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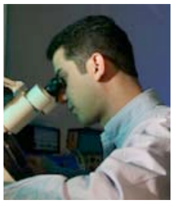



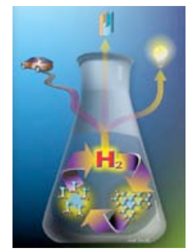

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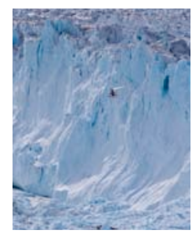

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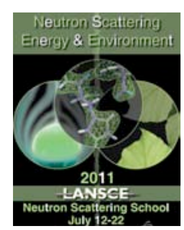

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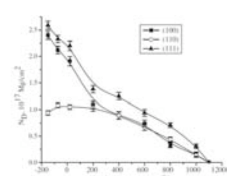

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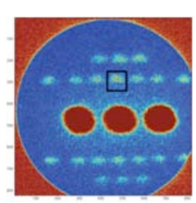

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AWARDS

Shadi Dayeh and Cristiano Nisoli receive Postdoctoral Distinguished Performance Awards

The awards recognize individual postdoctoral researchers or teams of no more than three who were the major contributors towards outstanding and unique research resulting in a positive and significant impact on the Laboratory's programmatic and or organizational efforts or status in the scientific community. Shadi Dayeh (Center for Integrated Nanotechnologies, MPA-CINT) and Cristiano Nisoli (Center for Nonlinear Studies/Physics of Condensed Matter and Complex Systems, CNLS/T-4) won Postdoctoral Distinguished Performance awards, and Juan Duque (Physical Chemistry and Applied Spectroscopy, C-PCS) and Katharine Page (Lujan Center, LANSCE-LC) received honorable mention.

Shadi Dayeh, a Distinguished J. Robert Oppenheimer Postdoctoral Fellow, was recognized for his outstanding contributions to the research and development community through his scientific accomplishments and creative ideas. His mentor, Tom Picraux (MPA-CINT) nominated him. Dayeh used the vapor-liquid-solid method to develop the most complete treatment of size-dependent growth of germanium nanowires. This comprehensive study potentially settles the controversial area of the size-dependent growth rate of nanowires. Dayeh has also worked on heterostructured nanowire growth and devices, and most notably uncovered issues surrounding the growth of core/shell germanium/silicon (Ge/Si) nanowires for field effect transistors that showed record on-current performance and utilized bandgap engineering in axial Ge/Si heterostructured nanowires for high on/off current switches. In addition, he has proposed a new research approach for neural probes that could open a new area of neuronal studies. Dayeh is the principal investigator of a Laboratory Directed Research and Development – Exploratory Research proposal on “High Density Neuronal Recording using Nanowire Capacitor Sensors.” He came to LANL as a Director’s Postdoctoral Fellow after earning his PhD in electrical and computer engineering/electronic materials and devices from the University of California – San Diego in 2008. Dayeh has served as vice president and president of the Los Alamos Postdoc Association, and he initiated an annual Los Alamos Postdoc Research day.

Cristiano Nisoli, a LANL Director’s Postdoctoral Fellow, was cited for his substantial impact in fields ranging from disordered systems to biophysics and condensed matter. Avadh Saxena (T-4 Group Leader) nominated him. Nisoli has made seminal contributions to the field of frustration, disorder, and thermodynamics out of equilibrium. He has introduced (in collaboration with Professor Schiffer’s group at Pennsylvania State University) and explained theoretically, a novel magnetic meta-material, now widely known as “artificial spin ice.” His research in quasi-one-dimensional systems has lead him to the exploration of pattern formations reminiscent of symmetries seen in flowers, leaves, or cacti; to the discovery of a new regime of topological excitations, which he termed “Dynamical Phyllotaxis;” and to the prediction of thermally induced failures in a variety of quasi-one-dimensional systems including nanotubes, nanowires, and DNA. Recently he has turned his attention to the thermomechanics of DNA. Nisoli’s work on artificial spin ice, recognized by an Outstanding Poster

Award at the Postdoc Research Day, has been featured on the cover of ***Nature***, in many ***Nature*** and ***Nature Physics*** editorials, and as a new field of research. His work on Dynamical Phyllotaxis was highlighted in a column of the American Mathematical Society, in ***Nature Materials***, as well as on many scientific websites. His research on thermally activated failures received honorable mention for the 2010 Leon Heller prize in theoretical physics. Nisoli was educated in Milano, Italy and the US, where he received his PhD from the Pennsylvania State University. He joined CNLS/T-4 as a postdoc in 2008.

Tom Intrator, Quanxi Jia, and James Werner win Postdoc Distinguished Mentor Awards
The awards recognize the positive impact and contributions that a mentor makes during a postdoc's appointment as well as demonstrating a level of mentoring substantially beyond what would normally be expected. Winners of the Postdoc Distinguished Mentor Awards are Tom Intrator (Plasma Physics, P-24), Quanxi Jia (MPA-CINT), and James Werner (MPA-CINT).

Tom Intrator was nominated by postdoctoral researcher Jason Sears (P-24), who described him as deeply passionate about preparing his postdocs for productive and rewarding careers as scientists. For example, Intrator facilitates postdoc attendance at conferences and workshops and is extremely proactive in identifying their next career opportunities, often personally making connections with future employers. According to Sears, Intrator has an unwavering commitment to his postdocs and encourages their independence while being available for consultation and feedback.

Quanxi Jia (MPA-CINT) was nominated by postdoctoral researchers Guifu Zou, Yingying Zhang, Mujin Zhuo, and Li Yan (MPA-CINT), who cited him for providing scientific guidance as well as the knowledge and skills to handle situations that cannot be learned by working in a laboratory. According to his nominators, Jia mentors his postdocs with their career goals in mind, ensuring that their research is closely aligned with these goals. Jia encourages his postdocs to publish in the highest impact scientific journals and works with them to garner international conference speaker invitations. He also inspires postdocs to collaborate with colleagues to broaden their background and skills.

James Werner was nominated by postdoctoral researcher Hsin-Chih Yeh (MPA-CINT), who cited him for providing excellent support, leadership, and a positive work environment. According to Yeh, Werner makes it a priority to give his postdocs new experiences and to recognize them for their work. For example, Werner and Yeh were part of a team that developed the NanoCluster Beacon, a technology to detect specific nucleic acid target sequences for diagnostics. When Technology Transfer Division selected NanoCluster Beacon as one of seven Laboratory entries to the 2011 R&D 100 Awards competition, Werner assigned Yeh to lead the award's internal application process. Werner's action recognized Yeh's major contribution to the research.

CHEMISTRY

Advances in rechargeable solid hydrogen fuel storage tanks

Scientists have developed a new single-stage method for recharging the hydrogen storage compound ammonia borane. The breakthrough makes potentially problematic hydrogen a more attractive fuel for vehicles and other transportation modes. In an article in the journal ***Science,*** LANL and University of Alabama researchers working within DOE's Chemical Hydrogen Storage Center of Excellence describe a significant advance in hydrogen storage science.

Hydrogen (H_2) is in many ways an ideal fuel. It possesses a high energy content per unit mass when compared to petroleum, and it can be used to run a fuel cell, which in turn can be used to power a very clean engine. Because H_2 has a low energy content per unit volume versus petroleum (it is very light and bulky), it is challenging to get enough on board a vehicle to power it a reasonable distance.

Work at LANL and elsewhere has focused on chemical hydrides, particularly ammonia borane, for storing hydrogen. The hydrogen storage capacity of ammonia borane approaches 20 percent by weight – sufficient that with appropriate engineering it should permit hydrogen fueled vehicles to go over 300 miles on a single "tank," a bench-mark set by the DOE. Although hydrogen release from ammonia borane has been demonstrated, its chief drawback to use has been the lack of energy-efficient methods to reintroduce hydrogen into the spent fuel to recreate ammonia borane.

The ***Science*** paper describes a simple scheme that regenerates ammonia borane from a hydrogen depleted "spent fuel" form (called polyborazylene) back into usable fuel via reactions taking place in a single container. This "one pot" method represents a significant step towards the practical use of hydrogen in vehicles by potentially reducing the expense and complexity of the recycle stage. Regeneration takes place in a sealed pressure vessel using hydrazine and liquid ammonia at 40 ^{o}C and necessarily takes place off-board a vehicle. The scientists envision vehicles with interchangeable hydrogen storage "tanks" containing ammonia borane that are used, and then sent back to a factory for recharge. Researchers include Andrew Sutton and John Gordon (Inorganic, Isotope and Actinide Chemistry, C-IIAC), Anthony Burrell and Tessui Nakagawa (Materials Chemistry, MPA-MC), Kevin Ott (Applied Energy, SPO-AE), and University of Alabama collaborators (D.A. Dixon, E.B. Garner III, J.P. Robinson, and M. Vasiliu). Reference: "Regeneration of Ammonia Borane Spent Fuel by Direct Reaction with Hydrazine and Liquid Ammonia", ***Science*** *331*, 1426 (2011); doi: 10.1126/science.1199003. The Chemical Hydrogen Storage Center of Excellence was one of three Center efforts funded by DOE. The Center of Excellence was a collaboration between LANL, Pacific Northwest National Laboratory, and academic and industrial partners. The work supports the Laboratory's Energy Security mission area and the Materials for the Future capability.

Figure 1. Artist's conception of the "one pot" regeneration of ammonia borane. Ammonia borane, on the left, releases hydrogen and is recycled back to polyborazylene on the right in a single vessel. Free hydrogen is available for a variety of applications. Design credit: Joshua Smith (Chemistry, C-DO)

COMPUTER, COMPUTATIONAL, AND STATISTICAL SCIENCES

Climate-driven fluctuations in freshwater flux in Greenland over the last 4000 years

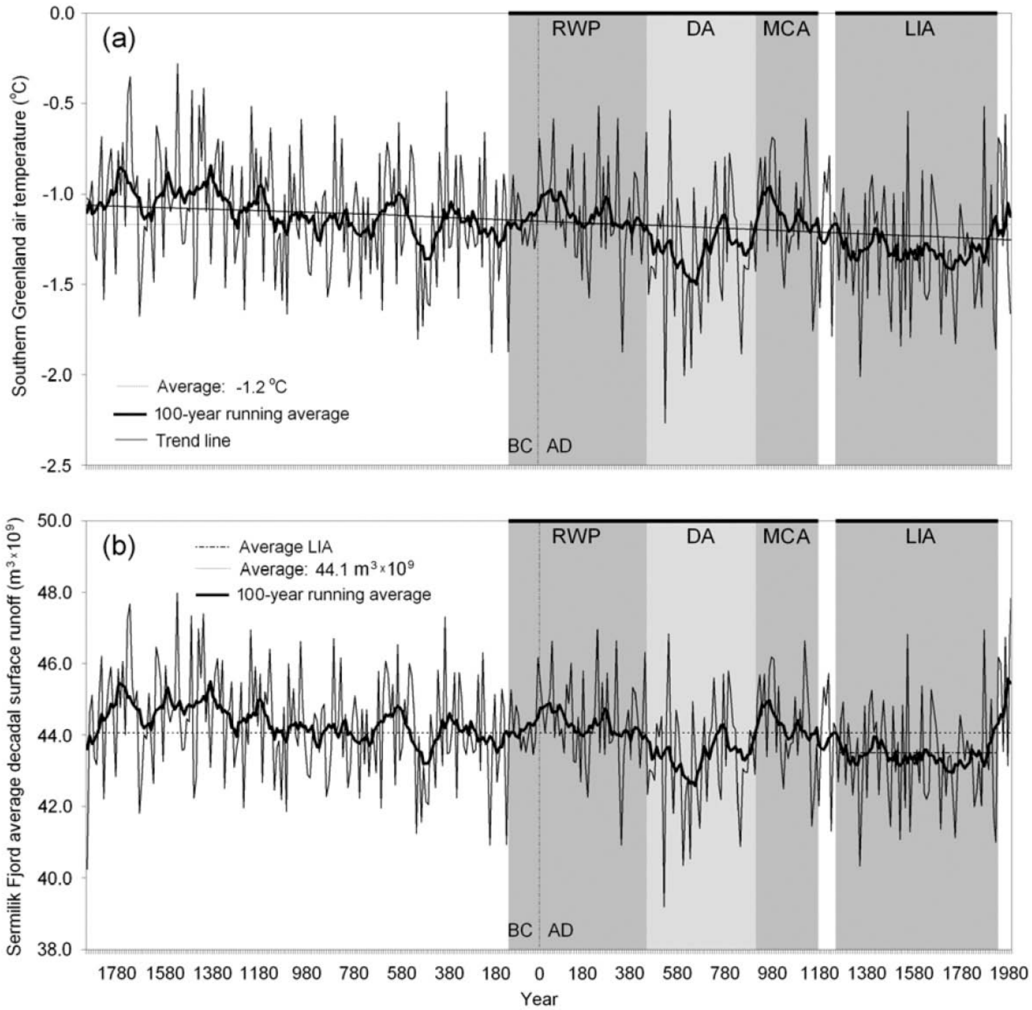
Global-mean and Arctic-mean instrumental temperature records show substantial variability on multidecadal to interannual time scales in addition to the global warming of approximately 0.7°C since the 1850s. The fluctuations modify the Arctic hydrological cycle and cryospheric elements such as the Greenland Ice Sheet, its outlet glaciers, marginal glaciers, and snow cover. These elements are indicators of present and past climate change, including atmospheric temperature and precipitation, and play a significant role in climate feedback mechanisms such as freshwater supply to the oceans. To understand and predict the impact of a likely shift from present climate conditions to a future warmer and wetter Arctic climate, the impact from past short- (annual to multi-decadal) and long-term (century to millennia) climate fluctuations must be assessed.

Sebastian Mernild (Computational Physics and Methods, CCS-2), Petr Chylek (Space and Remote Sensing, ISR-2), and collaborators have examined freshwater flux (surface runoff and ice discharge) variations and trends from the glaciated and snow-covered Sermilik Fjord. It is the largest fjord system in southeast Greenland draining the most extensive and active glacier outlets. This drainage may have a significant impact on freshwater output to the North Atlantic. The scientists' goal was to determine the freshwater flux from Sermilik Fjord to the ocean and the effect of short- and long-term climate fluctuations over the past four millennia. The researchers simulated the freshwater runoff from the Greenland Ice Sheet and the Sermilik Fjord catchment at annual resolution for the period 1900 - 2008 and at decadal resolution for the past four millennia. They used SnowModel, a state-of-the-art spatially distributed meteorological, snowpack, and ice melt modeling system to simulate the temporal and spatial surface runoff variability to the Sermilik Fjord. The simulations included available meteorological station data (1900 - 2008) and Greenland ice core estimated temperature data (1899 BC - 1980 AD).

Based on data and calculated subglacial melting and net precipitation for the fjord area, the scientists deduced the climate-driven fluctuation in simulated freshwater and the freshwater flux in the Sermilik Fjord for the period 1900 - 2008. The researchers estimated that the mean annual freshwater flux was $33.0 \pm 5.7 \times 10^9$ m^3 y^{-1}. During the last century, ice discharge has accounted for 81% of the freshwater flux. The scientists conclude that the Helheim outlet glacier, one of three major outlet glaciers, plays a dominant role as a freshwater source to both Sermilik Fjord and ultimately the Irminger Sea. Although mean atmospheric temperature and precipitation seem to be highly governed by the Atlantic Multidecadal Oscillation, the short term interannual surface runoff variations for Sermilik Fjord have a general trend of a 20-year periodicity possibly very weakly correlated to the North Atlantic Oscillation.

Photo. Helheim outlet glacier. Note helicopter in center of photo for scale of glacier front height. Credit: Sebastian Mernild

Simulated surface runoff over the past 4,000 years has averaged $4.4 \pm 0.2 \times 10^9$ m^3 y^{-1}. A very weak decreasing trend in runoff may be associated with Northern Hemisphere cooling since the Holocene Thermal Maximum. The simulations indicate centennial to sub-millennial scale variations in surface runoff concurrent with the well-known climate episodes such as the "Roman Warm Period" (110 BC -



430 AD), the "Dark Ages Cold Period" (440 - 910 AD), the "Medieval Climate Anomaly" (920 - 1170 AD), and the "Little Ice Age" 1250 - 1920 AD). During the Little Ice Age, the average surface runoff was about $0.7 \times 10^9 \ m^3 \ y^{-1}$ lower than today, while the increase in runoff for the Modern Warming, since the late 1800s, was the second fastest for the last 4,000 years.

Figure 2. (a) Southern Greenland decadal average temperatures estimated based on ice core data for 1899 BC - 1980 AD, and (b) Sermilik Fjord simulated average decadal surface runoff for 1899 BC - 1980 AD. Bold lines on the ordinate depict the Roman Warm Period (RWP), the Dark Ages Cold Period (DA), the Medieval Climate Anomaly (MCA), the Little Ice Age (LIA) and the Modern Warming, since the early 20th century. The average Little Ice Age runoff is illustrated in (b) as an example.

The scientists conclude that fluctuations in climate modify the Arctic hydrological cycle and the freshwater flux to the ocean. The overall pattern of freshwater production and glacier melting appears to be largely governed by the general regional climate development. Marginal areas of the Greenland Ice Sheet respond quickly to climate change. Increased melt-water outflow may potentially influence the strength of Atlantic Meridional Overturning Circulation (AMOC) and deep-water formation. However, the more immediate concern is the influence of warmer ocean waters on the Greenland Ice Sheet because large glacial outflows are grounded below sea level. ***The Holocene*** journal has accepted the paper for publication. Researchers include Mernild, Chylek, and collaborators M.-S. Seidenkrantz (University of Aarhus, Denmark), G.E. Liston (Colorado State University), and B. Hasholt (University of Copenhagen, Denmark). A LANL Director's Postdoctoral Fellowship and the DOE Office of Biological and Environmental Research, Climate and Environmental Sciences Division funded the Los Alamos scientists. The research supports the Laboratory's Energy Security Mission area and Information Science and Technology and Science of Signatures capabilities.

HIGH PERFORMANCE COMPUTING

First foreign electronic connection of the Enterprise Secure Network

The first foreign electronic connection has been completed to the Enterprise Secure Network (ESN). At the request of the United Kingdom (UK) government and under the auspices of the US-UK Mutual Defense Agreement (MDA), UK's Aldermaston Atomic Weapons Establishment and the UK Embassy in Washington, DC have been connected to the ESN. This fulfills a long-standing request of the MDA Working Groups and the NNSA administrator to connect the US and UK electronically. This electronic connection greatly facilitates communications between NNSA laboratories and plants with Aldermaston, allowing for file transfer and email. Aldermaston is the UK's "sister" laboratory to the US weapons laboratories. It is responsible for the production, development, and design of UK weapons.

After operational testing, the UK Gateway now has its first US and UK users. The first electronic classified data between the US and UK has been successfully transferred between countries. The ESN connection provides quick, secure email and file transport access from Aldermaston to NNSA/DOE managers, scientists, and engineers responsible for joint collaborative projects. Mike Boorman (HPC-5) is the Project Manager responsible for leading this effort. The work supports the Laboratory's Nuclear Deterrence mission area and the Information Science and Technology capability.

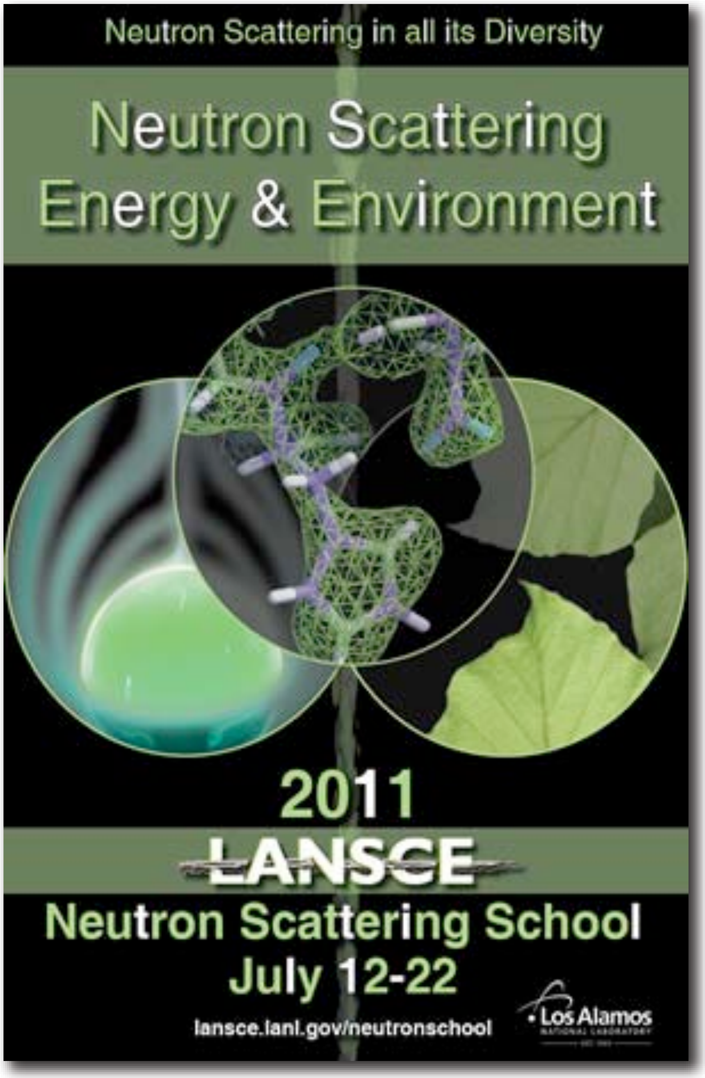
LANSCE

Neutron School will focus on energy and the environment

The Los Alamos Neutron Science Center (LANSCE) will hold its 2011 Neutron School on July 12 - 22 at in Los Alamos. The DOE, National Science Foundation, LANSCE, and New Mexico State University jointly sponsor the school. The annual school focuses on specific science topics to which neutron scattering makes a critical impact. This focus makes it distinct from other national neutron schools.

This year's theme focuses on the study of materials for energy and environment research. Novel approaches to energy production, storage, and distribution, pollution prevention, environmental cleanup and protection, carbon sequestration, and raw materials sources are urgently needed. The development of new functional materials and a better understanding of natural materials and processes will play a central role in this endeavor. Neutron scattering, in all its diversity, will contribute significantly to the arsenal of sophisticated materials characterization techniques for energy and environmental research.

The goal of the neutron school is to introduce a variety of neutron scattering techniques to the students and demonstrate how they complement other analytical methods to elucidate material structure and properties. In addition to introductory lectures on neutron scattering, experts will present contemporary research on materials science aspects of energy and environmental research. Afternoons will be devoted to hands-on neutron scattering experiments (small-angle scattering, reflectometry, powder diffraction, pair distribution function analysis, neutron vibrational spectroscopy, radiography) and data analysis. A variety of materials related to energy and environmental issues will be selected for these exercises.



James Rhyne (Lujan Center, LANSCE-LC) is the School Director, and local organizing committee members include Luke Daemen and Monika Hartl (LANSCE-LC), John Gordon (Inorganic, Isotope and Actinide Chemistry, C-IIAC), and Donald Hickmott (Earth and Environmental Sciences, EES-DO). Laboratory presenters include Kevin Ott (Applied Energy, SPO-AE) – keynote speaker, Greg Kubas (C-IIAC) – banquet speaker, and lecturers David L. Clark (Institutes, INST-OFF), S. Zoe Fisher (Bioenergy and Environmental Science, B-8), Victor Klimov (Physical Chemistry and Applied Spectroscopy, C-PCS), and Andrew Sutton (C-IIAC). Leads for the hands-on experiments include Katharine Page, Sven Vogel, Michel Mocko, Jarek Majewski, Rex Hjelm, and Luke Daemen (LANSCE-LC).

Potential students should apply before April 15: <http://lansce.lanl.gov/neutronschool>http://lansce.lanl.gov/neutronschoo. The school is open to graduate students and postdoctoral researchers only, and the number of participants is limited to 30. They will be selected based on a statement of interest and two letters of recommendation. Travel, hotel, and meals will be covered (details on web site). Technical contacts: *Luke Daemen* or *Monika Hartl*

MATERIALS SCIENCE AND TECHNOLOGY

Temperature dependence of lattice disorder in argon-irradiated magnesia single crystals

Magnesia (MgO) is a promising material for application in advanced nuclear fuel forms. An important criterion for selection of materials suitable for incorporation into nuclear fuels is their tolerance to a combination of irradiation-induced damage (produced primarily by fast neutrons and fission fragments) and elevated temperatures. During normal operating conditions in a nuclear reactor, the surface temperature of a fuel pellet is 800 – 1000 ^{o}C. Radiation damage evolution in MgO at these elevated temperature range has not been studied extensively.

To better understand dynamic annealing processes in ion-irradiated MgO single crystals of three low-index crystallographic orientations, Structure/Property Relations (MST-8) researchers Igor Usov, James Valdez, and Kurt Sickafus investigated argon (Ar) ion radiation damage evolution at LANL's Ion Beam Materials Laboratory. The researchers used Rutherford backscattering spectroscopy combined with ion channeling to analyze lattice damage. Damage recovery with increasing radiation temperature proceeded via two characteristic stages separated by 200 °C. The scientists observed strong radiation damage anisotropy at temperatures below 200 °C, with (1 1 0) MgO being the most radiation damage tolerant. The researchers attributed first stage damage recovery to radiation and/or ionization enhanced diffusion processes induced by the Ar ion bombardment. Above 200 °C damage recovery was isotropic, and almost complete recovery was reached at 1100 °C for all crystallographic orientations of MgO. The scientists conclude that thermally-activated point defect migration processes begin to contribute to the recovery of lattice damage at the elevated temperatures. Lattice recovery in MgO induced by high temperature irradiation is more efficient than recovery upon post-irradiation annealing. Reference: "Temperature Dependence of Lattice Disorder in Ar-irradiated (100), (110) and (111) MgO Single Crystals," ***Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms** 269*, 288 (2011); doi:10.1016/j.nimb.2010.12.024. DOE's Office of Basic Energy Sciences - Division of Materials Sciences and Engineering, DOE's High Temperature Superconductivity Program, and DOE's Advanced Fuel Cycle Campaign and Fuel Cycle R&D Program funded the research. The work supports the Laboratory's Energy Security mission area and the Materials for the Future capability. Technical contact: *Igor Usov*

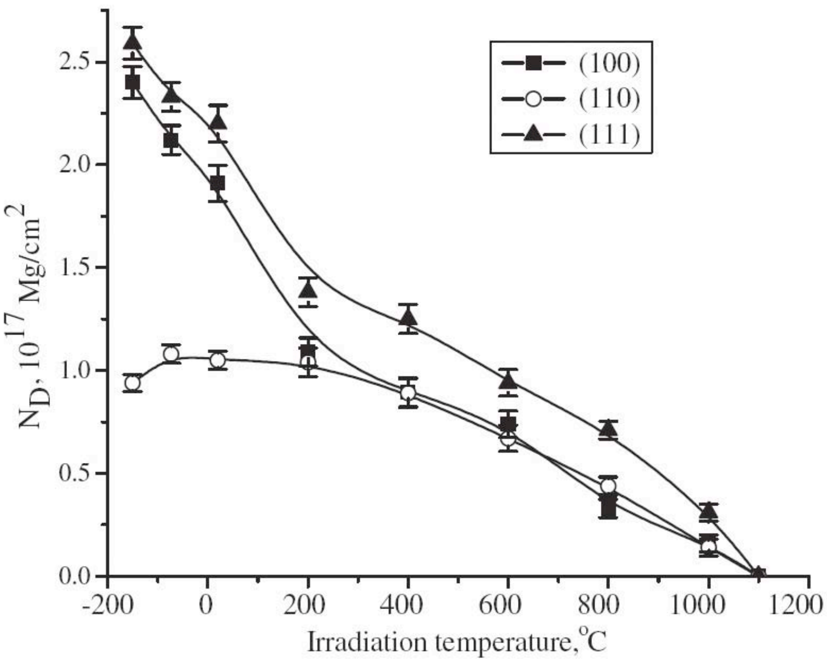


Figure 3. Damage parameter, N_D, versus irradiation temperature, T_{irr}, for MgO single crystal of three low-index orientations [(1 0 0), (1 1 0) and (1 1 1)] irradiated with 100 keV Ar ions to a fluence of 1 x 10^{15} Ar/cm^2. Error bars indicate statistical uncertainty.

PHYSICS

First neutron image collected at the National Ignition Facility (NIF)

On February 17, the LANL and Livermore National Laboratory (LLNL) neutron imaging team obtained its first neutron pinhole image at NIF. The target was a deuterium/tritium-filled directly-driven glass micro-balloon with a measured yield of 2 x 10^{14} neutrons. In a "direct-drive" experiment, all the laser beams impinge on the target. The pinhole assembly was aligned with remarkable precision, pointing within 40 micrometers of the target location and parallel to the line of site within 200 microradians. The measurement completed the operational qualification of this diagnostic.

The NIF neutron imaging system is designed to produce images from implosions of deuterium- and tritium-filled capsules. The Inertial Confinement Fusion project's ultimate goal is ignition of thermonuclear fuel in a laboratory setting. The neutron imaging system will play an essential role in understanding the performance of these implosions by providing key diagnostic information on the shape and compression of the implosion. The imaging system will take two pictures using two separate camera systems, one of direct neutrons from fusion reactions and one of scattered neutrons from the material surrounding the burning nuclear fuel.

The neutron imaging system forms magnified "pinhole" images of the neutrons generated in capsule implosions. Because neutrons are only generated in the regions of the fuel with sufficient temperature and pressure for fusion, these images provide a measure of the size and shape of the burning deuterium-tritium fuel. Some fusion neutrons are scattered within the material surrounding the burning core, losing energy in the scattering process. Due to the long flight path between the target and the neutron imaging detector, the primary 14 MeV fusion neutrons arrive at the detector approximately 50 ns before the down-scattered 10 - 12 MeV neutrons. Two fast-gated camera systems measure the distribution of the primary and the down-scattered neutron images. The data from the down-scattered neutrons provide a measure of the distribution of the "cold" fuel surrounding the burning core.

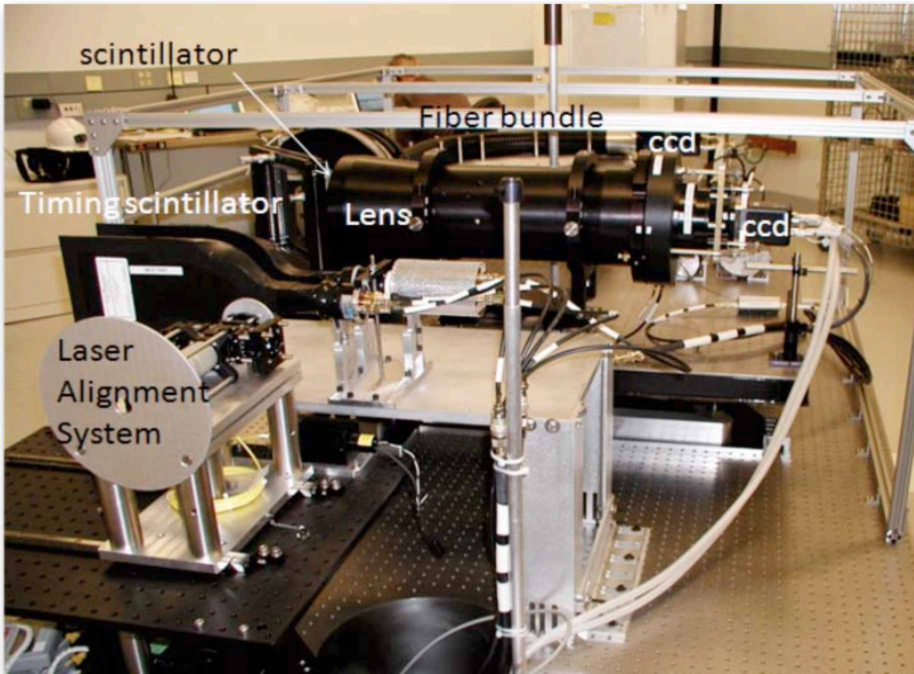


Photo. Neutron image collection system as installed in the neutron imaging annex at NIF. The neutrons interact with the scintillating fiber array, generating light that is directed towards to image collection systems. Light exiting the front of the scintillator is collected with an optical lens and transported to a micro-channel plate, for fast gating, and on to a CCD (charge-coupled device) camera. The light exiting the back of the scintillating fiber array is collected with a fiber taper and transported to a micro-channel plate for fast gating and through a fiber bundle to a second CCD camera.

The principles behind this imaging technique are similar to the principles for the standard pinhole cameras that are common in photography. The major difference lies in the penetrating ability of 10 - 14 MeV neutrons. The "pinholes" used to form neutron images are small tapered apertures machined in approximately 20 cm of gold or tungsten. The thick gold or tungsten is required to remove neutrons, and the tapered aperture is designed to provide a "sharp" edge for the neutron aperture. The triangular pinholes were machined in the surfaces of the gold layers. For a magnification factor of 85, the pinhole is located close to the source, within the NIF target chamber at 32.5 cm from the source, and the image was collected in the neutron imaging annex, which is 28 meters from the center of the target chamber.

Figure 4 shows the first image data of a directly driven glass micro-balloon. Each pinhole in the array points at a slightly different location at the target chamber center. Scientists used the neutron intensity through each pinhole to estimate the pointing of the pinhole array. Preliminary analysis revealed that the pinhole within the black box was pointed closest to the source, and the center of the black box was centered on the pinhole field of view. Researchers extracted this region of the image for further analysis to reconstruct the source distribution.

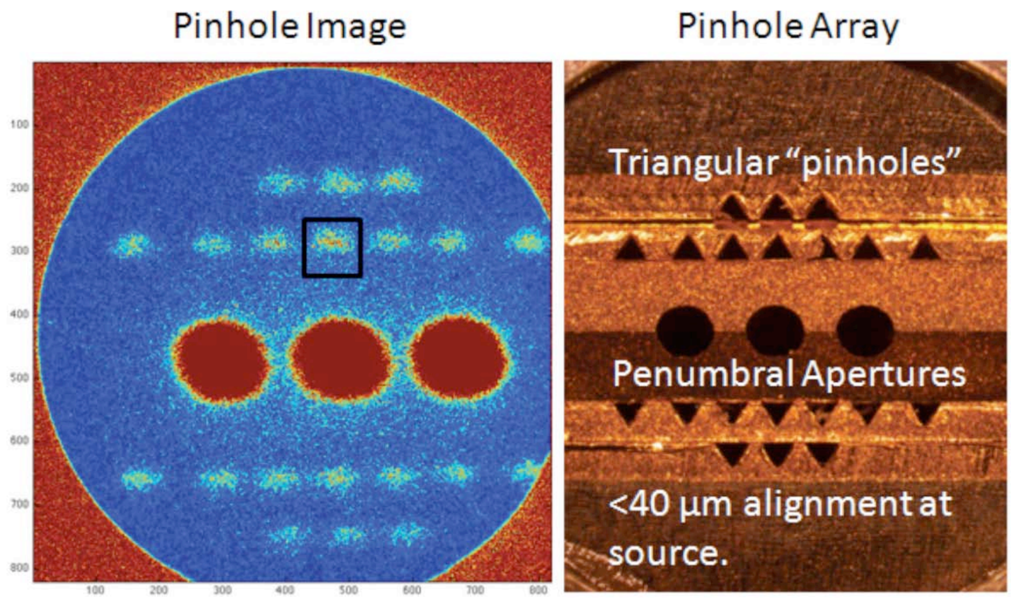


Figure 4. (*Left*): first neutron image from the micro-balloon target. (*Right*): microscope view of the pinhole array. The triangular "pinholes" form the pinhole images, while the penumbral apertures also provide information on the source distribution.

The results of this reconstruction show an oblate source, as expected in polar driven capsules. Because NIF is configured for hohlraum driven (indirect drive) implosions, the lasers are directed along the polar axes of the target. In this drive configuration the compressed core is expected to be prolate, because of the increased drive at the poles of the capsule. This result agrees with expectations of the capsule implosion and with the X-ray images of the same experiment. The X-ray images show different source distribution than the neutron images because the physics processes generating the X-rays differ from the processes generating the neutrons.

Physics, Materials Science and Technology, and Weapons Systems Engineering divisions performed the work in collaboration with a team from Lawrence Livermore National Laboratory. The LANL work was funded by the NNSA Inertial Confinement Fusion program (Steve Batha, program manager for Campaign 10) for the National Ignition Campaign. The research supports the Laboratory's Nuclear Deterrence and Energy Security mission areas and the Science of Signatures capability. Technical contact: *Frank Merrill*