector subcontractors can be reliably tracked and verified by sharing only zk-SNARKs and thereby not sharing any proprietary information.)

Dixon and his student, Zachary DeStefano, who is entering a doctoral program in computer security, set out to secure output from machine-learning systems called neural networks. Neural networks are complex algorithms that use many nodes, each with parameters that must be learned through experience, to simulate processing by neurons. Dixon and DeStefano's solution, unsurprisingly, involves ZKPs.

"The most powerful neural-network models are based on datasets much larger than what any one organization can house or efficiently collect," says DeStefano. "We live in an era of cloud computing, and neural-network computations are often subcontracted out. To validate critical results—or just to make sure you got what you paid for—you need a succinct, non-interactive way to prove that the correct neural network, set up exactly as you specified, processed the inputs you provided and no others."



Zero-knowledge proofs are considered probabilistically checkable: a mathematical operation reorganizes data so that evidence of a small, well-hidden error is replicated widely. Any random spot check will be overwhelmingly likely to capture one or more of these replicated errors, thereby revealing evidence of tampering or incorrect provenance. Conversely, the absence of such errors makes it overwhelmingly probable that the file is legitimate.

Last year, Dixon and DeStefano wrote a software program to do exactly that. It produces a zk-SNARK to validate both the inputs and the specific network execution for a system trained to recognize handwritten numbers. Without supplying a massively cumbersome log of all the scribbles in the dataset, of every single value of every variable the neural network adjusted, of what outputs the countless iterations produced, or of how the network learned to improve its accuracy, the proper processing was nonetheless successfully confirmed.

But with neural networks, there's another concern: their training. A ZKP is needed to account for the authenticity of the training set originally supplied to the neural network, which, often, the customer has no part in. Dixon and DeStefano are working on that now.

"We're working to help a distributed system for crowd-sourced training data audit itself," Dixon says. "The idea is to delegate neural-network training to the edge nodes, such as hospitals, and require them to furnish proofs that they did their jobs correctly." The neural network still seeks to improve its parameters through iteration, but instead of asking edge nodes for patient data explicitly, it only asks in what direction and by how much to shift the current-iteration parameters to achieve an improvement. Earlier research proved that the edge nodes can perform that computation, and Dixon and DeStefano are now demonstrating that zk-SNARKs can verify that the edge nodes did (or didn't do) exactly what they were supposed to. The result is a perfectly reliable neural network computation and a hugely valuable medical resource constructed from enormous quantities of verified patient data that were never actually shared. And by virtue of the zk-SNARKs, the system automatically recognizes and eliminates training information derived from faulty patient data, whether the error comes from a mistake or deliberate sabotage.

Eventually, Dixon hopes to see specific hardware designed to produce inherently self-verified data for neural-network training and general computation. Data would be quantum mechanically guaranteed and cryptographically certified upon creation, with subsequent zk-SNARKs generated as needed to verify the proper processing and the absence of tampering.

"Where we are now—verifying inputs and execution, securing data sources and supply chains—is just the beginning," says Dixon. "In a world concerned with massive-scale misinformation, it's difficult to overstate the public good that will ultimately come from this technology."

Find more information about zk-SNARK on the LANL website.

Work supported by the LDRD program was funded via project 20210529CR Information Science and Technology Institute (ISTI): Foundational Research in Information Science and Technology, and 20180719CR Rapid Response: Novel Computing. *(LA-UR-21-27618)*

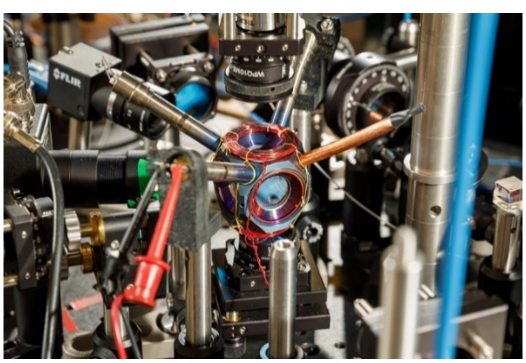
Sandia National Laboratories

HIGHLIGHTS

GPS-free navigation? Sandia device shows advanced wayfinding tech could become compact, fieldable

For over a year, an avocado-sized vacuum chamber with titanium metal walls and sapphire windows has contained a cloud of atoms at the right conditions for precise navigational measurements. It is the first device that is small, energy-efficient and reliable enough to potentially move quantum sensors—sensors that use quantum mechanics to outperform conventional technologies—from the lab into commercial use, said Sandia National Laboratories scientist Peter Schwindt.

Sandia developed the chamber as a core technology for future navigation systems that do not rely on GPS satellites. It was described earlier this year in the journal *AVS Quantum Science*.



A compact device designed and built at Sandia could become a pivotal component of next-generation navigation systems.
(Photo by Bret Latter)

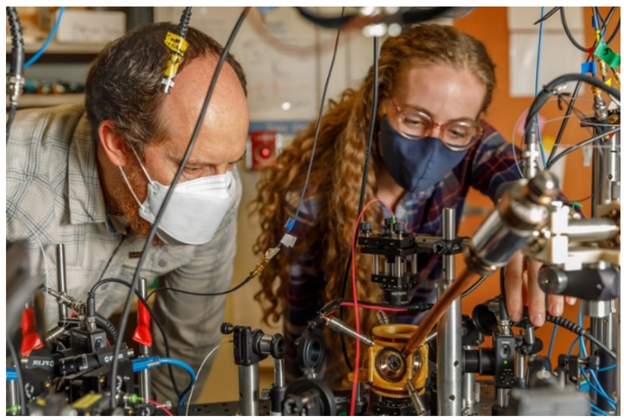
Countless devices around the world use GPS for wayfinding. It is possible because atomic clocks, which are known for extremely accurate timekeeping, hold the network of satellites perfectly in sync, but GPS signals can be jammed or spoofed, potentially disabling navigation systems on commercial and military vehicles alike. So instead of relying on satellites, Schwindt says future vehicles might keep track of their own position using on-board devices as accurate as atomic clocks, but that measure acceleration and rotation by shining lasers into small clouds of rubidium gas, like the one Sandia has contained.

Compactness key to real-world applications

Atomic accelerometers and gyroscopes already exist, but they are too bulky and power-hungry to use in an airplane's navigation system. That is because they need a large vacuum system to work—one that needs thousands of volts of electricity.

Quantum sensors are a growing field, and there are lots of applications you can demonstrate in the lab," said Sandia postdoctoral scientist Bethany Little, who is contributing to the research. "But when you move it into the real world there are lots of problems you have to solve. Two are making the sensor compact and rugged. The physics takes place all in a cubic centimeter (0.06 cubic inches) of volume, so anything larger than that is wasted space."

Little said her team has shown that quantum sensing can work without a high-powered vacuum system. This shrinks the package to a practical size without sacrificing reliability. Instead of a powered vacuum pump, which whisks away molecules that leak in and wreck measurements, a pair of devices called getters use chemical reactions to bind intruders. The getters are each about the size of a pencil eraser so they can be tucked inside two narrow tubes sticking out of the titanium package. They also work without a power source.



Sandia National Laboratories scientist Peter Schwindt, left, and postdoctoral scientist Bethany Little examine the vacuum package held in a yellow, 3D-printed mount. (Photo by Bret Latter)

To further keep out contaminants, Schwindt partnered with Sandia materials scientists to build the chamber out of titanium and sapphire. These materials are especially good at blocking out gasses like helium, which can squeeze through stainless steel and Pyrex glass. Construction took sophisticated fabrication techniques that Sandia has honed to bond advanced materials for nuclear weapons components. And like a nuclear weapon, the titanium chamber must work reliably for years.

The Sandia team is continuing to monitor the device. Their goal is to keep it sealed and operational for five years, an important milestone toward showing the technology is ready to be fielded. In the meantime, they are exploring ways to streamline manufacturing.

[Find more information about compact quantum sensors on the Sandia website.]

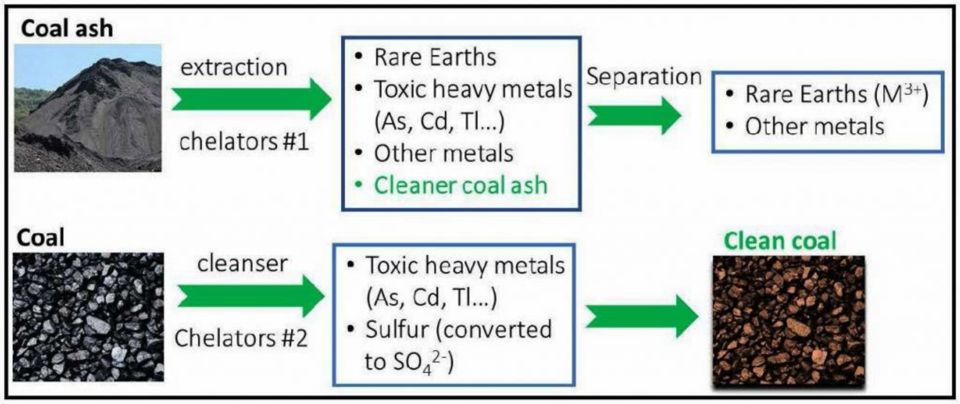
Funding was provided by Sandia's LDRD program. *(SAND2021-13053L)*

Sandia patent frees rare-earth metals from coal ash for phones, computers

A harmless food-grade solvent has been used to extract highly sought rare-earth metals from coal ash, reducing the amount of ash without damaging the environment and at the same time increasing an important national resource.

Coal ash is the unwanted but widely present residue of coal-fired power. Rare-earth metals are used for a variety of high-tech equipment from smart phones to submarines. The separation method, which uses carbon dioxide, water, and food-grade citric acid, is the subject of a Sandia patent application.

"This technique not only recovers rare-earth metals in an environmentally harmless manner but would actually improve environments by reducing the toxicity of coal waste dotting America," said Guangping Xu, lead Sandia researcher on the project. "Harmless extraction of rare-earth metals from coal ash not only provides a national source of materials essential for computer chips, smart phones and other high-tech products—including fighter jets and submarines—but also make the coal ash cleaner and less toxic, enabling its direct reuse as concrete filler or agricultural topsoil."



Comparison of extraction efficiency between Sandia's environmentally benign technology and existing method using strong acids, concentrated nitric acid, and hydrogen peroxide. (Graphic by Guangping Xu)

The method, if widely adopted, could make coal ash, currently an environmental pariah, into a commercially viable product, Guangping said.

Environmentally friendly method for mining rare-earth metals

The most common acids used as chemical separators in mining—nitric, sulfuric or phosphonic acids—also are able to extract rare-earth metals from coal ash but produce large amounts of acid waste, leaving the environment in worse shape than before. "Environmentally harmful acids would raise cleanup costs beyond economic feasibility in the United States," Guangping said. He found that in less than a day, at 70°C (158°F) and 1,100 pounds per square inch pressure (about 70 times ordinary atmospheric pressure), the method extracted 42% of rare-earth metals present in coal waste samples.

Chinese mines, where 95% of the world's resources of rare-earth metals are located, achieve less efficient separation while using environmentally damaging methods. "Theoretically, an American company could use this technique to mine coal and coal byproducts for rare-earth metals and compete with Chinese mining," said Guangping. "For U.S. national security purposes, it is reasonable to have alternate sources of rare-earth metals to avoid being at the mercy of a foreign supply."

Detoxifying coal ash for reuse alone should be worth the effort, he said. There's no shortage of coal ash as a raw material. According to a 2016 paper in the journal *Environmental Science and Technology*, "Approximately 115 million metric tons of coal combustion products are generated annually, and this sum includes 45 million tons of fly ash. These numbers remain of interest today, said Guangping, asserting that if "we don't detoxify and reuse the coal ash, then it will be abandoned in place and cost billions of dollars to clean up over the long term." To help make that outcome less likely, "we expect tests of our extraction techniques at larger volumes and on a variety of coal-based sources in the near future."

Find more information about the method to extract rare-earth metals from coal ash on the Sandia website.

The work is supported by Sandia's LDRD office. *(SAND2021-13054L)*

Sandia 3D-imaging workflow has benefits for medicine, electric cars, and nuclear deterrence

Sandia researchers created a method of processing 3D images for computer simulations that could have beneficial implications for several industries, including health care, manufacturing and electric vehicles.

At Sandia, the method could prove vital in certifying the credibility of high-performance computer simulations used in determining the effectiveness of various materials for weapons programs and other efforts, said Scott A. Roberts, Sandia's principal investigator on the project. Sandia can also use the new 3D-imaging workflow to test and optimize batteries used for large-scale energy storage and in vehicles.

"It's really consistent with Sandia's mission to do credible, high-consequence computer simulation," he said. "We don't want to just give you an answer and say, 'trust us.' We're going to say, 'here's our answer and here's how confident we are in that answer,' so that you can make informed decisions."

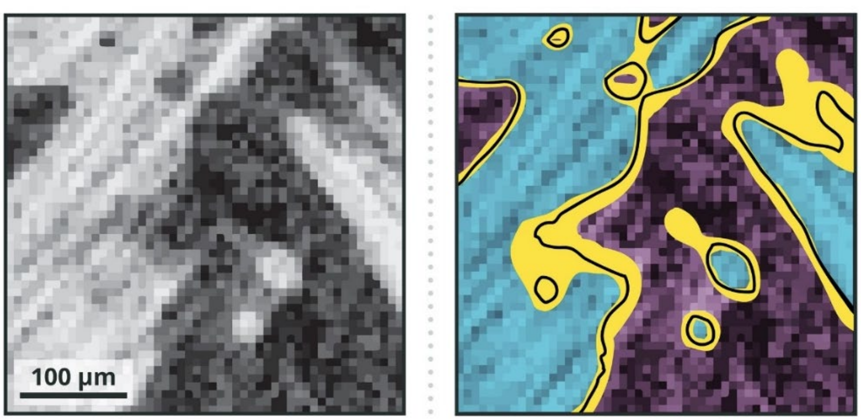
The researchers shared the new workflow, dubbed by the team as EQUIPS (Efficient Quantification of Uncertainty in Image-based Physics Simulation), in a paper published today in the journal *Nature Communications*.

"This workflow leads to more reliable results by exploring the effect that ambiguous object boundaries in a scanned image have in simulations," said Michael Krygier, a Sandia postdoctoral appointee and lead author on the paper. "Instead of using one interpretation of that boundary, we're suggesting you need to perform simulations using different interpretations of the boundary to reach a more informed decision."

EQUIPS can use machine learning to quantify the uncertainty in how an image is drawn for 3D computer simulations. By giving a range of uncertainty, the workflow allows decision-makers to consider best- and worst-case outcomes, Roberts said.

Workflow EQUIPS decision-makers with better information

Think of a doctor examining a CT scan to create a cancer treatment plan. That scan can be rendered into a 3D image, which can then be used in a computer simulation to create a radiation dose that will efficiently treat a tumor without unnecessarily damaging surrounding tissue. Normally, the simulation would produce one result because the 3D image was rendered once, said Carianne Martinez, a Sandia computer scientist. But, drawing object boundaries in a scan can be difficult and there is more than one sensible way to do so, she said. "CT scans aren't perfect images. It can be hard to see boundaries in some of these images."

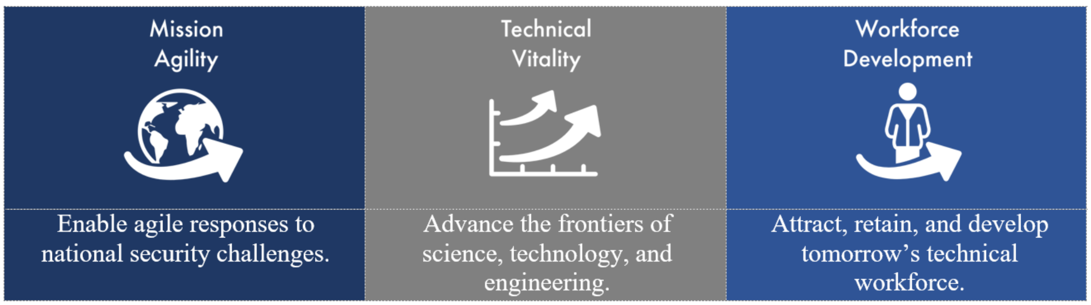


An illustration shows the uncertainty of drawing boundaries in scanned images used for high-consequence computer simulations. The gray-scale image on the left is a scan of material used as a thermal barrier. The illustrated image on the right shows the material segmented into two classes (blue and purple). The black lines show one possible interface boundary between the two classes of material. The yellow region depicts the segmentation uncertainty, meaning the black lines could be drawn anywhere within that area and still be valid.
(Illustration courtesy of Sandia)

Humans and machines will draw different but reasonable interpretations of the tumor's size and shape from those blurry images, Krygier said. Using the EQUIPS workflow, which can use machine learning to automate the drawing process, the 3D image is rendered into many viable variations showing size and location of a potential tumor. Those different renderings will produce a range of different simulation outcomes, Martinez said. Instead of one answer, the doctor will have a range of prognoses to consider that can affect risk assessments and treatment decisions, be they chemotherapy or surgery.

Find more information about the 3D-imaging workflow on the Sandia website.

The research, funded by Sandia's LDRD program, was conducted with partners at Indiana-based Purdue University, a member of the Sandia Academic Alliance Program. Researchers have made the source code and an EQUIPS workflow example available online. *(SAND2021-10839E)*



This newsletter, published quarterly, features LDRD and SDRD work done by Lawrence Livermore, Los Alamos, Nevada National Security Site and Sandia. For additional issues, visit NNSA-LDRD.lanl.gov. Per NNSS classification, this document is confirmed to be unclassified and approved for public release.

For more information

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