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HEADS UP!
NEW WEBSITE FOR ADEPS WSST

Singh to chair session at American Conference on Neutron Scattering

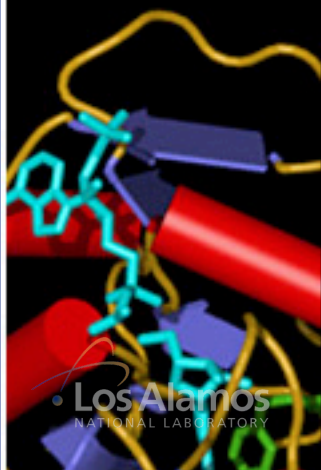
Lujan Center postdoctoral fellow focuses on soft-condensed materials at Los Alamos

Saurabh Singh, a postdoctoral fellow at the Lujan Neutron Scattering Center (LANSCE-LC), was recently selected to chair a session on lipids and membranes at the American Conference on Neutron Scattering 2012 conference. The conference is sponsored by the Neutron Scattering Society of America to stimulate, promote, and broaden the use of neutrons in science and technology and to integrate neutron scattering scientists in a wide spectrum of disciplines.

This year, from June 24-28, the conference is hosted by the National Institute of Standards and Technology in Washington, D.C.

ACNS is the most important forum for not only the U.S. neutron scattering society, but the event attracts scientists from all over the globe.

Singh began his work on neutron reflectometry in December 2011, and since then he has productively contributed to the neutron scattering investigations of soft-condensed materials (including bio-interfaces). During his short tenure at the Lujan Center he has already coauthored three journal articles and steered (with Ann Junghans, LANSCE-LC) the utilization of polyelectrolyte films in biostructures. His main research interests lie in the fabrication of multifunctional nanofilms using self-assembly techniques.



Colleagues,

Just by walking and driving around the TA-53 mesa it's clear we are going through a very intense maintenance period—from roofing activities to an intense accelerator maintenance schedule, from HVAC work to the WNR new building, and/or just general cleaning that's taking place. In addition to all that, we are starting to see an increasing number of summer students. Please be careful when driving around the site. In particular, please pay attention to pedestrians walking and crossing the roads.

We are now starting to focus on reviewing proposals and plans to accommodate user demand. For this upcoming run cycle some facilities received a record number of requests for beam time. For the past two weeks, review processes took place at WNR and Lujan Center. Overall, proposals continue to increase not just in numbers, but also in the breadth of proposed science and mission connections.

Coupled with LANSCE's Users Program, we hosted a tour for participants of the National User Facility Organization (NUFO) annual meeting June 18-20 in Santa Fe. For additional information go to lansce.lanl.gov. The tour was scheduled to take place on the afternoon of June 19 and featured LANSCE, the NHMFL, and CINT as the three major LANL user facilities. Around 60 people were expected to attend the tour. This was a great opportunity for us to feature our science, our people, and the connections we have with other user facilities at LANL.



'Let me take this opportunity to welcome Mark Bourke as the selected Lujan Neutron Scattering Center Leader. Mark returns to LANSCE, where he began his Los Alamos career in 1990 as a postdoctoral researcher ...'

Let me take this opportunity to welcome Mark Bourke as the selected Lujan Neutron Scattering Center Leader. Mark returns to LANSCE where he began his Los Alamos career in 1990 as a postdoctoral researcher using neutron diffraction to study constitutive response in materials of engineering relevance. Previously, he served as deputy group leader for Materials Science in Radiation and Dynamic Extremes (MST-8) at LANL. Mark holds a BSc in physics and a PhD in mechanical engineering from Imperial College, London University. In 1993, Mark joined the staff of LANL, becoming instrument scientist for the NPD (Neutron Powder Diffractometer). In 1997 he played a pivotal role proposing to the Office of Science the construction of the SMARTS (Spectrometer for Materials Research at Temperature and Stress) instrument. Since 2008, he has been a member of the MaRIE (Matter-Radiation Interactions in Extremes) core team, which is developing and implementing a strategy for an experimental facility to be located on the LANSCE mesa. He is chair of an International Atomic Energy Agency (IAEA) collaborative research program titled "Development, Characterization and Testing of Materials of Relevance to Nuclear Energy Sector Using Neutron Beams." Please join me in welcoming Mark back and thanking Jim Rhyne for his leadership and contributions in bringing the Lujan Center to its recognized scientific stature worldwide.

Have a great and safe summer

LANSCE Deputy Division Leader Alex Lacerda

A furnace with rotating load frame for in situ high temperature deformation and creep experiments

A novel sample environment at LANSCE extends the capabilities for in situ studies in support of neutron diffraction users at the Lujan Center. H. Matt Reiche (New Mexico State University and LANSCE-LC) and Sven C. Vogel (LANSCE-LC) spearheaded the development with design support from Eric Larson (LANSCE-LC) and in collaboration with Paula Mosbrucker and Mark Daymond (Queen's University, Kingston, Canada).

For material scientists and engineers working on optimizing material properties, it is crucial to understand and ultimately predict the microstructural evolution of metals and alloys during thermo-mechanical treatment. Material properties of the polycrystalline aggregate are strongly influenced by the orientation distribution of all crystals (i.e., texture). The ability to study the distinct influences of elevated temperatures and uni-axial stress on the texture, temperature dependent lattice strains, and phase transformation kinetics of a material in situ provides unique insight into, for example, variant selection during phase transformations or deformation mechanisms active during creep.

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Figure 2, right: Texture of the α -phase (left column) and β -phase (right column) of an extruded Zr-2.5Nb sample at room temperature measured with the sample changer (a) before and (f) after heating and 20% compression in the axial direction, which is the original extrusion direction shown about the center. The radial direction is horizontal and the hoop direction vertical. Revelation of critical factors influencing this material's texture is provided by in situ measurements (b) through (e) using the presented furnace. Pre- and post-treatment conditions of the sample are confirmed in (a/b) and (e/f), respectively. The Burger orientation relationship determines the transition of $(0002)_{hcp/\alpha}$ to maxima in $(110)_{bcc/\beta}$ during a temperature increase to 975°C . The resulting textures at high temperature are shown in (c). The $(222)_{bcc/\beta}$ planes align with the applied compression direction (d).

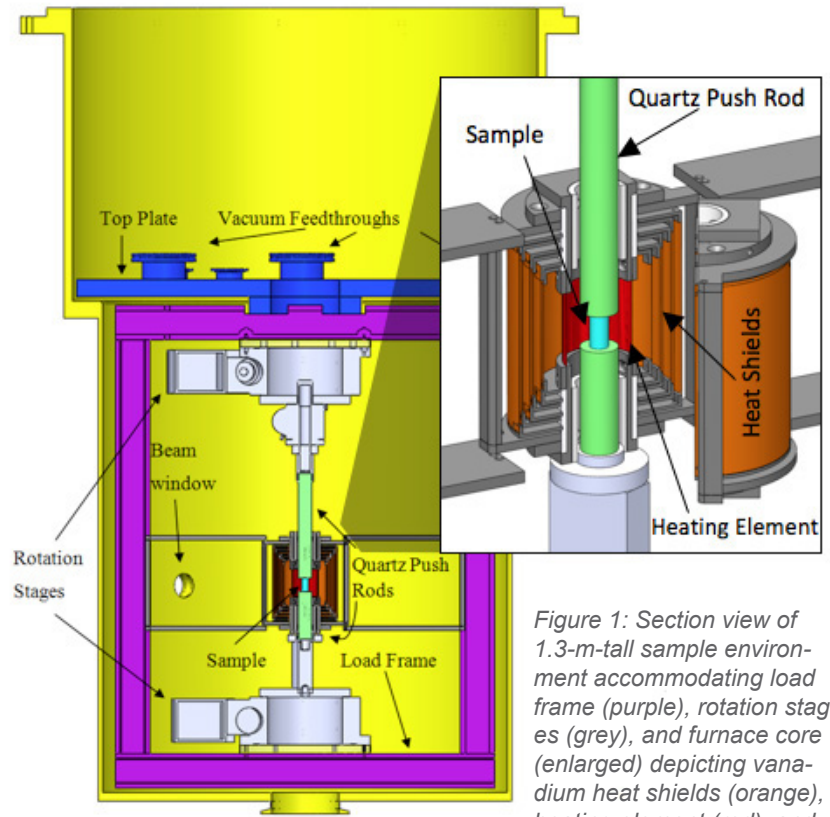
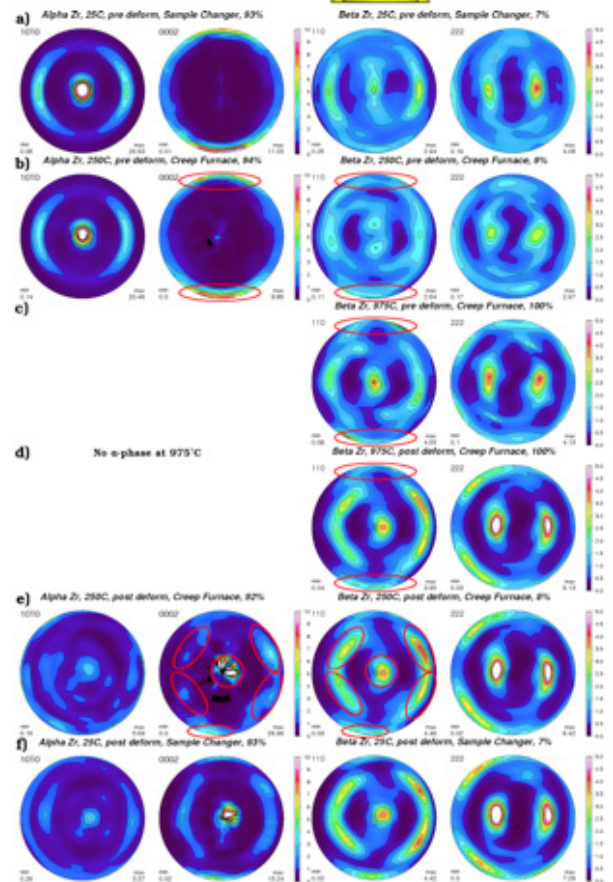


Figure 1: Section view of 1.3-m-tall sample environment accommodating load frame (purple), rotation stages (grey), and furnace core (enlarged) depicting vanadium heat shields (orange), heating element (red), and sample (light blue).



Furnace... Therefore, a resistive furnace was designed (Figure 1) and commissioned that allows for the acquisition of neutron diffraction data while the centimeter-sized specimen is under uni-axial stress ($\leq 2700\text{N}$) at elevated temperatures ($\leq 1000^\circ\text{C}$). Additional rotation ($\leq 80^\circ$) around the vertical compression axis of the sample allows for texture measurements in the HIPPO (High Pressure – Preferred Orientation) diffractometer at LANSCE.

This apparatus revealed quantitative insights (Figure 2) on the development of texture and lattice plane dependent stains throughout deformation and phase changes (at $\sim 860^\circ\text{C}$) simulating various thermo-mechanical processing steps of Zr-2.5wt%Nb, an alloy used for pressure tubes in CANDU® nuclear reactors.

Reference: "A furnace with rotating load frame for in situ high temperature deformation and creep experiments in a neutron diffraction beam line," *Rev. Sci. Instrum.* **83**, 053901 (2012). This work benefits from NSERC Industrial Research Chair in Nuclear Materials which Queen's University funds, as well as, Lujan Neutron Scattering Center at LANSCE, which the DOE Office of Basic Energy Sciences funds.

Proton transfer investigated using neutrons

A team including researchers from the Lujan Neutron Scattering Center recently performed an experimental and theoretical study on short, strong hydrogen bonding in tetraacetylene (TAE), a model system for proton transfer.

Proton transfer is one of the most important reactions in biology and biochemistry. For example, proton-driven machines populate cell membranes and are necessary for biological processes. More generally, proton transfer reactions are of central importance in

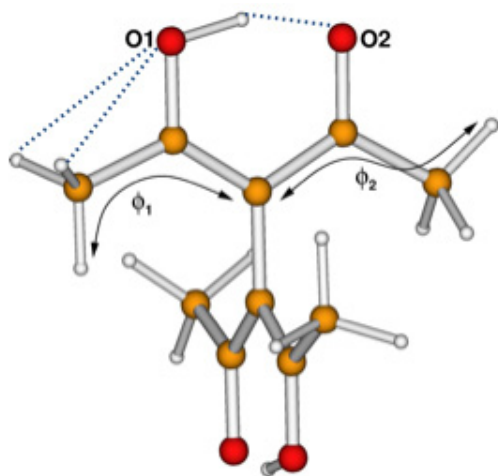


Figure 3: Ball-stick-representation of a molecule of tetraacetylene. Examples for intramolecular hydrogen bonds are displayed as dotted lines.

many areas of study concerning redox systems, ionic reactions, and chemical catalysis. Numerous proton transfer mechanisms are possible and still poorly understood in spite of years of study. Modeling the structures and dynamics of protons and of proton transfer with ab initio techniques requires difficult and costly quantum chemical calculations, few of which have been validated experimentally in detail.

The team's research, which appears in the *Journal of Physical Chemistry*, highlights a novel mechanism for facilitating proton transfer or stabilization of hydrogen-bond geometry mediated by the dynamics of adjacent functional groups in a very short, strong hydrogen bond. These have been implicated as possible intermediates in enzyme catalysis, for example, where such a process would have enormous complexity that is difficult to unravel with anything like the detail as in our model system.

Hydrogen bonding occurs when hydrogen is shared between electronegative atoms that can be located on different parts of the same molecule (intramolecular) or on different molecules (intermolecular). A hydrogen atom bound to an electronegative atom can interact strongly with another electronegative atom or even be transferred between atoms. Hydrogen bonding plays an important role in biochemistry as it is for example present in proteins, nucleic acids, as well as between single strands of DNA stabilizing the double helix. Hydrogen bonding strongly influences structure and dynamics of materials and thus model systems with short, strong hydrogen bonds are of great interest to scientists across various research fields.

Tetraacetylene (TEA), $(\text{CH}_3\text{CO})_2\text{CH}=\text{CH}(\text{COCH}_3)_2$, is a highly symmetric molecule with short, strong intramolecular hydrogen bonds (Figure 3), which are of special interest for proton transfer. Periodic density functional theory (DFT) calculations of the structure and the dynamics of the crystalline TAE as well as molecular dynamics simulations were performed and validated against experimental neutron scattering data. Potential energy surfaces (PESs) for the hydrogen bond were derived to determine the factors that govern proton transfer.

The methyl groups (CH_3 -groups) on each "side" of the TAE molecule form weak intermolecular hydrogen bonds in the solid to the oxygen atom (of the intramolecular H-bond) of a neighboring molecule. We showed experimentally that the movement of the methyl groups (mainly rotation) is strongly correlated with the position of the proton between the oxygen atoms and vice versa, thereby supporting or hindering the proton transfer process, a mechanism interfering with proton transfer that had not been recognized hitherto.

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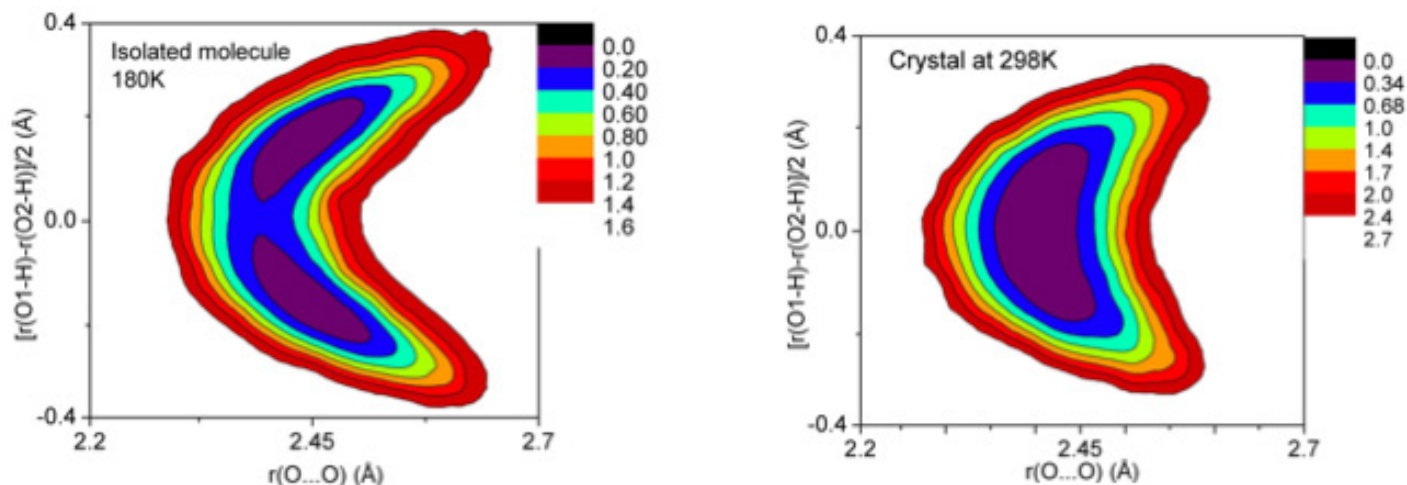


Figure 4: PES of the hydrogen bond in an isolated molecule (left) and in a crystal (right). The well in the crystal is 0.1 Å wide in the O...O coordinate (energy < 0.34 Kcal/mol) and 0.4 Å along the approximate O...H coordinate. At low temperature, the reorientation of the methyl groups leads to a preferred O-atom for the bridging proton. The amplitude of methyl torsions becomes larger with increasing temperature, so that free energy minimum for the proton becomes flat, in stark contrast with the isolated molecule case.

Proton... Incoherent inelastic neutron scattering (IINS) is particularly sensitive to H-atom motion, so that the proton in the hydrogen bonds and the methyl group dynamics could be studied with ease. While the computational determination of the electronic structure of hydrogen-bonded systems is difficult, the neutron vibrational spectrum can readily be obtained from such computational studies. In fact, the simplicity of the neutron-nucleus interaction permits one to calculate the position and intensity of the vibrational modes for direct comparison with the experimental neutron vibrational spectrum. This is a powerful tool for the validation of ab initio calculations, which have become an indispensable part of spectroscopic studies.

The correlations between the movement of the various parts of the system with that of the bridging H-atom on its PES were determined from experiment and computations. Calculations on a fully periodic system representing the crystal reveal the important effect of the intermolecular interactions on the potential energy surface of the hydrogen bond when compared with the result for an isolated molecule (Figure 4).

The IINS data were collected on the Filter Difference Spectrometer FDS at the Lujan Center.

Reference: Gordon J. Kearley (ANSTO), Jernej Stare (National Institute of Chemistry, Slovenia), Ramzi Kutteh (University of Sydney), Luke Daemen (LANSCE-LC), Monika Hartl (LANSCE-LC), and Juergen Eckert (University of South Florida), "Methyl Dynamics Flattens Barrier to Proton Transfer in Crystalline Tetraacetylene," *J. Phys. Chem. A*, **116** (9), 2283–2291 (2012).

Technical contact: L. Daemen

Bulk texture evolution nanolamellar composites during accumulative roll bonding

In bulk multi-phase composite metals containing an unusually high density of heterophase interfaces, the bi-metal interface controls all defect-related processes. Quite unconventionally, the constituent phases play only a secondary role. With the "right" characteristics, these bi-material interfaces can possess significantly enhanced abilities to absorb and eliminate defects. Through their unparalleled ability to mitigate damage accumulation induced under severe loading and/or severe environments, they provide their parent composite with a highly effective healing mechanism and an unrivaled robustness not possible in existing advanced structural materials.

Atom-by-atom fabrication of copper-niobium (Cu-Nb) nanolamellar composites prepared via physical vapor deposition (PVD) exhibit orders-of-magnitude increases in desirable properties such as strength, resistance to radiation damage, resistance to shock damage, and thermal stability when compared with their bulk counterparts. Modeling indicates that the desired properties of the nanolamellar composites are tied to the specific atomic structure that is exhibited at the interfaces between the two materials. The atomic structure of PVD Cu-Nb promotes recombination and annihilation of defects leading to a self-healing interface. These unique properties make the material attractive for nuclear power, transportation, energy, and defense applications. Los Alamos researchers and a collaborator have investigated scalable

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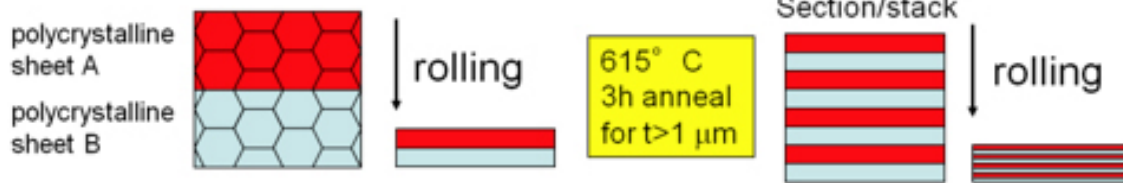


Figure 5. Schematic of the accumulative roll bonding process.

Bulk... fabrication methods that can produce bulk material (as the potential applications require) that are geometrically similar to PVD multilayers but with different interfacial structures. Having a different interfacial structure would allow researchers to distinguish the effect of the high density of heterophase interfaces from the interfacial structure in determining the desirable properties listed above. The journal *Acta Materialia* published the research.

The researchers examined accumulative roll bonding (ARB) as a scalable method to fabricate Cu-Nb composites that are geometrically similar to those produced by the physical vapor deposition method. The ARB process begins with two 1 mm thick plates of fully annealed, high purity Cu and Nb as shown in Figure 5. A pass with a 60% reduction in overall thickness is made through a rolling mill to induce bonding between the two stacked plates. After the pass is performed, the new, single plate is cut, restacked, and sent through the mill on another 60% reduction pass. This process is repeated with intermittent annealing steps to offset the differences in work hardening between Cu and Nb. The scientists successfully manufactured bulk sheets of Cu-Nb multilayer composites with more than 14,000 layers and individual layer thicknesses as small as 10 nm.

Because the ARB Cu-Nb has a layered morphology similar to PVD Cu-Nb, the researchers conducted a bulk texture study at the Lujan Neutron Scattering Center to examine the evolution of the interfaces from the ARB process. The scientists found that the interfaces in ARB Cu-Nb evolve towards an atomic structure that is fundamentally different from that exhibited in PVD due to the extreme strain infused during the ARB process. White arrows in Figure 6 indicate where confined layer slip, a deformation mechanism, is observed. Confined layer slip was observed in the PVD Cu-Nb system at this same layer thickness. This finding indicates that the same deformation mechanisms are present and active despite the difference in fabrication and interfacial structure.

Now the researchers are determining how the difference in interfacial structure of Cu-Nb affects thermal stability, radiation damage resistance, strength, and shock resistance.

John Carpenter and Duncan Hammon (Materials Technology-Metallurgy, MST-6), Nathan Mara (Center for Integrated Technologies, MPA-CINT), Irene Beyerlein (Fluid Dynamics and Solid Mechanics, T-3), Sven Vogel (LANSCE-LC), and Jonathan LeDonne

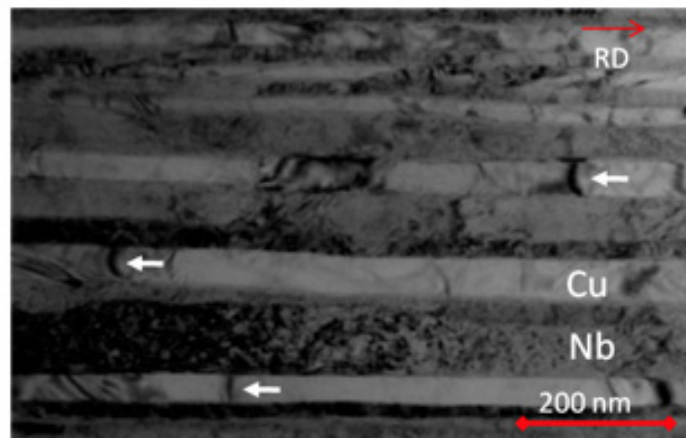
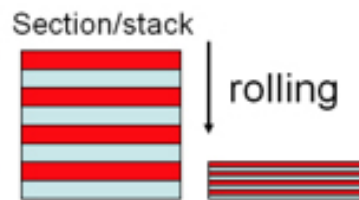


Figure 6. Bright Field TEM image of ARB Cu-Nb nanolamellar multilayers with individual layer thicknesses of 48 nm. Red arrow indicates rolling direction and white arrows indicated evidence of confined layer slip.

(Carnegie Mellon University) conducted the research. Reference: "Bulk Texture Evolution of Cu-Nb Nanolamellar Composites during Accumulative Roll Bonding," *Acta Materialia* **60**, 1576 (2012).

The Laboratory Directed Research and Development (LDRD) program funded the research, and the DOE Office of Basic Energy Sciences sponsors the Lujan Neutron Scattering Center at LANSCE. The work supports the Lab's Energy Security and Global Security mission areas and the Materials for the Future science pillar.

Technical contact: John Carpenter

Celebrating service

Congratulations to the following AOT and LANSCE Division employees celebrating service anniversaries this month:

Jeffrey Casados, AOT-MDE	40 years
Lawrence Rybarcyk, AOT-ABS	25 years
Henry Alvestad, AOT-ABS	20 years
Lawrence Castellano, AOT-RFE	15 years
Jacob Sandoval, AOT-RFE	10 years
Haruo Miyadera, AOT-ABS	5 years

New website for ADEPS Worker Safety and Security Team

The ADEPS WSST has a resource and information page located on the ADEPS internal website:

int.lanl.gov/org/padste/adepts/wsst.shtml

The site includes the team's most recent meeting minutes as well as links to a wide range of related safety and security information, including

- Environment, Safety, Health (ADESH)
- Security and Safeguards (ADSS)
- National Safety Council
- Occupational Medicine
- Occurrence Reporting
- Safety Short
- Voluntary Protection Program (VPP)
- Mesalib

WSST is all about

- Driving worker involvement in resolving issues
- Improving safety and security
- Representing all workers
- Facilitating communication between workers and managers

The WSST will work hard to address any issue you have. You will get a response from the WSST within a week and will be periodically kept abreast of progress on your issue.

Your ADEPS WSST members are

- ADEPS: Jeff Schinkel
- LANSCE-DO: Howard Nekimken
- LANSCE-LC: Eric Larson
- MPA-CMMS: Michael Torrez
- MPA-MC: Eve Bauer, chair
- MST-6: Erik Luther
- MST-8: Thomas Sisneros
- P-25: Jeff Bacon, co-chair

AOT & The Pulse

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