LA-UR-16-21843
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Title: MST e-News March 2016

Author(s): Kippen, Karen Elizabeth

Intended for: Newsletter
Web

Issued: 2016-03-17

MST e-News

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INSIDE

Los Alamos NATIONAL LABORATORY EST. 1943

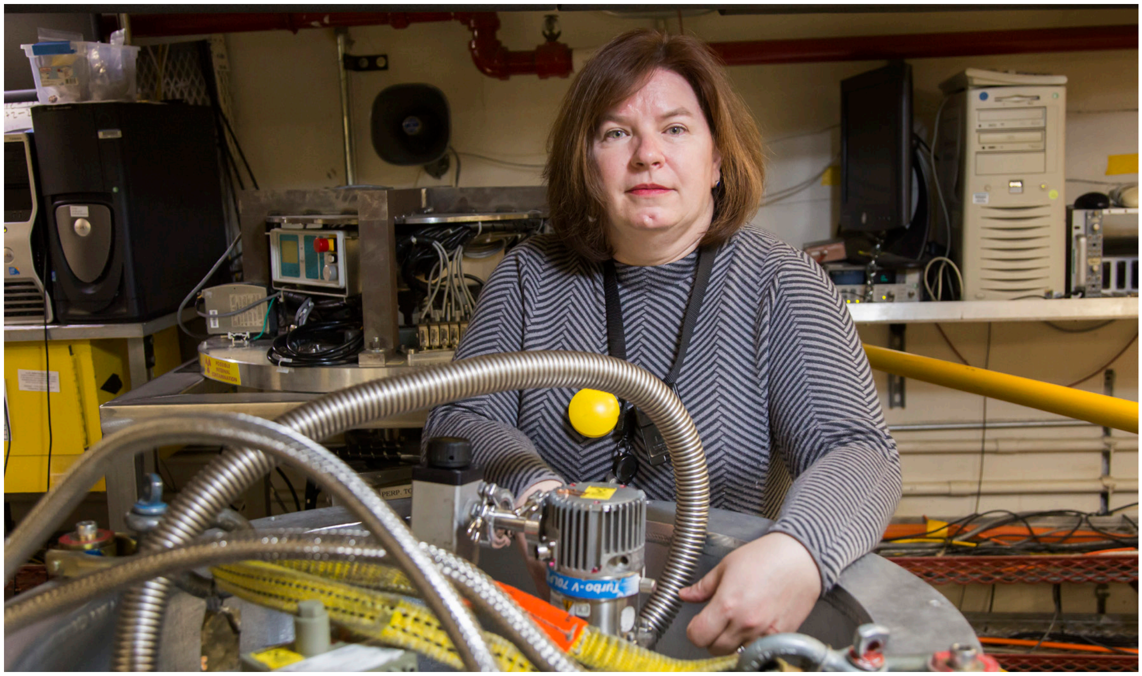

Photo by Richard Robinson, NIE-CS

Alice Smith recently began a new experiment using the Lujan Center's HIPPO (high-pressure/preferred orientation) diffractometer to study delta phase ^{242}Pu-Ga alloys under high-pressure and high-temperature conditions. Franz Freibert (MST-16) is the principal investigator, Smith is co-PI, and Jianzhong Zhang (Materials Science in Radiation and Dynamics Extremes, MST-8) is instrument scientist.

"It's hard not to be excited by science, and Los Alamos is a great place to do science."

Alice Smith

Detecting plutonium's secrets using neutrons and x-ray diffraction

By Diana Del Mauro, ADEPS Communications

By age 8, Alice Smith had discovered the joy of playing with microscopes and other instruments in her father's university hospital genetics laboratory. "I didn't make him very happy because I was messing up everything, but it paid off in the end," she said.

Given strong support from her physician father and electrical engineer mother, Smith said her path was set in eighth grade when she was accepted into an elite Romanian high school dedicated to math and science. At Louisiana State University she earned her PhD in physics and developed a passion for running synchrotron experiments and working with neutrons.

Ten years ago, as a postdoctoral researcher, she was drawn to the Lujan Neutron Scattering Center at Los Alamos to learn new experimental techniques using neutrons. Now a staff scientist in Nuclear Materials Science (MST-16), Smith performs studies of actinides, a series of radioactive metallic elements, for the Laboratory's fundamental science and nuclear weapons missions. She is the group's instrument

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From Deniece's desk . . .

Greetings. I am so honored and excited to be the Deputy Division Leader of MST. I started my LANL career in MST almost 30 years ago and as stated in the LANL purpose, I have truly been given the opportunity to do things I would have never imagined. I want to share with you some of the goals I hope to accomplish as DDL to keep MST Division productive, innovative, and essential. I have divided these goals into two broad categories: capabilities and operations.

> *"I want to share with you some of the goals I hope to accomplish as DDL to keep MST Division productive, innovative, and essential."*

MST needs to have vibrant, sustainable capabilities. Capabilities can be described in three areas: personnel, equipment, and infrastructure.

Personnel - I believe the true strength of our capabilities resides in our people. The people are the innovative, problem solving life blood of our science program. To keep the personnel part of our capability strong I want to focus on teaming, cross-training, mentoring, and true succession planning.

Equipment – The best people cannot do excellent science without equipment and materials. We need to develop and execute an equipment investment plan where we replace our aging and outdated equipment and invest in new, modern equipment. All equipment needs to be well maintained and accessible when needed. We can also take better advantage of equipment owned by other organizations across LANL as well as elsewhere in the United States.

Infrastructure – Many of our facilities are old and in need of attention (example Sigma). Some of our facilities are new and receiving attention (RLUOB). We need to work with NNSA to ensure all of our facilities get the attention they need.

MST needs to work/operate efficiently. The topic of increased work efficiency is ripe with opportunities for improvement both large and small. I have picked two areas to focus on first: Eliminate unneeded "requirements" and instill a shared fate mentality across work teams.

Eliminate unneeded "requirements" – We at LANL are famous for solving a problem by adding new rules, more paperwork, and additional controls until we can no longer work effectively. We must explore ways to streamline work authorization by implementing qualified worker programs and general training for operations that include common hazards. Work control documents should be simple and concise and designed for the worker not the auditor.

Shared fate – A simple definition for shared fate is an "all-for-one, one-for-all" type mentality, or put another way "we all succeed or fail together." To succeed, we need teams comprised of scientists, engineers, technicians, technologists, safety SMEs, security SMEs, facility SMEs, financial analysts, etc. to work together towards common goals. The result is a better-informed, more supportive, and more responsible workforce where everyone's goal is to complete the given job on-time, within budget, safely, and securely. To become a shared fate organization, we need to understand each other's needs and drivers and ensure that everyone is adequately informed and funded to succeed.

These are my thoughts. I am interested in your thoughts and ideas about MST directions and goals.

MST Deputy Division Leader Deniece Korzekwa

Smith cont.

scientist for x-ray diffraction and has mastered other techniques.

"Science remains my main focus," she said. "Changing the type of materials makes it more interesting; the same for changing techniques."

In 2012 the National Nuclear Security Administration gave Smith a Certificate of Appreciation for her role in making new plutonium pits for W88 warheads. Using x-ray diffraction, she and technician Fritz Sandoval (MST-16) tested the structural character of each pit, a critical component for initiating a weapon's nuclear chain reaction. Since 2007, the Lab has manufactured new pits to replace pits destroyed as part of the surveillance process of the U.S. Stockpile Stewardship Program.

Smith is driven to help complete the picture of plutonium phase stability and phase transformations, seeking to understand the mechanisms behind plutonium's erratic behavior so eventually scientists can control plutonium's behavior. At the Lujan Center, the only United States neutron scattering center that can accept highly radioactive materials samples, Smith leads the first long-term study using neutrons to observe plutonium-239's natural aging process.

"Quite a few people said the measurements wouldn't happen because I wouldn't be able to get any signal," she said. Smith said she doesn't like the word "impossible," and forged ahead, proving them wrong.

Undaunted by the numerous requirements of this complex, ongoing work, Smith said, "You tend to forget about the hardships when you accomplish a task. The next time, you rely on that experience and it doesn't seem so impossible or hard anymore."

She also characterized the plutonium sample for a notable experiment in which Los Alamos and Japanese researchers detected the faint signal of plutonium-239's nuclear magnetic resonance signature, a Rosetta stone for deciphering the atomic-scale electronic properties of the most complex element in the periodic table.

Her postdoctoral mentor, Luke Daemen, now at Oak Ridge National Laboratory, described Smith as meticulous and determined. "What stands out is Alice's deep concern for science and an extraordinary steadfastness in pursuing and resolving scientific questions despite difficulty or adversity," he said.

Smith said working at a large national lab gives her access to numerous experimental techniques and researchers from different fields. "It's hard not to be excited by science, and Los Alamos," she said, is "a great place to do science. I'm sure in 10 to 15 years we will be able to access measurements that are thought to be impossible today."

Los Alamos has proposed an experimental facility called Matter-Radiation Interactions in Extremes (MaRIE) where Smith could study materials in extreme conditions, such as temperature and pressure, and observe changes in real time. "Time-resolved experiments are a big deal because many times the changes can occur on very short time scales, and we can't see those changes with the instruments we have today," she said.

Alice Smith's favorite experiment

What: Measuring the local structure of ^{239}Pu-Ga alloys by neutron pair distribution function (nPDF)

Why: Long-term phase stability in binary Pu alloys affects mechanical properties, microstructure, corrosion behavior, and most important, structural integrity, and is critical for a variety of applications, from metallurgy to nuclear energy and weapons research. For a better understanding of the mechanism behind the phase stability, we need a detailed picture of the short- to medium-range plutonium lattice distortions at the atomic level, and how this is influenced by alloying elements.

When: 2012-2013

Where: Lujan Neutron Scattering Center, Los Alamos National Laboratory

Who: Alice Smith, Scott Richmond, Tarik Saleh, Michael Ramos, Fred Hampel, Dan Schwartz (MST-16); Katharine Page, Joan Siewenie (Spallation Neutron Source, Oak Ridge National Laboratory)

How: The nPDF approach enables science on different length scales previously out of reach for plutonium and other actinides. Along with an overview of the average structure, it provides valuable and unique information on the short- and especially medium-range order in materials—a region not covered by extended x-ray absorption fine structure, Bragg diffraction, or small-angle scattering.

The "a-ha" moment: Plutonium-239 was previously thought by many to be unsuitable for neutron scattering measurements due to its large absorption cross section. Redesigned sample containers and a more appropriate sample geometry allowed us to acquire the signal needed to study our samples by both diffraction and the more challenging nPDF.

Carlos Tomé named Laboratory Fellow

Carlos Tomé (Materials Science in Radiation and Dynamics Extremes, MST-8) has been selected as a 2015 Los Alamos National Laboratory Fellow.

"The Laboratory Fellows Organization recognizes researchers for innovative scientific and technical advances in their respective fields," said Laboratory Director Charlie McMillan.

Piotr Zelenay (Materials Synthesis and Integrated Devices, MPA-11), Michael Bernardin (Weapons Physics, ADX), and Avadh Saxena (Physics of Condensed Matter and Complex Systems, T-4) were also named Fellows.

"The exciting work by Michael, Avadh, Carlos, and Piotr exemplifies the essential science we do at Los Alamos that helps enable continuing success in our national security mission," McMillan said. "I commend each of them for this prestigious achievement."

Tomé, who joined the Laboratory in 1996, is known as one of the world's leading experts in the micromechanics of polycrystalline metals and possesses an outstanding publication record with more than 11,000 citations having far-reaching and influential impact. He has co-authored a now-classic reference book in the field of materials modeling, *Texture and Anisotropy*, a book with more than 1,400 citations. His influence outside of Los Alamos is extensive. For example, a symposium was held in his honor in 2011 at the Minerals, Metals, and Materials Society (TMS) annual meeting, which included more than 90 presentations by researchers from around the world. The TMS's Structural Materials Division awarded him the 2013 Distinguished Scientist/Engineer Award. The theories, models, and numerical codes that he has developed with colleagues are widely used in academia, national laboratories, and industry.

The selection committee ranked this year's nominations on the basis of the following:

- sustained, high-level achievements in programs of importance to the Laboratory;
- a fundamental or important discovery that has led to widespread use;
- having become a recognized authority in the field, including outside recognition and an outstanding record of publications.

Established in 1981, the Fellows organization comprises technical staff members appointed by the Laboratory Director in recognition of their sustained outstanding contributions and exceptional promise for continued professional achievement. Limited to 2 percent of the Laboratory's technical staff, Fellows advise management on important issues, promote scientific achievement, and organize symposia and public lectures. The organization administers the annual Fellows Prize for Outstanding Research in Science or Engineering and the Fellows Prize for Outstanding Leadership in Science or Engineering.

Origins of radiation tolerance in complex materials

Knowing what makes some complex materials radiation tolerant is important for improving nuclear fuels and nuclear waste storage. A report in the journal *Nature Communications* provides new insight into the matter, generalizing the previous understanding and providing a new path for developing radiation-tolerant materials for use in extreme environments. The research aims to understand at a fundamental level: 1) how materials respond to being irradiated, and 2) how that response depends on fundamental properties of the material, such as its crystal structure and crystal chemistry. The researchers examined oxide ceramics that have potential application for storing nuclear waste and the development of advanced nuclear fuels.

The investigators discovered that fundamental differences in the structure of the material play a key role in how those materials respond to irradiation.

The relative ease in swapping cations is key to radiation tolerance. Using a combination of experimental characterization and a variety of simulation techniques, the Los Alamos researchers determined that different types of complex oxides have a fundamentally different response to irradiation. Decades of work on one class of complex oxides, pyrochlore ($A_2B_2O_7$), have revealed that there are correlations between the ability of the cations (A and B) to swap position and the radiation tolerance of the material. Pyrochlores in which A and B can easily be swapped (such as when A=Er and B=Zr) are radiation tolerant. In contrast, for pyrochlores in which this swapping is difficult (A=Er and B=Ti), the material quickly amorphizes under irradiation. This transformation from a crystalline to an amorphous structure is inherently bad for performance because it is accompanied by changes in volume and the ability of other species to leach from the material.

However, different oxides produced different results. The researchers examined another class of complex oxides, spinels (AB_2O_4), to determine if the same relationship holds. They irradiated three different chemistries of spinels and examined how the spinels responded to the irradiation damage.

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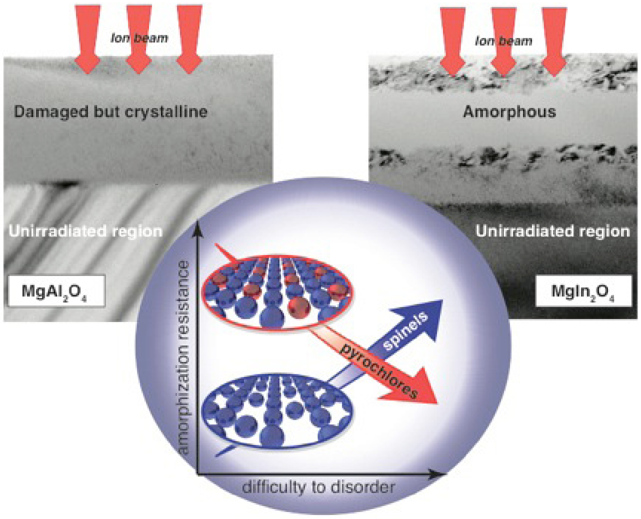

Schematic highlights the relationship between the energetics of disordering and amorphization resistance as a function of the cation structure of the derivative compound, spinel, or pyrochlore. In spinels that have cation vacancies relative to the basic rocksalt structure, amorphization resistance is proportional to the difficulty to disorder the compound. The kinetics of reordering, facilitated by the cation vacancies, is faster as the disordered phase becomes less favorable. These kinetics are absent in fluorite-derivative compound that have the same cation density as the basic fluorite structure. Energy builds faster in compounds that have higher energies to disorder. These compounds are thus less resistant to amorphization.

Origins cont.

The team found the opposite behavior from what was observed in pyrochlores: if the A and B cations are hard to swap in spinels, the material is more, not less, radiation tolerant. The investigators used atomistic simulation methods to examine these results. They attribute this difference to the fundamental manner in which the A and B atoms are arranged. There are holes in the cation structure in spinels that facilitate rearrangement back to the ordered structure. These holes do not exist in pyrochlore. Once the cations swap in pyrochlore, they are stuck there. Due to the holes, spinels can rearrange easily to recover the original structure. Thus, the fundamental difference is related to the holes—cation structural vacancies—that exist in one material but not the other.

The new insight from combined experimental and modeling efforts generalizes the understanding that had been developed from the study of pyrochlores and provides new opportunities for identifying radiation-tolerant oxides for nuclear applications.

Reference: “Opposite Correlations between Cation Disordering and Amorphization Resistance in Spinels versus Pyrochlores,” *Nature Communications* **6**, 8750 (2015). Authors: Blas Uberuaga, Ming Tang, James Valdez, and Yongqiang Wang (Materials Science in Radiation and Dynamics Extremes, MST-8); and collaborators with Thermo-Calc Software Inc., Loughborough University, and the University of Tennessee. The DOE Office of Science (Basic Energy Sciences, Materials Sciences and Engineering Division) funded this work, which supports the Laboratory’s Energy Security mission area and Materials for the Future science pillar. Researchers performed ion irradiations at the Ion Beam Materials Laboratory at Los Alamos, a DOE user resource supported by the DOE Office of Basic Energy Sciences and Office of Nuclear Energy, Laboratory Directed Research and Development, and University of California lab-fee research.

Technical contact: Blas Uberuaga

3D printing on the nanoscale to help MST-7 researchers develop high-performance materials of the future

Science Campaigns invest in new technology

The Engineered Materials Group (MST-7) is using 3D printing on the nanoscale to help invent novel materials with functionalized and engineered properties. With unprecedented speed and control, researchers have made foams, physics package holders, and other structures (see figures) using the group’s new 3D printer. Within a few hours, they can write one or many copies of an object. Unlike typical 3D printing technologies, this model from Germany can produce materials with submicrometer resolutions, which Los Alamos researchers need to address important questions in microfluidics, life sciences and biomimetics, foams, photonic crystals, and metamaterials.

Soon, researchers will print foam structures with regular void/ligament geometries, which can be engineered to have varying properties, and create templates for depositing metal or other materials, or optical waveguides. They will explore the possibility of making tailorable photoresists.

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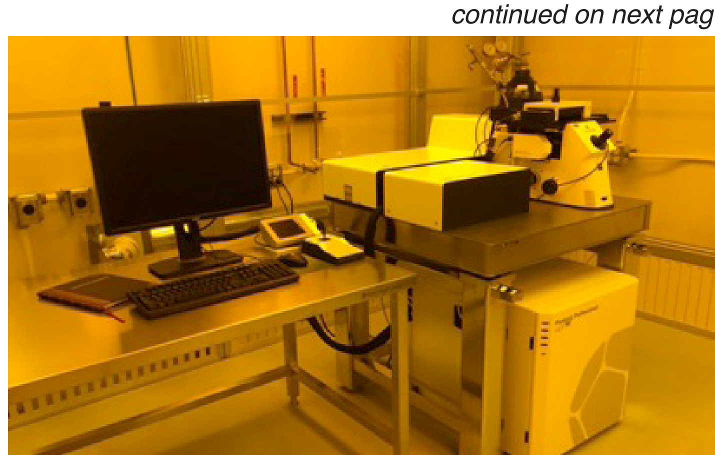
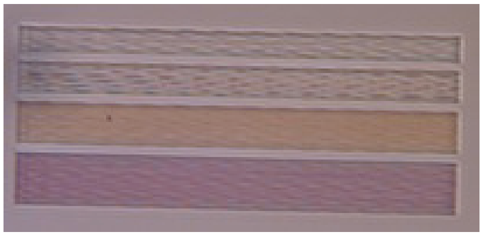


The Nanoscribe Photonic Professional GT 3D printer in a yellow-light illuminated laboratory at Los Alamos.



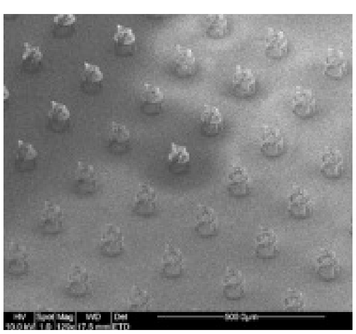
Transmission visible light microscope image of a grating.

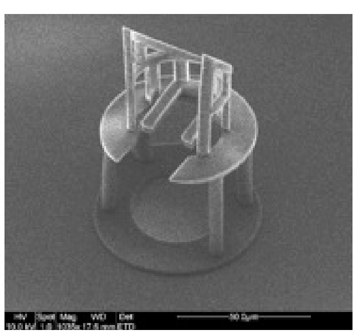
3D printing cont.

The production of meso- and nano-scale materials with engineered (non-stochastic) structures is critical to a variety of science questions of interest to Los Alamos National Laboratory. Ranging from the controlled porosity of a foam for use in weapons programs and campaigns, to basic science such as nanophotonics, researchers are expected to create materials with highly tailored and controllable microstructures. They create materials with engineered structures, three-dimensional functionally graded materials, and materials that integrate multiple constituents—all while individualizing the materials for each experiment in order to probe specific questions. High-performance materials of the future are derived from understanding the interplay of experimental requirements, characterizing the materials to assure the requirements are met, and developing new models of how both materials structure and properties affect performance.

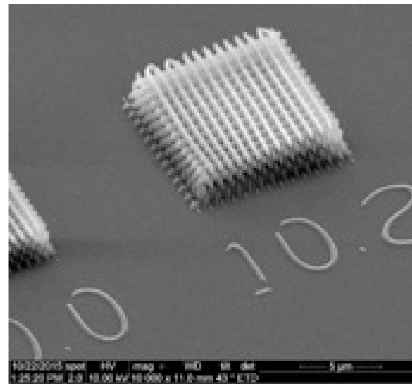
The following MST-7 researchers specified the instrument, oversaw installation, and attended user training: Ross Muenchausen, Dominic Peterson, Brian M. Patterson, Matthew Herman, Joseph Torres, Nik Cordes, and Tana Cardenas. The Nanoscribe Photonic Professional GT laser lithography system uses a near-infrared laser that can write structures at rates of up to 10 mm/s. Resolutions down to less than 200 nm, and write areas as large as 100 mm x 100 mmx2-3 mm tall are possible. The laser prints directly into a highly viscus resin, requiring no support structure (unlike traditional 3D printing technologies). The Lab's Science Campaigns (Acting Program Director Kimberly Scott) purchased the printer, which supports the Lab's Nuclear Deterrence mission area and Materials for the Future science pillar.

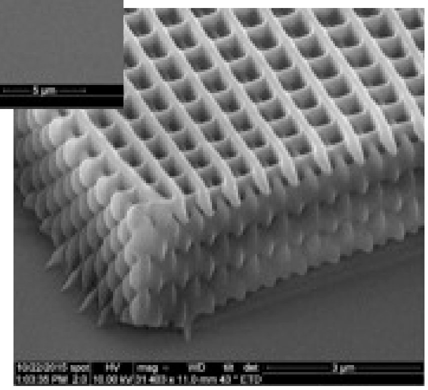
Technical contact: Brian M. Patterson





Electron microscope images of a Los Alamos-designed, greatly scaled down, mirror physics package holder for the Cepheus campaign at the National Ignition Facility. Left shows an array of holders that can be rapidly printed with various geometries. Right image shows the close up image of one structure.





A 3D-printed "wood-pile" structure. The lack of support structure during printing means that no residual polymer is left behind. Open porosity, however, is required to remove any remaining liquid resin.

Celebrating service

Congratulations to the following MST Division employees celebrating service anniversaries recently:

Lydia Apodaca, MST-6..30 years
Blas Uberuaga, MST-8..15 years
Michael Blair, MST-7 ....10 years

MSTe NEWS
Materials Science and Technology

Published by the Experimental Physical Sciences Directorate.

To submit news items or for more information, contact Karen Kippen, ADEPS Communications, at 505-606-1822, or kkippen@lanl.gov.

For past issues, see www.lanl.gov/org/padste/adeps/mst-e-news.php.

Los Alamos NATIONAL LABORATORY EST.1943

Hydrotest component fabrication key to Lab's weapons deliverables

Metallurgy (MST-6) continues to be vital to the Laboratory weapons mission by fabricating experimental hardware for the Los Alamos National Laboratory Hydrotest Program. The Hydrotest Program is an essential element of the Laboratory's stockpile stewardship mission. Over the past several months, the MST-6 Forming/Machining Team and the MST-6 Welding Team have played a key role in the manufacture of this experimental hardware. David Alexander, MST-6 Forming/Machining Team leader, has worked with scientists Kester Clarke and Dan Coughlin as well as research technologist Jeff Scott to form and heat treat numerous components for the Hydrotest Program. The forming and heat treating equipment is shown below.

Left: MST-6 500-ton hydraulic press used to form components for the Lab's Hydrotest Program. Right: MST-6 heat treatment furnace used to heat treat components for the Lab's Hydrotest Program.

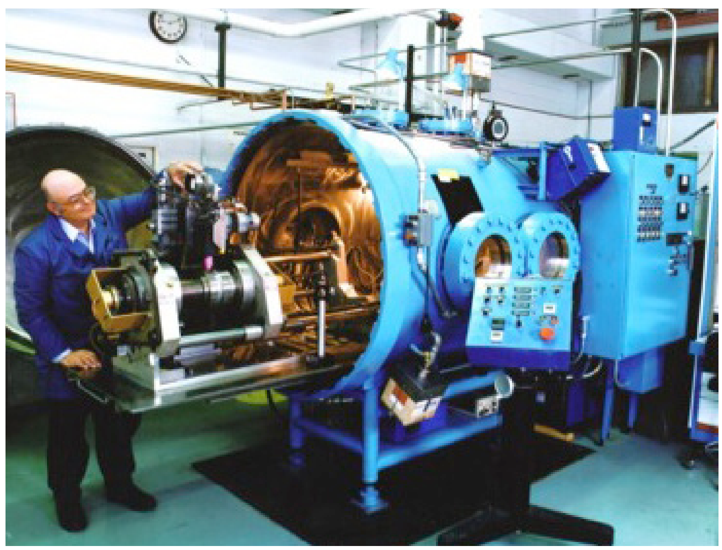
In addition to forming and heat treating components, MST-6 also supports the Hydrotest Program with component assembly, welding, and joining activities. Dan Javernick, the MST-6 Welding and Joining Team leader, works with scientists and engineers on his team to produce high-quality and reproducible welds and brazes for the weapons program. Javernick performs all of the brazing activities with MST-6 research technicians Jesse Martinez and Matt Strandy. A photograph of the brazing furnace is shown below.

Brazing equipment used to support hydrotest component fabrication in MST-6.

MST-6 welding and joining engineer Matt Dvornak works with Martinez and Strandy for assembly and electron beam welding activities. Paul Burgardt, American Welding Society Fellow and Los Alamos National Laboratory (MST-6) associate, works closely with these MST-6 personnel to ensure quality assemblies and welds are made for the Hydrotest Program. A photograph of the electron beam welding equipment is shown below.

MST-6 electron beam welding equipment used to support the hydrotest welding.

Finally, MST-6 scientist Carl Cross, an American Welding Society Fellow, works with both Martinez and Burgardt on semi-automatic gas metal arc welding of certain hydro components. The photo below shows Burgardt and the gas metal arc welding equipment.



Semi-automatic gas metal arc welding equipment used by MST-6 to manufacture certain hydrotest components. Lab associate Paul Burgardt is shown in the photograph.

For more information concerning the forming, heat treating, assembly, and welding of hydrotest components, please contact MST-6 Group Leader Dane Spearing or MST-6 Deputy Group Leader Patrick Hochanadel.

HeadsUP!

ADEPS Environmental Action Plan for FY16

ADEPS remains committed to managing its environmental impacts with forethought and action. Our 2016 Environmental Action Plan was developed from an overarching review of the potential impacts of our work activities and identifies certain, concrete steps we can take to decrease the potential for, and severity of, any environmental damage from our work.

We remain focused on three areas: *Clean the Past, Control the Present*, and *Create a Sustainable Future*. These objectives parallel Los Alamos National Laboratory institutional objectives, with the specific targets fine-tuned to fit our directorate.

Clean the Past: Reduce environmental risks from historical operations, legacy and excess materials, and other conditions associated with activities no longer a part of current operations.

Target 1: Continue salvaging and recycling surplus equipment, materials, etc.

Action 1: Reduce, salvage, and recycle
Action 2: Transportainer assessment, clean-out, removal
Action 3: Combined effort: MPA/MST clean-up of rad-contaminated vacuum pumps and other legacy items from 03-34
Action 4: Transfer hazardous chemicals from LANSCE to ORNL-SNS and dispose of the rest of the hazardous chemicals from 53-015.

Target 2: Identify and execute ADEPS Footprint Reduction Project

Action 1: Relocate occupants, supplies, and equipment from 53-044, 53-045, 53-046, and 53-047 such that these buildings can be readied for D&D via the LFO-FOD.

Control the Present: Control and reduce environmental risks from current, ongoing operations, missions, and work scope.

Target 1: Annual: One environmental MOV per manager per quarter

Target 2: Annual: Communicate EAP and EMS information to directorate staff

Action 1: Ample use of posters, division newsletter articles, group meetings
Action 2: Integrate ADEPS EMS EAP message with ADEPS WSST Team
Action 3: Host a "zero waste" meeting or event

Target 3: Annual: Maintain control of chemicals

Action 1: Annual chemical inventory with 95% goal for each ADEPS division
Action 2: Utilize LANL chemical re-use resources (ChemDB & Chemicals eStockroom)

Target 4: Submit projects or work improvement activities for P2

Create a Sustainable Future: Ensure mission is entwined with effective environmental stewardship

Target 1: Sponsor or participate on building a "Green Team"

Action 1: Participate on the 03-1415 Green Team

Target 2: Incorporate MaRIE planning to include future potential environmental hazards and mitigations on our 2.10's and 2.4

Additionally:
Each of us can contribute in small, but important ways, such as turning off lights in areas when not in use, calling attention to a leaking faucet or toilet so it can be fixed, turning off computer peripherals when not in use, and being attentive to purchases to support "green" procurements wherever possible. Other actions to consider are:

- Using the blue and green recycling bins.
- Sharing chemicals, minimizing chemical inventories, purchasing safer alternatives, recycling and disposing properly.
- Salvaging all unnecessary or unused (and not needed) equipment.
- Nominating a deserving colleague for a P2 Award!!

Please remember to let us know of any environmental actions so we can tally them in our end-of-year report. You can send information to any of the ADEPS Environmental Action Plan contacts:

ADEPS – John Gustafson, johngus@lanl.gov
MPA Division – Jeff Willis, jwillis@lanl.gov
MST Division – Dianne Wilburn, dianne@lanl.gov
P Division – Steve Glick, sglick@lanl.gov

The ADEPS plan in greater detail can be found at the LANL EMS web page at int.lanl.gov/environment/ems/index.shtml; then click on Tools - "EMS Action Plans."