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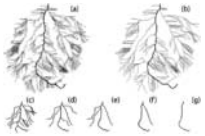

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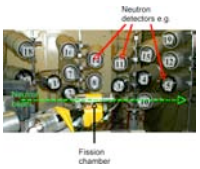

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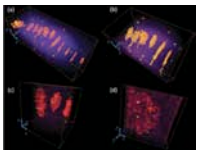

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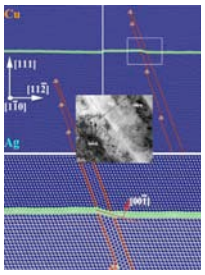

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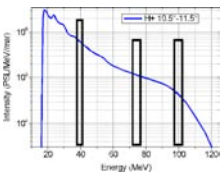

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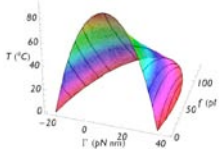

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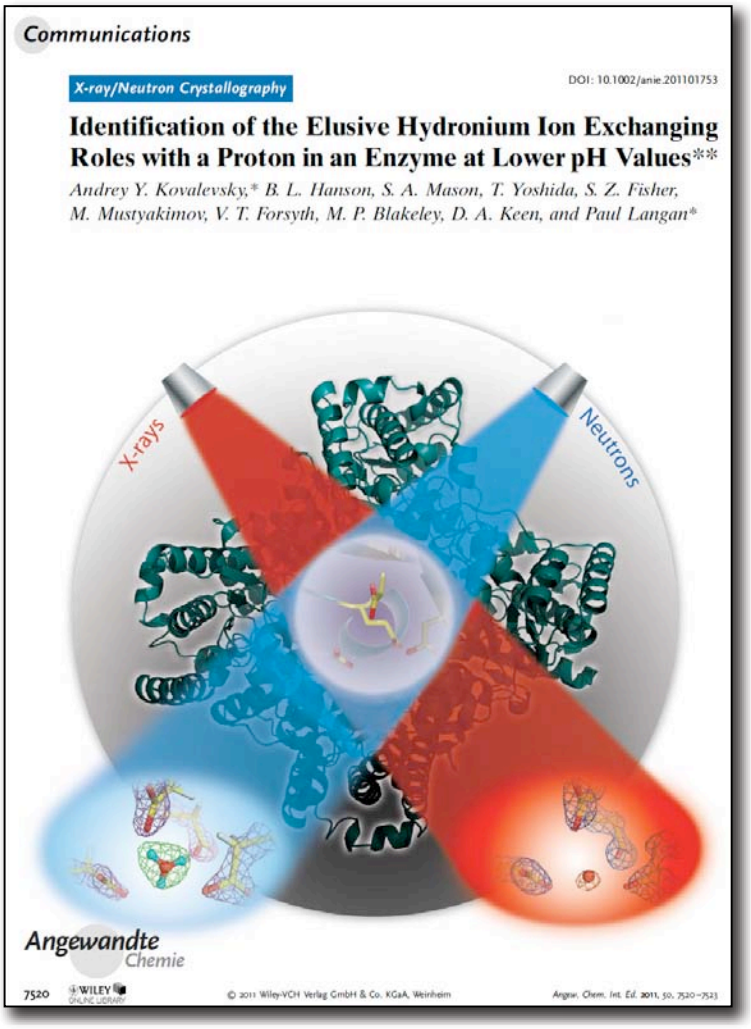
PADSTE HIGHLIGHTS August 17, 2011

BIOSCIENCE

First proof of hydronium ion's role in an enzymatic process

LANL researchers and collaborators have employed neutrons for an unprecedented view of the critical role that the elusive hydronium ion plays in the transfer of protons during enzyme-catalyzed reactions. Prior to this work, no one had ever directly witnessed the role of the hydronium ion, a water molecule bound to an additional hydrogen ion, in the catalytic mechanisms of enzymes. Scientists took an interest in an enzyme that has the potential to allow conversion of sugars in woody biomass into alcohol, a potential alternative fuel, because the enzyme loses its effectiveness when the pH value of the milieu is lowered — a common occurrence in the interior of industrial yeast cells fermenting alcohol.



The scientists used neutrons from the Los Alamos Neutron Science Center (LANSCE) to examine the mechanism of the biological reactions. The hydronium ion appears as a pyramid-shaped mass in the enzyme's active site where the chemical reaction occurs. The researchers discovered a crucial change as the system fell into the acidic range of the pH scale (below 6). The hydronium ion facilitating the binding of a metal ion cofactor crucial to the conversion of the sugar molecule into its fermentable form suddenly becomes dehydrated. The space occupied by the relatively large hydronium ion collapses into a tiny volume occupied by the remaining proton (a positively charged hydrogen ion). The spatial change in the molecular structure prevents the enzyme from attacking the sugar. This explains why pH has such an important role in the process and renders the enzyme inactive under acidic conditions. The hydronium ion has a key role in the transport of protons in these types of biochemical systems. The research provides insight for the role of hydronium ions in biological systems and could aid in treatment of peptic ulcers or acid reflux disease, or enable more efficient conversion of woody waste into biofuels.

Figure 1. A hydronium ion has been found to interchange with metal cofactors in the active site of an enzyme. Under more acidic conditions, the hydronium ion is dehydrated to a proton, and the binding site collapses.

LANL scientists include Andrey Kovalevsky, Suzanne Fisher, and Marat Mustyakimov (Bioenergy and Environmental Science, B-8); Thomas Yoshida (Chemical Diagnostics and Engineering, C-CDE); and Paul Langan (B-8, currently at Oak Ridge National Laboratory). Collaborating institutions are the University of Toledo, Ohio; the Institut Laue Langevin, France; Keele University, England; and the ISIS facility in Oxfordshire, England. Reference: "Identification of the Elusive Hydronium Ion Exchanging Roles with a Proton in an Enzyme at Lower pH Values," ***Angewandte Chemie International Edition*** *50*, 7520 (2011); doi: 10.1002/anie.201101753. Laboratory's Directed Research and Development Program (LDRD), the DOE Office of Biological and Environmental Research, and the National Institutes of Health supported different aspects of the LANL research. The work supports the Lab's Energy Security mission area and the Materials for the Future science pillar.

CHEMISTRY

Industrial Hygiene Laboratory obtains international accreditation

The Industrial Hygiene (IH) Laboratory in Chemical Diagnostics and Engineering (C-CDE) passed their American Industrial Hygiene Association (AIHA), LLC assessment, which addressed new international requirements. This international accreditation is effective through May 1, 2013. AIHA is an international accreditation body that was recently accepted as a full member of the International Laboratory Accreditation Coopertaion (ILAC), a signatory of the ILAC Mutual Recognition Arrangement (MRA), a full member of the Inter American Laboratory Accreditation Cooperation (IAAC), a signatory of the IAAC Multi Lateral Arrangement (MLA), and a full member and signatory of the Asia Pacific Laboratory Cooperation (APLAC) Mutual Recognition Arrangement (MRA). This international recognition allows AIHA accredited laboratories to provide accredited services worldwide.

The IH Laboratory has been accredited since 2000. It provides ISO 17025 accredited analyses for beryllium and a suite of 11 metals under its accreditation. Every two years the accreditation agency assesses laboratories to ensure they are adhering to their rigorous standards and implementing their continually changing requirements. The laboratory also must pass quarterly blind performance evaluation samples, and the analysts must pass biannual blind performance evaluation samples. The personnel are dedicated to the high quality standards required of them and continuously improve processes to ensure that customers receive accurate and timely results. The team performs analyses for the Facilities Operations Director at TA-55 and for the Plutonium Manufacturing and Technology program. The work supports the Lab's Nuclear Deterrence mission area and the Materials for the Future science pillar.

Photo. C-CDE's Industrial Hygiene Laboratory Personnel. Front Row (left to right): Claudine Armenta, Yolanda Giles, April Longhair, and Sandra Cruz (TL). Back Row: Holly Dodge, Tom Yoshida, Adam Pacheco, Charlotte Holland, and Melissa Montoya. Not Pictured: Michael Schappert.

EARTH AND ENVIRONMENTAL SCIENCES

New watershed classification system developed

A paper co-authored by Chandana Gangodagamage (Earth System Observations, EES-14) is a featured article on the American Geophysical Union's ***Water Resources Research*** Website (http://www.agu.org/journals/wr/wr1107/2010WR009252/**)**. The article titled "Revisiting Scaling Laws in River Basins: New Considerations Across Hillslope and Fluvial Regimes," proposes the use of "directed distance from the divide" as the scale parameter in an alternative to Horton's stream order or upstream contributing area for performing detailed probabilistic analysis of landscapes over a broad range of scales. Gangodagamage conducted research for the paper while working on a Ph.D. from the University of Minnesota Department of Civil Engineering. Postdoctoral Associate Patrick Belmont and Professor Efi Foufoula-Georgiou University of Minnesota) also contributed to the research and paper.

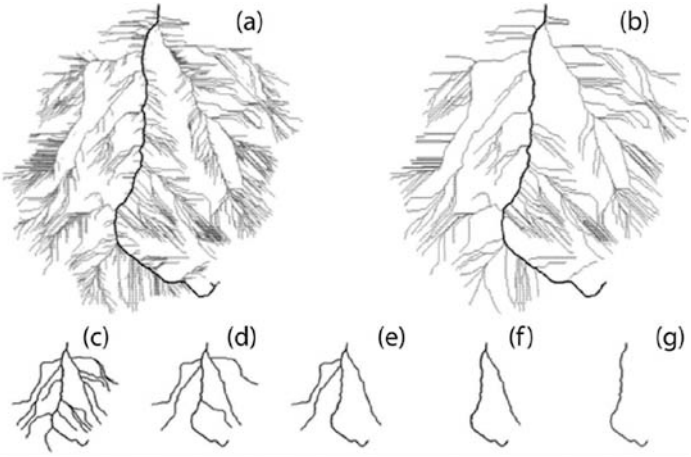


Figure 2. A new stream ordering system based on flow path distance *l* called "directed distance from the divide." (a) Basic network of flow path segments for $l > 50$ m. (b) Flow path segments with $l < 100$ m are eliminated from Figure 2a at their corresponding tributary junctions. (c) Flow path segments with $l < 200$ m are eliminated from the network at their tributary junctions. Flow path segments *l* less than (d) 300 m, (e) 400 m, (f) 500 m, and (g) 600 m.

Models of watershed behavior are beginning to incorporate lidar (light detection and ranging) topography measurements with resolutions of the order of 1 m^2, but this increase in the availability of high-quality data outpaces the ability to make the best use of them. At issue is the conceptual lens through which the data are analyzed, particularly when investigating hydrologic behavior at different scales. Scaling parameters break down the masses of data into groupings that fit within certain constraints to be analyzed for trends. Watershed research traditionally used either stream order – a measure based on how many tributaries a body of water has – or the upstream catchment area to make these divisions. To best make use of the available high-resolution topography data, Gangodagamage and collaborators proposed a new scaling parameter based on the "directed distance from the divide." For each point in a watershed, the technique calculates the longest distance from that point to a drainage divide, taking into account variations in topography and recognizing that water only flows downhill. When two paths converge, the shorter is treated as a tributary to the longer. This process is repeated until the entire watershed culminates in one major river. From these calculations, the watershed can be broken down and analyzed using ensemble statistics based on flow paths of different lengths. In addition to their theoretical investigation of the technique, the authors analyzed a watershed in Mendocino County, California, at three different spatial scales. The scientists found that directed distance from the divide provides new information, more clearly delineating transitions in geomorphic process regimes relative to other common scaling parameters. Reference: ***Water Resources Research*** 47, W07508 (2011); doi:10.1029/2010WR009252. A doctoral dissertation fellowship to Gangodagamage from the University of Minnesota supported his research. Technical contact: *Chandana Gangodagamage*

LANSCE

Measuring the fission neutron spectrum at LANSCE

Scientists from LANL, Japan (Kyushu University), and France (CEA Bruyères-le-Châtel) have measured the energy distribution of neutrons from neutron-induced fission. The data are used as constraints in the Los Alamos model of nuclear fission to obtain information on the total kinetic energy of the fission fragments. Moreover, the data will improve the evaluated data libraries, which are used in applications to nuclear energy, criticality safety, and nuclear weapons development.

A nucleus of uranium, plutonium, or certain other elements can be induced to fission, or split into two lighter nuclei, by the addition of a neutron. When fission occurs, the two fission fragments can emit energetic neutrons, which then can induce further fissions. This is the principle of the chain reaction. For reactors, the chain reaches a steady state, whereas for weapons and other super-critical systems, the number of fissions increases exponentially with time. Because the probability of fission depends on the neutron energy, the energy spectra of the neutrons from fission must be known in order to calculate the neutron multiplication of a fissionable system. Although several measurements have been made of the neutron emission spectrum from fission induced by thermal neutrons (neutron energy distribution characteristic of room temperature), very few measurements have been performed for fission induced by fast neutrons (neutrons with a kinetic energy in excess of 0.1 MeV). The two measurements for the important isotope plutonium-239 (^{239}Pu), are inconsistent. Therefore, the researchers' goal in the measurements at the Weapons Nuclear Research (WNR) facility at LANSCE is to make significant improvements in these basic data.

The approach uses a double time-of-flight technique. The WNR neutron source is pulsed to give the "start" signal, and the time of flight of neutrons to the fission detector located 22.7 meters away gives the energy of the neutron inducing the fission. An electronic pulse created when fission takes place is the "stop" signal for the timing. The fission pulse is also used as the "start" signal to time neutrons from fission in the fission chamber to neutron detectors placed 1 meter away. These detectors are called the FIGARO (Fast Neutron-Induced Gamma-Ray Observer) array. By collecting data from many fission events, a distribution of the energies of the fission neutrons is obtained and can be compared with predictions of the Los Alamos Model. The fission chamber, which was supplied by the French colleagues, and the neutron detectors are pictured in the photo. Samples of the results, shown in Figure 3, are compared with data in the Evaluated Neutron Data File, ENDF/B-VII.0, which is used around the world for applied calculations, and with predictions of the revised Los Alamos Model. Their results are in agreement with the data in ENDF/B-VII.0. Scientists are continuing the work to reduce the size of the error bars and to extend the measurements to neutrons with energies below 1 MeV. The work supports the Lab's Nuclear Deterrence and Energy Security mission areas and the Science of Signatures and Materials for the Future science capabilities.

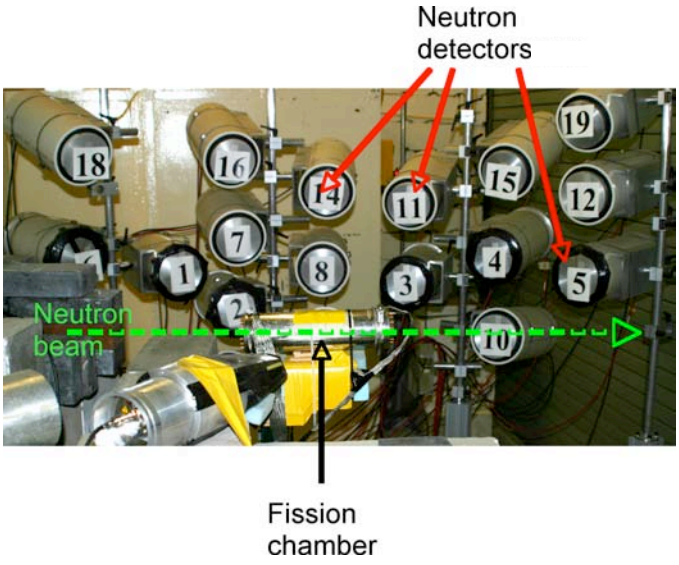


Photo. Fission chamber and neutron detectors (numbered).

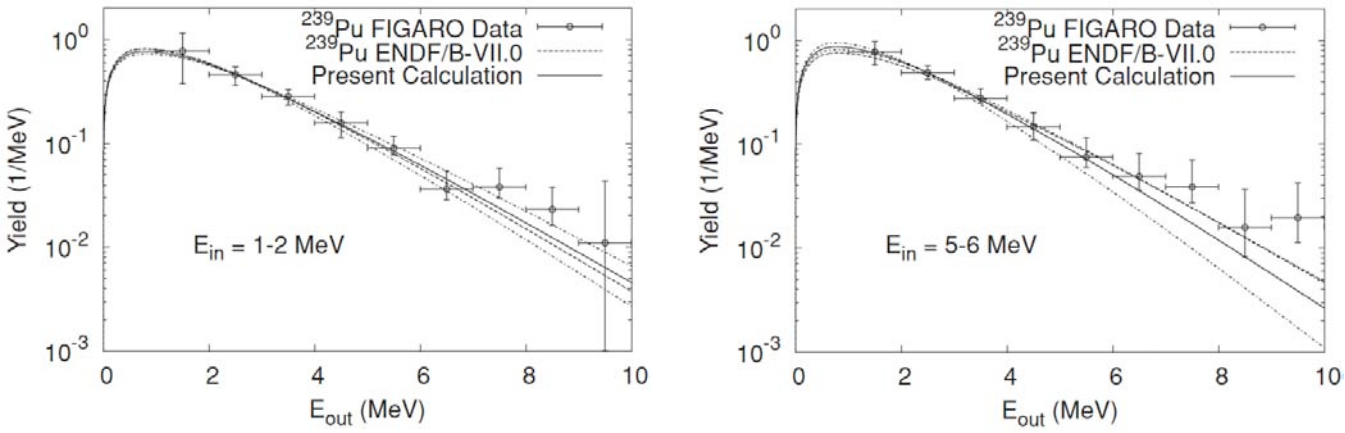


Figure 3. Sample results of the prompt fission neutron spectra for two incident neutron energies, 1-2 MeV and 5-6 MeV. The data (FIGARO) are compared with those in the Evaluated Nuclear Data Library (ENDF) and with predictions of the modified the Los Alamos Model (Present Calculation). Scientists adjusted input parameters of the latter to fit the present data.

Scientists participating in the research include Shusaku Noda [Kyushu University, Neutron Science (LANSCE-NS), and Nuclear and Particle Physics, Astrophysics and Cosmology (T-2)], Robert Haight, Ronald Nelson, Matthew Devlin, and John O'Donnell (LANSCE-NS); Audrey Chatillon, Thierry Granier, Gilbert Belier, and Julien Taieb (CEA); Toshihiko Kawano and Patrick Talou (T-2). Reference: "Measurement and Analysis of Prompt Fission Neutron Spectra from 1 to 8 MeV in Neutron-induced Fission of ^{235}U and ^{239}Pu Using the Double Time-of-flight Technique," ***Physical Review C*** *83*, 034604 (2011); doi:10.1103/PhysRevC.83.034604. Technical contact: *B. Haight*

MATERIALS PHYSICS AND APPLICATIONS

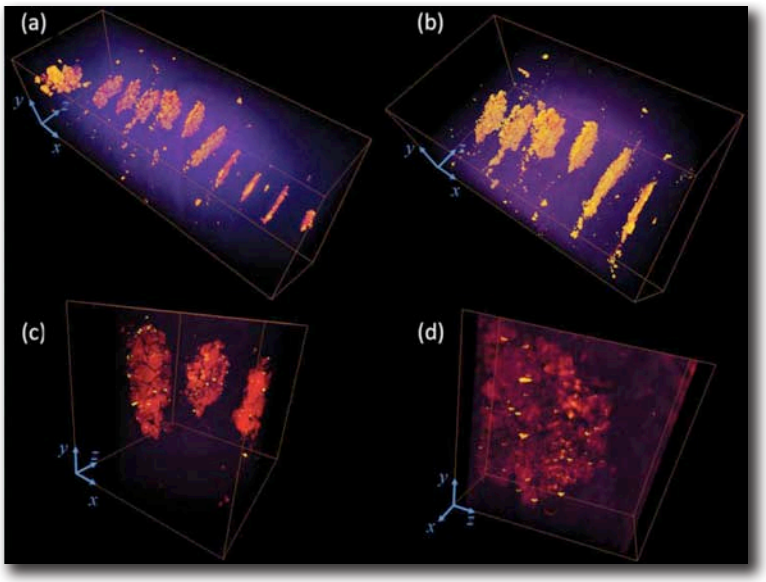
Making metamaterials with sound waves in five minutes or less

In an important step in metamaterials development, Dipen Sinha (Sensors and Electrochemical Devices, MPA-11) and collaborators have identified fast and inexpensive tools for engineering these materials. Director's Postdoctoral fellow Farid Mitri (MPA-11), under the direction of Sinha and with material scientist Fernando Garzon (MPA-11), have described how to build artificial materials with unusual properties, such as negative refractive index that can lead to invisibility cloaking, in a mere five minutes or less. Until now, metamaterial synthesis was cost-prohibitive and required expensive equipment. The journal ***Review of Scientific Instruments*** published the research, and numerous scientific Web sites featured the work.

Metamaterials are manmade structures exhibiting exotic properties. These materials can manipulate electromagnetic and acoustic waves to create invisibility cloaks, subwavelength focusing, and shielding. The combination of these intriguing properties poises metamaterials to make a significant impact on the technological world.

Sinha, Mitri, and Garzon have developed an easy and inexpensive method for fabricating a three-dimensional (3D) periodic structure using the radiation force induced by high-frequenc (greater than 1 MHz) acoustic waves in a resonator cavity. The process arranges nanoparticles in a host polymer matrix

(e.g., epoxy). Changing the frequency of the acoustic waves can easily modify this arrangement. The scientists characterized its internal skeleton with X-ray micro-computed tomography (XμCT) to assess the quality of the manufacturing process. The particles can be made from any material and can be even hollow microspheres. This is important to create acoustic metamaterials where the particles behave as local mechanical resonators. The scientists used the state-of-the-art technique based on the radiation force of ultrasound standing (or stationary) waves in a rectangular chamber to pattern clusters of 5-nm-diameter diamond nanoparticles in parallel planes within a 3D matrix of epoxy before solidification. The periodic pattern became permanent with full cure of the epoxy matrix to form a 3D metamaterial structure. A wide variety of patterns and shapes can be created by applying the appropriate ultrasound field.



The ultrasound field was activated for 5 minutes, a duration corresponding to the epoxy curing cycle. During this time, clusters of diamond nanoparticles were trapped and patterned due to the acoustic radiation force that directs them toward the nodes of the standing wave field to form parallel periodic planes. The manufacturing time may be further reduced by selecting a faster curing epoxy (less than 1 minute). This is a bench-top and inexpensive fabrication approach.

Figure 4. XμCT renderings of a polymer nanocomposite metamaterial assembled using 1 MHz ultrasound standing wave field in which approximately 5-nm diameter diamond nanoparticles are clustered in a host fluid (epoxy) cured during 5 minutes to create the surrounding solid structure. (a) The 3D rendering using the 2°ø detector lens (resolution apprroximately 10 microns), in which all the patterned planes (i.e., 12 planes) of diamond-nanoparticle clusters are visible. [(b)–(d)] 3D rendered images at higher resolutions using the 4°ø, 10°ø, and 20°ø lenses, respectively.

This technique is particularly suited for creating materials with the length-scale (periodicity of the pattern) in the range of 1-100 micron where there is a gap in existing fabrication technology. For example, lithography techniques are available for small-scale fabrication (sub-micron length-scale), and mechanical machining techniques are used for materials created with mm-size objects.

An advantage of this fabrication technique is that the particles may consist of any material (metal, insulator, semiconductor, superconductor, piezoelectric, nanowires, or nanotubes, and even biological materials), and a wide range of geometries (cylindrical, hexagonal, and other symmetries) is possible. The researchers' goals are to develop novel sensors and devices based on this fabrication technique that extend beyond metamaterials. Reference: "Characterization of Acoustically Engineered Polymer Nanocomposite Metamaterials using X-ray Microcomputed Tomography," ***Review of Scientific Instruments*** *82*, 034903 (2011); doi:10.1063/1.3553207. A Laboratory Director's fellowship provided financial support for the research. Cristian Pantea (MPA-11) provided the diamond-nanoparticle powder

and experimental assistance, and Mark. A. Nelson (formerly MPA-11) assisted while using the X-ray computed tomography system. The work supports the Lab's Global Security and Energy Security mission areas and the Materials for the Future science pillar. Technical contact: *Dipen Sinha*

MATERIALS SCIENCE AND TECHNOLOGY

Two novel mechanisms of deformation twinning in face-centered-cubic metals

Crystal twinning results in an intergrowth of two separate crystals in a variety of specific configurations. A twin boundary separates the two crystals. There are three modes of formation of twinned crystals: growth twins, annealing or transformation twins, and deformation or gliding twins. Deformation twinning is a typical deformation mechanism, accomplished by the glide of twinning dislocations. The presence of twin boundaries can strengthen materials on the order of ten times higher in nanotwinned copper (Cu) due to the discontinuity of slip systems. However, it is difficult in single-phase face-centered-cubic (fcc) metals with medium to high stacking fault energies. Therefore twinning in these cases usually requires extreme conditions, such as shock and/or cryogenic temperatures. LANL researchers observed two novel twinning mechanisms in face-centered-cubic crystal. One is zero-strain twinning and de-twinning mechanism in single phase, and the other is interface-facilitated twinning mechanisms in composites. LANL scientists' research provides new insight for understanding deformation mechanisms in fcc crystals and controlling twins in composites.

Figure 5 shows the atomistic structure of the incoherent twin boundary (ITB) in Cu by high-resolution transmission electron microscopy (HRTEM) and molecular statics modeling . The HRTEM micrograph of S3{112} ITBs reveals that the atomic structure has a regular repeatable pattern with a unit containing three {111} planes, which corresponds to a set of Shockley partial dislocations with a repeatable sequence b_2:b_1:b_3 on every {111} plane. A noteworthy characteristic of the three partial dislocations is that the sum of their Burgers vectors in one unit equals zero. In situ TEM observation and atomistic simulations both synthesize the zero-strain twinning and de-twinning mechanism, in which twinning or de-twinning can be accomplished through the collective glide of S 3{112} ITBs, as shown in Figure 6. References: "Detwinning Mechanisms for Growth Twins in Face-centered Cubic Metals,"***Acta Materialia*** *58*, 2262 (2010), doi:10.1016/j.actamat.2009.12.013; "High Resolution Transmission Electron Microscope Observation of Zero-Strain Deformation Twinning Mechanisms in Ag," ***Physical Review Letters*** *106*: 175504 (2011); doi: 10.1103/PhysRevLett.106.175504].

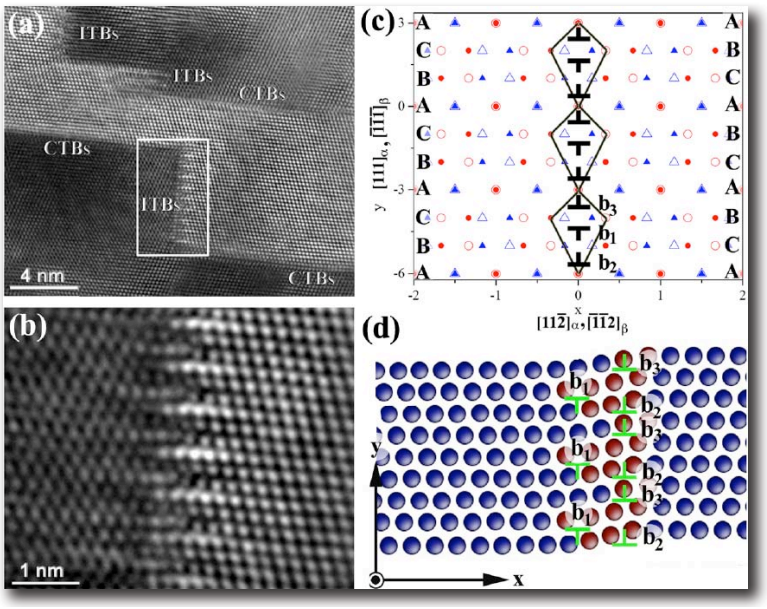


Figure 5. (a) HRTEM micrograph of grain boundaries. (b) Magnified HRTEM micrograph showing narrow and straight Σ3{112} ITBs. (c) Dichromatic pattern of a [110]Σ3{112}||{112} twin boundary

showing the atomic structure of the boundary consisting of a unit of three {111} planes and the corresponding Shockley partial dislocations. (d) Atomistic simulation of the relaxed atomic structure.

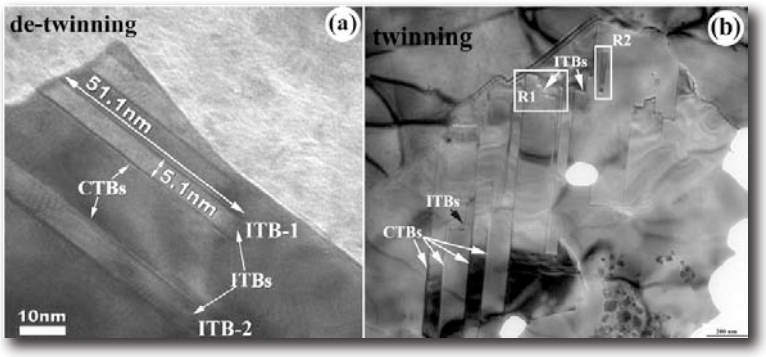


Figure 6. (a) In situ HRTEM observation of detwinning in Cu via the collective glide of the ITBs. (b) The HRTEM observation of twinning in silver through the collective glide of the ITBs.

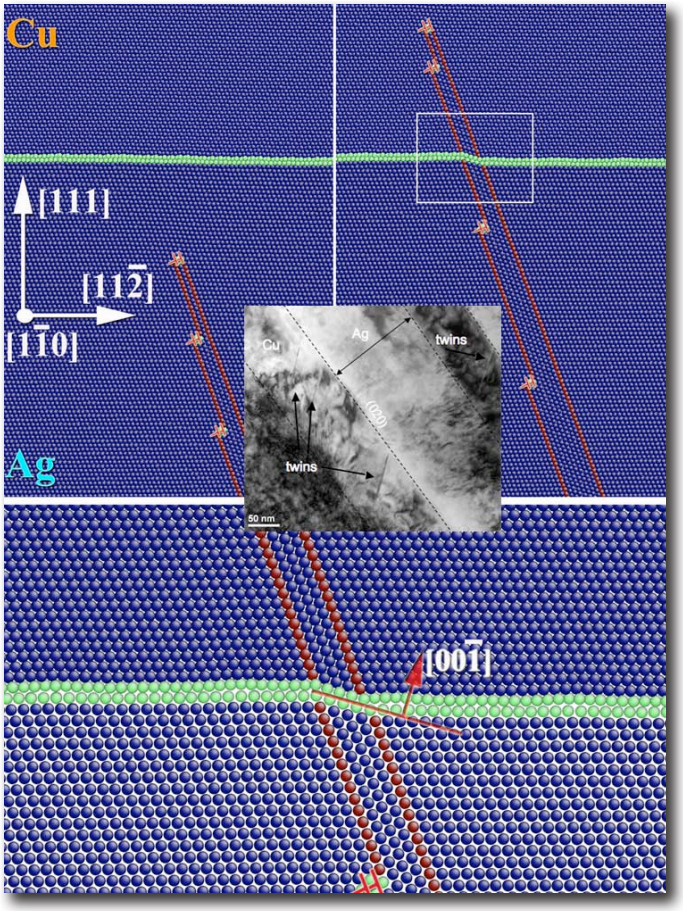


Figure 7. Interface-facilitated twinning in Cu through the twin transmission across the copper-silver (Cu-Ag) interface. Atomistic simulations show the initial, final, and the magnification of the twin transmission region. TEM image shows the fine twins in Cu.

The researchers proposed and demonstrated the interface-facilitated twinning mechanism, particularly for the materials that are hard twinned. They synthesized Ag-Cu eutectic-layered composites via a flux-

melting technique and then rolled the material. The (Ag-Cu) interface facilitates extensive deformation twinning in Cu during room temperature, low strain-rate loading conditions. This result demonstrates that twins in Ag can provide an ample supply of twinning partials to Cu to support and sustain twin growth in Cu during deformation. Atomistic simulations reveal that this "ideal" Ag-Cu interface allows transmission of twinning partials from the Ag phase into the Cu phase. As a consequence, the proposed twin nucleation and growth processes transform the interface plane from {111} to {100}, in agreement with experimental observation. Interface-driven twinning as revealed by this study suggests the exciting possibility of altering the roles of dislocation slip and twinning through the design of hetero-phase interface structure and properties. Researchers include Jian Wang (Structure/Property Relations, MST-8), Irene Beyerlein (Physics and Chemistry of Materials, T-1), Nathan Mara and Dhriti Bhattacharyya (Center for Integrated Nanotechnologies, CINT), David Alexander (Metallurgy, MST-6), and Carl Necker (B-61 Systems Engineering, W-1). References: "Texture Evolution via Combined Slip and Deformation Twinning in Rolled Silver–copper Cast Eutectic Nanocomposite," ***International Journal of Plasticity*** *27*, 121 (2011); doi:10.1016/j.ijplas.2010.05.007 , and "Interface-facilitated Deformation Twinning in Copper within Submicron Ag–Cu Multilayered Composites," ***Scripta Materialia*** *64*, 1083 (2011); doi:10.1016/j.scriptamat.2011.02.025. This research was supported as part of the Center for Materials at Irradiation and Mechanical Extremes, an Energy Frontier Research Center funded by the DOE Office of Science, Office of Basic Energy Sciences. The work supports the Lab's Energy Security mission area and the Materials for the Future science pillar. Technical contacts: *Jian Wang, Amit Misra, and Irene Beyerlein*

Rusty Gray shares metallurgical wisdom at National Science Foundation workshop

The American automotive industry has an eye on magnesium (Mg), a material that has promise of bolstering fuel-efficiency. However, this lightweight material is costly, more difficult to fabricate than other materials, and suffers from a poor performance record in regards to its high-strain rate ductility.

During a National Science Foundation "Magnesium Science and Technology" workshop, George "Rusty" Gray (Structure/Property Relations, MST-8) outlined one path that magnesium research could take given a better understanding of its service performance and its predictive capability. In his keynote lecture, he reviewed the high-strain-rate and shock response of magnesium and addressed how dynamic properties influence the future design for platform material applications.

The automotive, aerospace, and defense industries await such developments. While magnesium can offer the benefit of significant weight savings in structural applications, the use of magnesium in current transportation and defense material systems poses unique challenges as well as opportunities. Widespread use of magnesium is not practical yet – and it may never be in many applications due to its limited fracture resistance under impact loading due to shear localization. In what Gray called a "decadal grand challenge," engineers and scientists should take what they know about scientific mechanisms and governing physics to build more robust, lightweight materials. Progress on dynamic deformation and fracture predictive modeling requires new insight on deformation twinning, which is an active deformation mechanism in some materials and can even become a predominate mechanism at high strain rates. Los Alamos research has focused on materials with the hexagonal close-packed crystal structure and has included detailed microstructural characterization and modeling.

Gray serves on the National Materials Manufacturing Board, an organization of the National Academies. A LANL Fellow, Gray earned his bachelor's and master's degrees in metallurgical engineering from South Dakota School of Mines and Technology and his doctorate in metallurgical engineering from Carnegie Mellon University. Technical contact: *R. Gray*

PHYSICS

LANL sets new world records in laser-ion acceleration

Manuel Hegelich (Plasma Physics, P-24) led an international collaboration of scientists from P-24, Plasma Theory and Applications (XCP-6), Polymers and Coatings (MST-7), Ludwig-Maximilians University – Munich, and Queen's University – Belfast in an experiment on LANL's ultra-high intensity laser facility, Trident. The researchers accelerated protons to approximately 120MeV and carbon ions to approximately 1GeV using a 130 TW laser pulse.

These results represent a major break-through in laser-driven ion acceleration, increasing the previous record by almost a factor of two after more than 10 years of stagnation. In 2000, the Nova petawatt system at Lawrence Livermore National Laboratory demonstrated approximately 60 MeV protons using a process called Target-Normal Sheath Acceleration. This result sparked the hope of efficient and compact laser ion accelerators. The Trident laser reproduced these results using approximately one-fifth the pulse energy of Nova, and made slight improvements to approximately 67 MeV using special cone targets. However, many applications require energies of 100 MeV or more (e.g. approximately 140 MeV for proton tumor therapy, approximately 1 GeV for active interrogation). One new mechanism examined for a more efficient acceleration mechanism is the "Break-Out Afterburner" (BOA), which operates in the Transparent-Overdense Regime of plasma physics. BOA was discovered at LANL in VPIC simulations in 2006, and experimentally demonstrated for the first time with carbon ions at Trident in 2008. P-24's Relativistic Laser Matter Interaction Team and LANL/ Ludwig-Maximilians University graduate student Daniel Jung as responsible instrument scientist implemented the BOA mechanisms to accelerate protons for the first time. Interacting the 130TW Trident pulse at normal incident with a specially developed 280 nm thin, hydrocarbon target, designed for specific Trident pulse parameters using VPIC simulations and than developed by postdoc Chris Hamilton (MST-7), LANL researchers achieved up to 120 MeV protons from the interaction.

Scientists observed high-energy protons on all shot targets using both a newly developed ion wide angle spectrometer (iWASP), as well as stacks of CR-39 nuclear track detectors. Estimates from the CR-39 detectors suggest more than 10^7 protons above 100 MeV and more than 10^{10} protons above 20 MeV. In addition to the specific target design, newly developed focus and target alignment systems ensure a high intensity interaction (greater than $5x10^{20}$ W/cm^2), and contribute to the increase in particle energies. Using these improvements, the team could also increase their own record energy of 0.5GeV for laser-driven carbon acceleration by a factor of two to approximately 1 GeV. Proton and carbon ion energies are now within range of requirements for medical applications, isotope production, and other applications as drivers or probes for high energy density physics or material science experiments. Advances in laser technology allow for the construction of high-repetition rate, high average power drivers suitable for useful applications, making this technology a topic of interest for further study with regards to the MaRIE facility. The High Energy Density Laboratory Physics joint DOE Office of Science/NNSA program and the Domestic Nuclear Detection Office of the Department of Homeland Security funded the research. The work supports the Lab's Materials for the Future science pillar.

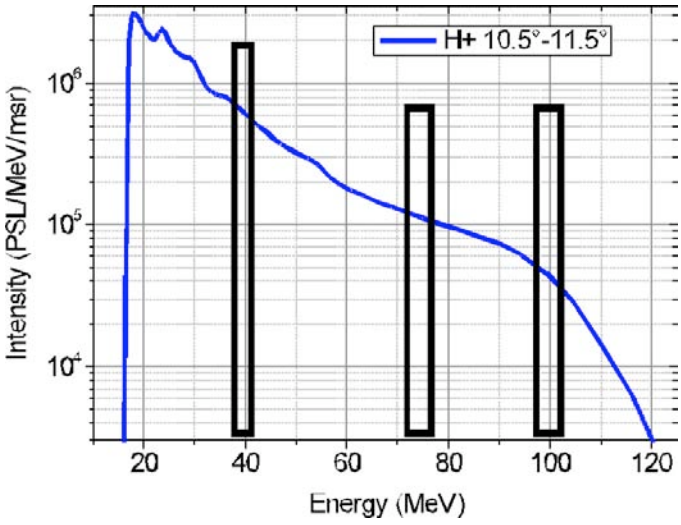


Figure 8. Proton spectrum from a relativistic laser-matter interaction of an approximately $5x10^{20}$ W/cm^2 ultrahigh contrast laser pulse with a 280 nm thin hydrocarbon target, measured with the iWASP spectrometer. The black squares mark the spectral locations where CR39 was placed, i.e., where protons of that initial energy range out, leaving a measurable track, used as independent confirmation.

THEORETICAL

Understanding the behavior of DNA under external mechanical load

DNA is a highly refined nanomechanical object, whose physical properties are unlike any other natural or synthetical polymer. In its helical form, in which the double strands are joined, DNA possesses remarkably large bending and torsional rigidities, which are orders of magnitude larger than those of a single strand. Because the two strands of DNA can open locally for transcription and replication or completely, in DNA denaturation, these unique physical properties are exploited in the mechanism of life by the protein machinery involved in transcription, repair, and packaging of DNA. Enzymes act as powerful motors. For example, helicases unwinds DNA to open a portion of it, whereas gyrase rewinds it. Therefore understanding the behavior of DNA under external mechanical load in a thermal bath becomes fundamental to illuminate biology and for nanotechnological applications, where DNA is the basis for novel functionalized materials.

In the past twenty years, direct single molecule manipulation has revolutionized our understanding of key aspects of DNA, revealing new couplings and transitions. In these experiments, performed with magnetic or optical tweezers, a few micrometer long strand of DNA is stretched to a tension of the order of pico-Newtons (pNs), and sharp transitions are activated at positive and negative applied torques. A still debated overstretching transition is observed for DNA under tension of approximately 60 pN at zero torque. As more refined measures have been performed under tension and stretch, tentative tension–torque phase diagrams for the stability of B–DNA have been proposed, as well as various phenomenological theories. However, most of these models are purely mechanical and do not take into consideration the effect of temperature. Other models neglect fundamental phenomena, such as the role of tension or denaturation at overwinding. Therefore, the models of qualitative behavior cannot provide a phase diagram in the tension-torque plane.

Cristiano Nisoli (Physics of Condensed Matter and Complex Systems, T-4 and Center for Nonlinear Studies, CNLS) and Alan R. Bishop (Acting Principal Associate Director for Science, Technology and Engineering, PADSTE) have shown that it is the interplay between the strong covalent bonds of the backbones and weak hydrogen interactions between bases, the thermal bath in which DNA is immersed, and the proximity of physiological conditions to the denaturation temperature, that make DNA highly and non-linearly responsive to mechanical and thermal changes. The scientists proposed a minimal model of the symmetry of the macromolecule and of a few relevant interactions, which takes into account the steric dependence of the base bonds. By performing statistical mechanics, they could predict for the first time phase diagrams for stability of DNA in the tension-torque plane of DNA. They find that those transitions seen experimentally correspond to DNA melting, or complete separation of the two strands, which happens at different temperatures when different mechanical loads are applied. The agreement with more than twenty available experimental measures at room temperature is excellent, and University of California –Santa Barbara collaborators are experimentally testing their predictions at different temperature. The LANL scientists computed the behavior of DNA's critical temperature as a function of applied torque and tension. The result shows the initial stabilizing effect of overwinding in preserving DNA helical structure at temperatures well above denaturation –a mechanism exploited by extremophile bacteria. Nisoli and Bishop are using their novel framework to study the conformational changes induced on DNA by mechanical actions at different temperatures and salt concentrations. Reference: "Thermomechanics of DNA: Theory of Thermal Stability under External Load", ***Physical Review Letters*** 107, 068102 (2011); 10.1103/PhysRevLett.107.068102. A LANL Director's Funded Postdoctoral Fellowship funded Nisoli's research, which supports the Lab's Energy Security mission area and the Materials for the Future science capability.

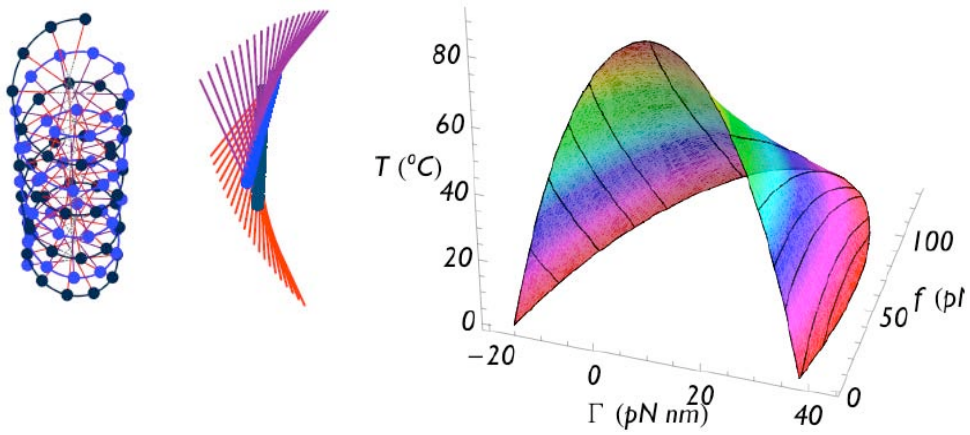


Figure 9. Schematics of the DNA model showing (*left*): closed double helix, (*middle*): open strands twisting with bases pointing outwards, (*right*): predicted critical surface for denaturation of B-DNA in (T), torque (Γ) and tension (f). Solid lines on the surface correspond to critical lines at fixed torque Γ.