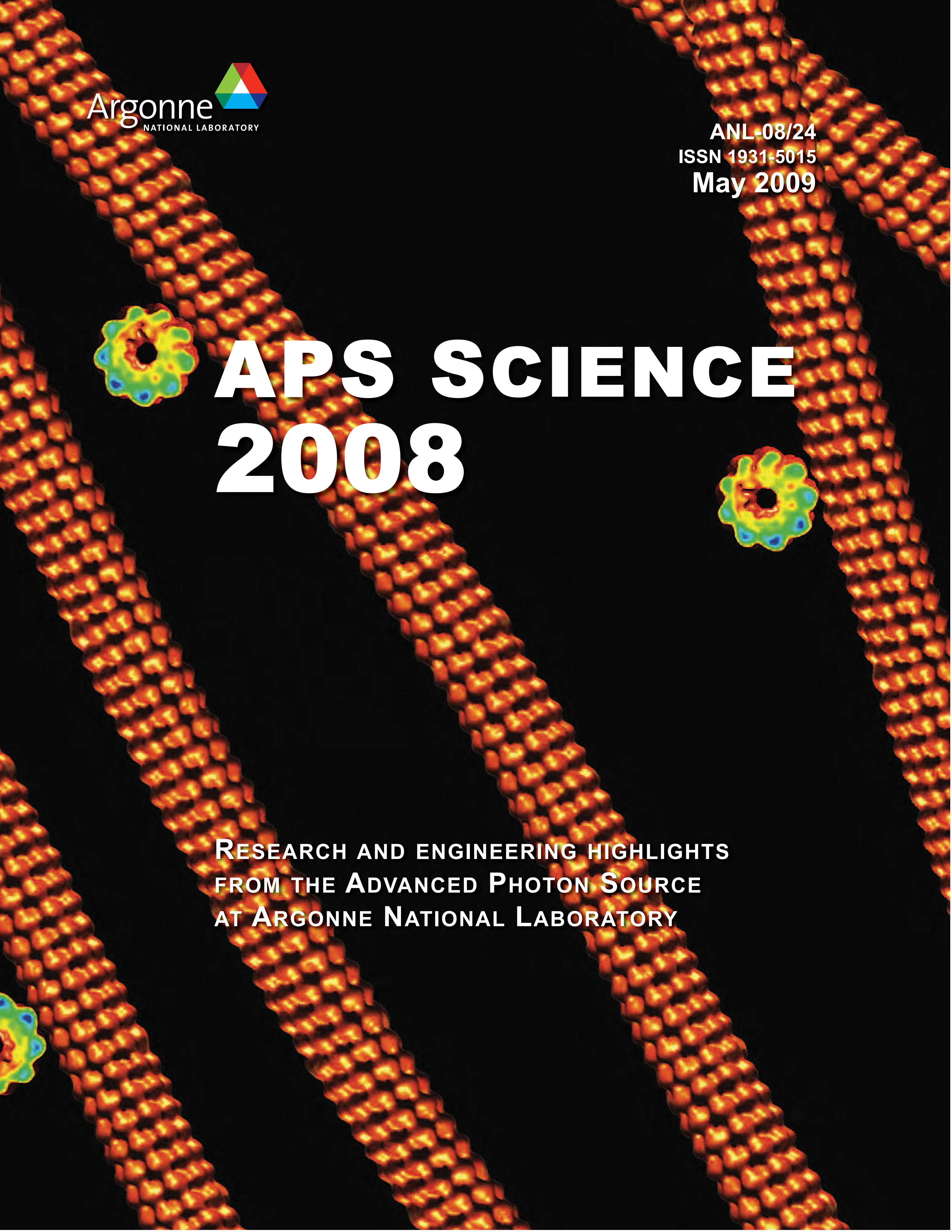

Argonne
NATIONAL LABORATORY

ANL-08/24
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May 2009

APS SCIENCE 2008

Research and engineering highlights
from the Advanced Photon Source
at Argonne National Laboratory

ANL-08/24
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About Argonne National Laboratory

Argonne is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC under contract DE-ACO2-06CH11357. The Laboratory's main facility is outside Chicago, at 9700 South Cass Avenue, Argonne, Illinois 60439. For information about Argonne and its pioneering science and technology programs, see www.anl.gov.

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On the cover: Segments of the potyvirus soybean mosaic virus; several virions are also shown in cross-section. The symmetry and low-resolution structure of this virus are very similar to those of the potexvirus potato virus X, suggesting that flexible filamentous plant viruses share a common coat protein fold and approximate helical symmetry. See the article "Revealing the Structural Secrets of Plant Viruses" on page 56.

Argonne
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May 2009

APS SCIENCE 2008

THE ANNUAL REPORT OF THE ADVANCED PHOTON SOURCE AT ARGONNE NATIONAL LABORATORY

About this enhanced version of *APS Science 2008* (Web connection required for all links):

- Referenced journal articles are linked to at least the paper's abstract (depending on subscription requirements)
- Hyperlinks are indicated by blue rectangles or complete URLs
- To access animations, QuickTime clips, or additional info, look for this icon (and the corresponding link[s]): ▮
- Email addresses for contact persons are live
- Includes list of 2008 APS publications
- Articles preceded by ** in the Table of Contents are expanded from the versions in the printed book

Argonne is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC
The Advanced Photon Source is funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences

THE ADVANCED PHOTON SOURCE FACILITY AT ARGONNE NATIONAL LABORATORY

The APS occupies an 80-acre site on the Argonne campus, about 25 miles from downtown Chicago, Illinois.
For directions to Argonne, see www.anl.gov/Visiting/anlil.html.

ACCESS TO BEAM TIME AT THE APS

Beam time at the APS can be obtained either as a general user (a researcher not associated with a particular beamline) or as a partner user (e.g., a member of a collaborative access team [CAT], a partner user proposer, or a member of a collaborative development team). If you are a CAT member, contact your CAT for instructions on applying for CAT beam time. At minimum, 25% of the time at all operating beamlines is available to general users, but many offer considerably more general user time—up to 80% on X-ray Operations and Research beamlines, for example.

How general users can apply for beam time at the APS:
1) First-time users should read the information for new users found on our Web site at http://www.aps.anl.gov/Users/Prospective/ before applying for beam time. Also, certain administrative requirements must be completed. In particular, a user agreement between the APS and each research-sponsoring institution must be in place.

2) To choose the appropriate technique(s) and beamline(s), see the beamlines directory in the "Data" section of this volume or at https://beam.aps.anl.gov/pls/apsweb/beamline_display_pkg.beamline_dir.

3) Submit a proposal via the Web-based system. Proposals are evaluated before each user run. For more information see the proposal system overview at: www.aps.anl.gov/Users/Scientific_Access/General_User/General_User_Proposal/Instructions/Proposer/.

CONTACT US

For more information about the Advanced Photon Source or to order additional copies of this, or previous, issues of *APS Science*, send an e-mail to apsinfo@aps.anl.gov, or write to APS info, Bldg. 401, Rm. A4115, Argonne National Laboratory, 9700 S. Cass Ave., Argonne, IL 60439. Visit the APS on the Web at www.aps.anl.gov.

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Future Light Sources

The APS Light Source

APS Users

lightsources.org For news from, and information about, light sources worldwide, visit www.lightsources.org

WELCOME FROM THE DIRECTOR

We at the Advanced Photon Source (APS) are immensely grateful for the support of the Department of Energy (DOE) and the U.S. Congress that has enabled us to operate fully even in this difficult economic environment, and for the prospect of future investment in the APS Renewal. Because APS researchers address key problems in energy, the environment, human health, and the economy, we have an important role to play in solving these problems for our nation and the world.

You can find inside this volume highlighted research that could lead to cleaner (page 54) or more efficient (pages 28, 30, and 50) energy, better energy storage (page 52), a better understanding of climate (pages 122 and 106,) improved health (pages 60, 62, 72, 78, and 84), new materials for manufacturing (page 47), information technology (pages 10 and 14), improved agriculture (pages 56 and 112) and civil engineering (pages 31 and 34). Other research addresses our curiosity as to where life came from (page 64) and how civilizations behaved 3,000 years ago (page 8).

With the support of our users; Argonne National Laboratory; the University of Chicago Argonne, LLC; and our sponsors in the DOE, we aim to remain at the forefront of x-ray science for the foreseeable future. To this end we arranged a workshop in October 2008 to identify the key scientific drivers for the renewal of the APS (page 65). "Members of the APS Scientific Advisory Committee [SAC] participated in the October 20-22, 2008, retreat to discuss and help structure the all-important renewal proposal for the APS. They took active part in the breakout sessions during the first two days and offered advice about the structure and content of the proposal during the close-out session," said our SAC chairman, Professor Miles Klein from the University of Illinois at Urbana-Champaign.

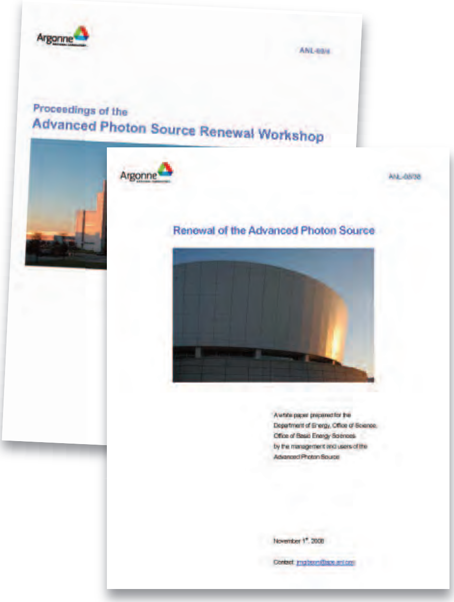
Professor Larry Lurio (Northern Illinois University), Chair of the APS Users Organization (APSUO) Steering Committee, noted: "Maintaining this impressive scientific output is one of the main challenges faced by the APS user community. As user programs continue to grow, access to the facility becomes increasingly competitive. While a healthy competition for beam time can strengthen the scientific program, the problem of limited access can also make it more challenging to nurture new science or to find dedicated time for the larger and most ambitious projects. The APSUO has worked over the past year to address these issues. We collaborated with APS management in developing plans so that experienced users, who can work more independently, may obtain beam time that might otherwise go unused. We also worked with the SAC to keep issues of beam time access in the forefront during scientific reviews. Most important, we coordinated and promoted advocacy efforts so that APS users can help inform the public and the U.S. Congress about the benefits of APS-supported research, and make the case for continued support for the facility."

The Advanced Photon Source Scientific Advisory Committee, January 20, 2009. Back row, l. to r.: Soichi Wakatsuki, High Energy Accelerator Research Organization (KEK); Laurence Lurio, Northern Illinois University, *ex officio;* Janos Kirz, Lawrence Berkeley National Laboratory; Denis T. Keane, Northwestern University, *ex officio;* Donald J. Weidner, Stony Brook University; Glenn A. Waychunas, Lawrence Berkeley National Laboratory; William G. Stirling, European Synchrotron Radiation Facility; Piero A. Pianetta, SLAC National Accelerator Laboratory; Dan A. Neumann, National Institute of Standards and Technology. Front row, l. to r.: Britt Hedman, Stanford Synchrotron Radiation Laboratory; J. Murray Gibson, Argonne National Laboratory; Miles V. Klein (Chair), University of Illinois at Urbana-Champaign; Wei Yang, National Institutes of Health. Not pictured: Howard M. Einspahr, Bristol-Myers Squibb (retired); Dame Louise N. Johnson, University of Oxford Laboratory of Molecular Biophysics.

Our partner users, in particular the collaborative access teams (CATs), remain a vibrant component of the APS. Denis Keane (Northwestern University), the Chair of our Partner User Council (PUC), reports: "The focus of much of the effort of the PUC in 2008 related to planning for the APS Renewal. Myself, as PUC chair, and Bob Fischetti [Argonne Biosciences Division], as Chair of the Life Sciences Council (a group formed this year to represent the life sciences CAT directors), both serve on the APS Renewal Steering Committee. Several PUC members responded to the call for beamline renewal proposals in March 2008. An informal pizza lunch—open to all beamline scientists from both X-ray Operations and Research (XOR) beamlines and non-XOR beamlines—was jointly sponsored by the PUC and the APSUO in June to facilitate communication from the APS 'floor' to the members of the Renewal Steering Committee. Many members of the PUC were either on the various renewal science teams or gave valuable input to the teams as they prepared their science cases over the summer of 2008. The PUC, in co-operation with the APSUO, worked with the APS on the October 2008 Renewal Workshop, with a joint APSUO/PUC meeting in September to review the preliminary renewal science cases before their presentation at the October workshop. The PUC will continue to work with the APS as the renewal takes shape so that the entire facility, including non-XOR beamlines, will see innovations and improvements to produce more high-impact science."

In this report you will also find descriptions of engineering and accelerator research and development work that is designed to keep the APS not only as reliable as possible, but also to enhance the performance. Long-range research and development focuses on the next-generation hard x-ray source, which could ultimately complement the APS, and we are particularly enthusiastic about the x-ray free-electron laser oscillator concept pioneered by Kwang-Je Kim and Yuri Shv'ydko (page 134).

J. Murray Gibson
(jmgibson@aps.anl.gov)



Proceedings of the
Advanced Photon Source Renewal Workshop

Renewal of the Advanced Photon Source

A white paper prepared for the
Department of Energy, Office of Science,
Office of Basic Energy Sciences
by the management and users of the
Advanced Photon Source

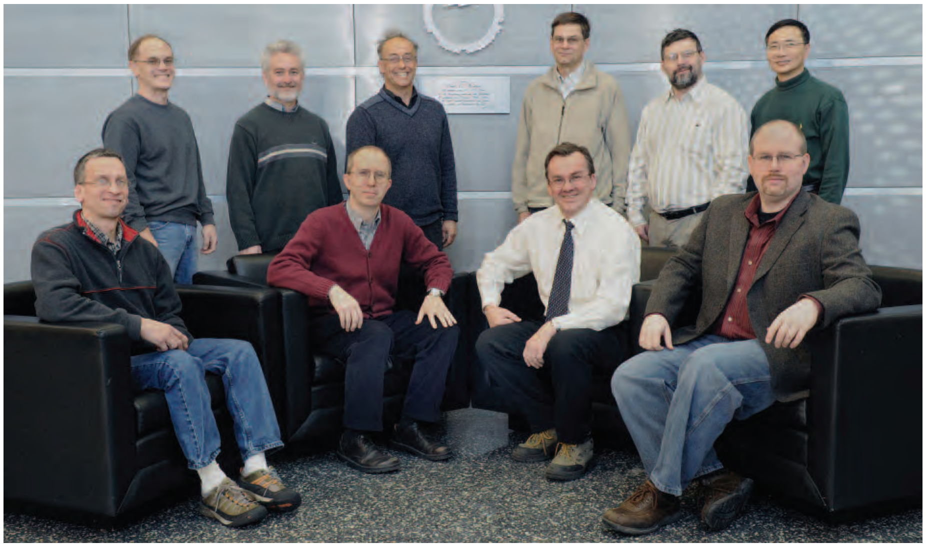
November 1st, 2008

Contact:

The white paper "Renewal of the Advanced Photon Source" is available online.

The "Proceedings of the Advanced Photon Source Renewal Workshop" are available online here. Printed copies can of either or both be obtained by sending a request to apsinfo@aps.anl.gov.

The Advanced Photon Source Users Organization Steering Committee, January 19, 2009. Back row, l.to r.: Linda Young, Argonne National Laboratory(ANL); Anne M. Mulichak, The University of Chicago; Peter J. Eng, The University of Chicago; David M. Tiede, ANL; Paul G. Evans, University of Wisconsin-Madison; Nino Campobasso, Glaxo SmithKline, Inc.; Nadia E. Leyarovska, ANL. Front row, l. to r.: J. Murray Gibson, ANL; Laurence Lurio (Chair), Northern Illinois University; Paul H. Fuoss (Vice-Chair), ANL; Susan B. Strasser, ANL. Not Pictured: Carl C. Correll, Rosalind Franklin University of Medicine and Science; Timothy J. Graber, The University of Chicago; Simon G.J. Mochrie, Yale University; Alfonso Mondragon, Northwestern University.



Present at the January 19, 2009, meeting of the Advanced Photon Source Partner User Council Executive Board were: Back row, l. to r.: John Chrzas, SER-CAT, University of Georgia; Robert F. Fischetti, GM/CA-CAT, Argonne National Laboratory (ANL); Mark L. Rivers, GSECARS, The University of Chicago; Keith E. Brister, LS-CAT, Northwestern University; Thomas C. Irving, Bio-CAT, Illinois Institute of Technology; Guoyin Shen, HP-CAT, Carnegie Institution of Washington. Front row, l. to r.: Jörg Maser, CNM/XOR, ANL; Denis T. Keane (Chair), DND-CAT, Northwestern University; J. Murray Gibson, Advanced Photon Source, ANL; Robert A. Gordon, PNC/XOR Advisory Board, Simon Fraser University. Not present for this meeting: Bruce A. Bunker, MR-CAT, Notre Dame University; Keith Moffat, BioCARS, The University of Chicago; P. James Viccaro, ChemMatCARS, The University of Chicago; Lisa J. Keefe, IMCA-CAT, The University of Chicago; Andrzej Joachimiak, SBC-CAT, ANL; Malcolm S. Capel, NE-CAT, Cornell University; John P. Hill, IXS-CAT, Brookhaven National Laboratory; Stephen R. Wasserman, SGX-CAT, SGX Pharmaceuticals, Inc.; Chris J. Benmore, BESSRC/XOR Advisory Board, ANL; Paul Fenter, BESSRC/XOR Advisory Board, ANL; J. Kent Blasie, CMC/XOR Advisory Board, University of Pennsylvania; Roy Clarke, MHATT/XOR Advisory Board, University of Michigan.

APS sectors:

Sectors 1-4: XOR 1-4
X-ray Operations and Research (XOR)

Sector 5: DND-CAT
DuPont-Northwestern-Dow Collaborative Access Team (CAT)

Sector 6: MU/XOR
Midwest Universities/XOR

Sector 7: XOR 7

Sector 8: XOR 8

Sector 9: XOR/CMC
XOR/Complex Materials Consortium

Sector 10: MR-CAT
Materials Research CAT

Sectors 11 and 12: XOR/BESSRC
XOR/Basic Energy Sciences Synchrotron Radiation Center

Sectors 13 through 15: CARS
Center for Advanced Radiation Sources:
  GeoSoilEnviroCARS—sector 13
  BioCARS—sector 14
  ChemMatCARS—sector 15

Sector 16: HP-CAT
High Pressure CAT

Sector 17: IMCA-CAT
Industrial Macromolecular Crystallography Association CAT

Sector 18: Bio-CAT
Biophysics CAT

Sector 19: SBC-CAT
Structural Biology Center CAT

Sector 20: XOR/PNC
XOR/Pacific Northwest Consortium

Sector 21: LS-CAT
Life Sciences CAT

Sector 22: SER-CAT
Southeast Regional CAT

Sector 23: GM/CA-CAT
General Medicine and Cancer Institutes CAT

Sector 24: NE-CAT
Northeastern CAT

Sector 26: CNM/XOR
Center for Nanoscale Materials/XOR

Sector 30: XOR/IXS
XOR/Inelastic X-ray Scattering

Sector 31: SGX-CAT
SGX Pharmaceuticals, Inc.

Sector 32: XOR 32

Sectors 33 and 34: XOR/UNI
XOR/University-National Laboratory-Industry

The Advanced Photon Source (APS), a national synchrotron radiation research facility at the U.S. Department of Energy's (DOE's) Argonne National Laboratory in Illinois, provides this nation's brightest x-ray beams for science. Research by APS users extends from the center of the Earth to outer space, from new information on combustion engines and microcircuits to new drugs and nanotechnologies whose scale is measured in billionths of a meter. The APS, which is funded by the DOE Office of Science, Office of Basic Energy Sciences, enhances America's competitiveness in such areas as superconductors, semiconductors, pharmaceuticals, polymers, and catalysts, and promises to have far-reaching impact on our technology, economy, health, and fundamental knowledge of the materials that make up our world.

At the APS, a "sector" comprises the radiation sources (potentially one of the two bending magnets, and one insertion device, although the number of insertion devices in the straight sections of the storage ring can vary), and the beamlines, enclosures, and instrumentation that are associated with a particular storage ring sector. The APS has 35 sectors, 34 of which are dedicated to user science and experimental apparatus. The 35th has limited space for instrumentation and is used primarily for accelerator-related studies.

X-ray Operations and Research (XOR) sectors comprise those beamlines operated by the APS. Some XOR sectors have historic CAT origins, e.g., XOR/PNC.

Collaborative access team (CAT) sectors comprise beamlines operated by independent groups made up of scientists from universities, industry, and/or research laboratories.

To access the APS as **general users** (GUs), researchers submit proposals that can be active for up to two years. These proposals are reviewed and rated by one of nine proposal review panels comprising scientific peers, generally not affiliated with the APS. Beam time is then allocated by either of two APS Beam Time Allocation Committees.

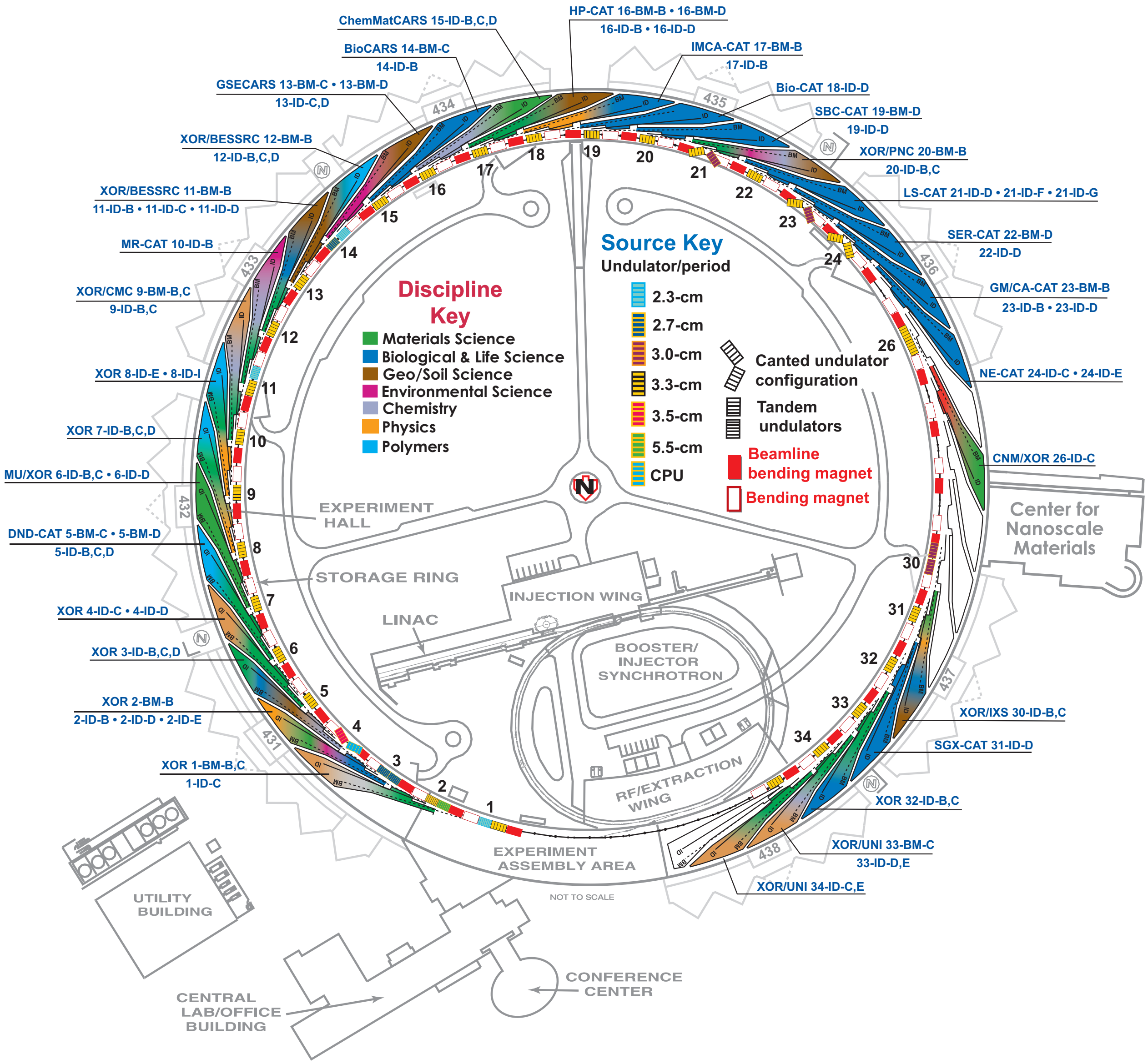
Those users who propose to carry out research programs beyond the scope of the GU program may apply to become **partner users** on any beamline operated by the APS. Prospective Partner User Proposals are peer reviewed by a subset of the APS Scientific Advisory Committee. Final decisions on the appointment of partner users are made by APS management.

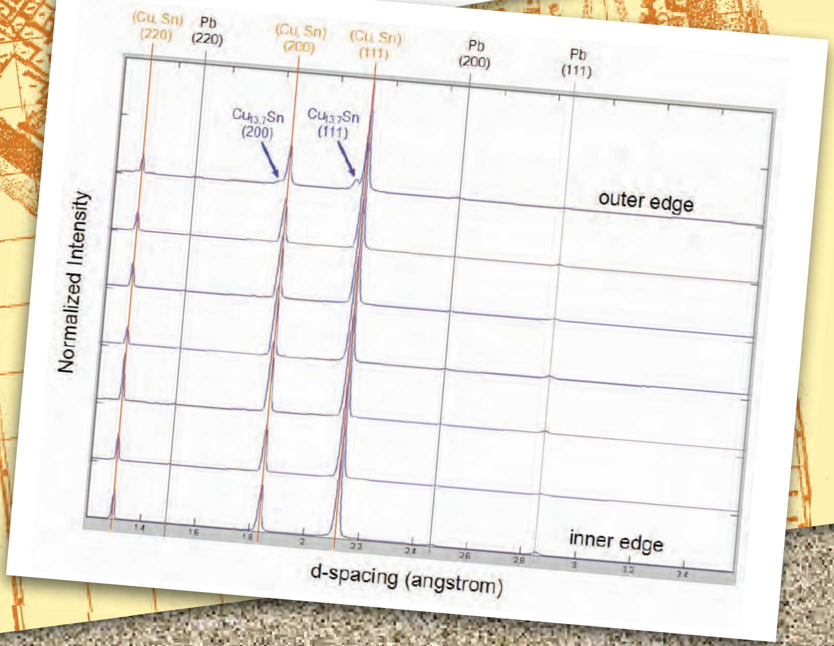
Beamlines, sector designations, disciplines, techniques, radiation sources, and general-user status for particular beamlines are displayed with the science highlights that follow.
This information in total can be accessed here

THE ADVANCED PHOTON SOURCE

Sector Allocations & Disciplines

Source Configuration





Photograph above: Excavating near the recently revealed city wall at Tell en-Nasbeh, 1927 (courtesy of the Badè Museum of Biblical Archaeology, Pacific School of Religion).

Fig. 1 (right top): O-shaped bangle 2665c from the Badè Museum collection at the Pacific School of Religion, 7 mm. diameter, 74.40 g, dating to the 10-6th century BCE.

Fig 2 (bottom right): Normalized intensity as a function of d-spacing for a typical bangle (2665c) at seven different positions from the inner edge to the outer edge of the bangle in 1 mm steps. Beam size: 100 x 100 μm^2.

Map of Tell en-Nasbeh (courtesy of Aaron J. Brody, Badè Museum of Biblical Archaeology, Pacific School of Religion).

BRINGING ANCIENT CULTURES TO LIGHT

An interdisciplinary team of researchers utilized two APS beamlines and a variety of synchrotron techniques to analyze the bronze alloys of Iron Age bracelets excavated in the 1930s at Tell en-Nasbeh, an archaeological site 12-km north of Jerusalem, which is associated with the Biblical town of Mizpah in Judah. The bracelets were used as mediums of exchange, symbols of wealth, and at times as utilitarian objects. The results of this journey back in time indicate that commerce often trumped hostilities in those ancient hills.

In the 1980s, Garman Harbottle, a senior chemist at Brookhaven National Laboratory, foresaw that synchrotron radiation could be used to solve questions about the composition, origins, and method of fabrication of ancient artifacts. In recent years, beamlines at the APS have been used to study ancient Chinese bronzes; astrolabes from Lahore, Pakistan; and now, these Iron Age bronze bracelets.

The non-destructive research at the APS revealed not only the composition and mode of fabrication of the original alloy, but when placed in an archeological and socioeconomic perspective, the findings also suggest that despite enmity between Judah and nearby Edom, trade between the warring kingdoms was thriving (Fig. 1).

The bracelets are part of a larger collection housed in the Badè Museum at the Pacific School of Religion in Berkeley, California. Five O-shaped bangles from Iron Age II (1,000-586 BCE) from family tombs outside the walls of the site were tested, while two C-shaped bangles tested were found on the tell itself and date from the late Iron Age (IIB) to the early Persian era (8-5th centuries BCE).

Chemical analysis of a bangle fragment performed in 1930-31 was deemed unreliable because drilling through the bangle's surface to the core introduced bits of corroded exterior material into the interior bulk material. Non-invasive, high-energy x-ray diffraction and x-ray fluorescence (XRF) at XOR beamline 1-ID allowed analysis in discrete steps from the corroded surface to the interior, revealing the composition of the original alloy. Most of the bangles were found to consist of lead, tin, and copper in four phases—Cu; Sn; an intermetallic phase, Cu13.7Sn; and Pb (Fig. 2).

The presence of lead in the bronze suggests that the metal workers may have discovered a means to create a strong, easily molded alloy while lowering the cost of production, as tin was a rare and costly metal imported from afar. The transition in composition from the surface to the core indicates that the molten alloy was subjected to rapid cooling. The bangles were formed in either rod-shaped molds, and then hammered into shape, or in circular-shaped molds. Residual strain in the bulk alloy could be the result of bending after casting, or from annealing after casting in a circular mold.

The research team used energy-dependent XRF at MR-CAT beamline 10-ID to detect the presence of arsenic, which has an energy level so close to that of Pb that traditional XRF measurements cannot distinguish between the two. None of the bangles contained more than trace amounts of arsenic, a likely indication that they were fabricated from a regional source. There were no mining activities at Nasbeh, but in the Iron Age, extensive mining and smelting took place at Wadi Feinan, a site in Edom about 300 kilometers SE from Nasbeh and a possible source of the leaded-tin bronze bangles. Thus, despite ongoing hostilities between Edom and Judah, economic trade between the two tribes likely occurred along well-established routes. — *Elise LeQuire*

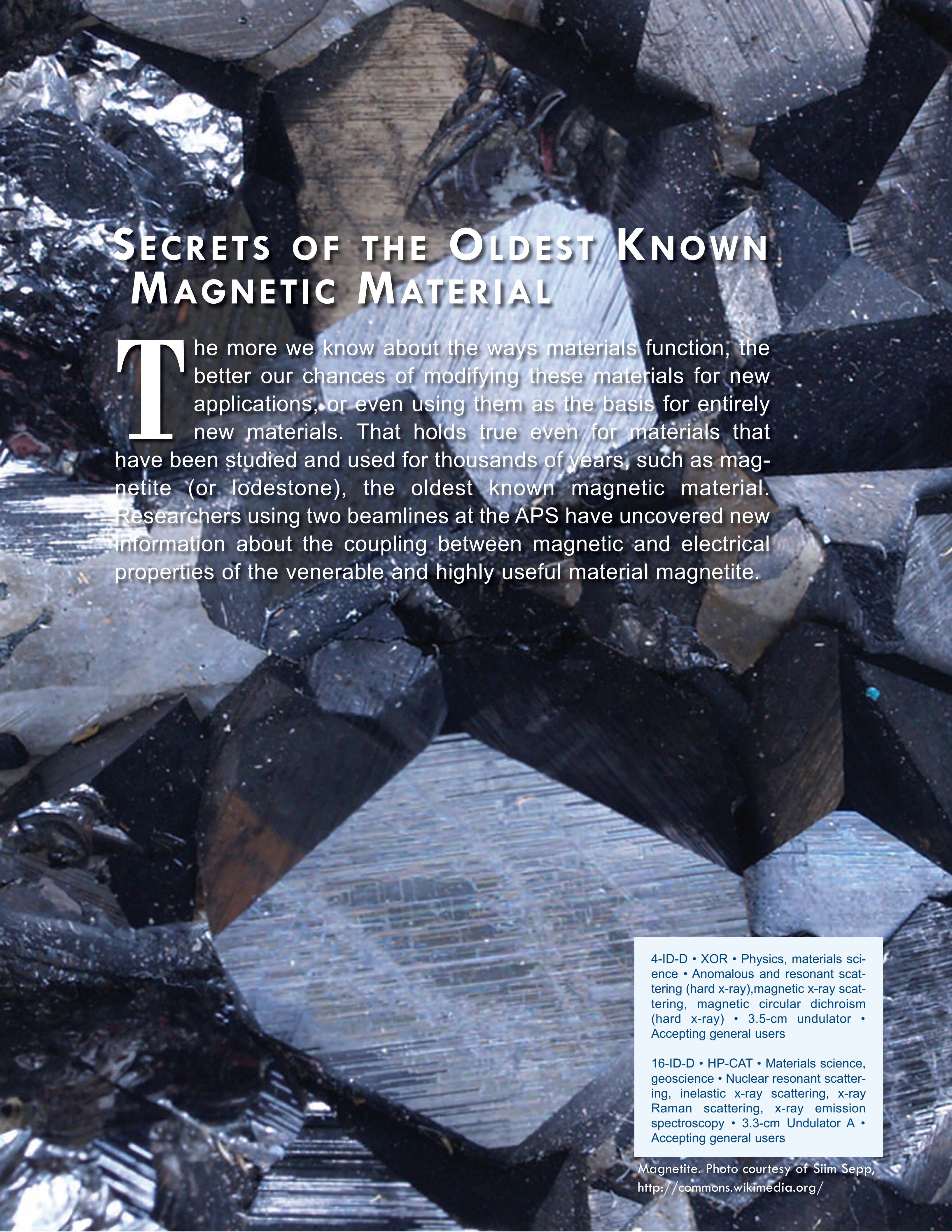
Learn more about this research here.

See: Elizabeth S. Friedman[1], Aaron J. Brody[2], Marcus L. Young[3], Jon D. Almer[4], Carlo U. Segre[1], Susan M. Mini[4,5], "Synchrotron radiation-based x-ray analysis of bronze artifacts from an Iron Age site in the Judean Hills," J. Archaeo. Sci. **35,** 1951 (2008). DOI: 10.1016/j.jas.2007.12.006
Author affiliations: [1]Illinois Institute of Technology, [2]Badè Museum of Biblical Archaeology, [3]Northwestern University, [4]Argonne National Laboratory, [5]Northern Illinois University
Correspondence: friedman@iit.edu

MR-CAT operations are supported by the U.S. Department of Energy (DOE) and the MR-CAT partnership of three universities (University of Notre Dame, University of Florida, and Illinois Institute of Technology), two Argonne National Laboratory Divisions (Chemical Sciences and Engineering, Environmental Research), the Environmental Protection Agency, and two companies (BP and UOP). Use of the Advanced Photon Source is supported by the DOE, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CHI1357.

1-ID • XOR • Materials science, physics, chemistry • High-energy x-ray diffraction • 3.3-cm Undulator A • Accepting general users

10-ID • MR-CAT • Materials science, environmental science, chemistry • Microfluorescence (hard x-ray), x-ray absorption fine structure (XAFS), diffraction anomalous fine structure, micro-XAFS • 3.3-cm undulator A • Accepting general users



Magnetite. Photo courtesy of Siim Sepp, http://commons.wikimedia.org/

SECRETS OF THE OLDEST KNOWN MAGNETIC MATERIAL

The more we know about the ways materials function, the better our chances of modifying these materials for new applications, or even using them as the basis for entirely new materials. That holds true even for materials that have been studied and used for thousands of years, such as magnetite (or lodestone), the oldest known magnetic material. Researchers using two beamlines at the APS have uncovered new information about the coupling between magnetic and electrical properties of the venerable and highly useful material magnetite.

4-ID-D • XOR • Physics, materials science • Anomalous and resonant scattering (hard x-ray),magnetic x-ray scattering, magnetic circular dichroism (hard x-ray) • 3.5-cm undulator • Accepting general users

16-ID-D • HP-CAT • Materials science, geoscience • Nuclear resonant scattering, inelastic x-ray scattering, x-ray Raman scattering, x-ray emission spectroscopy • 3.3-cm Undulator A • Accepting general users

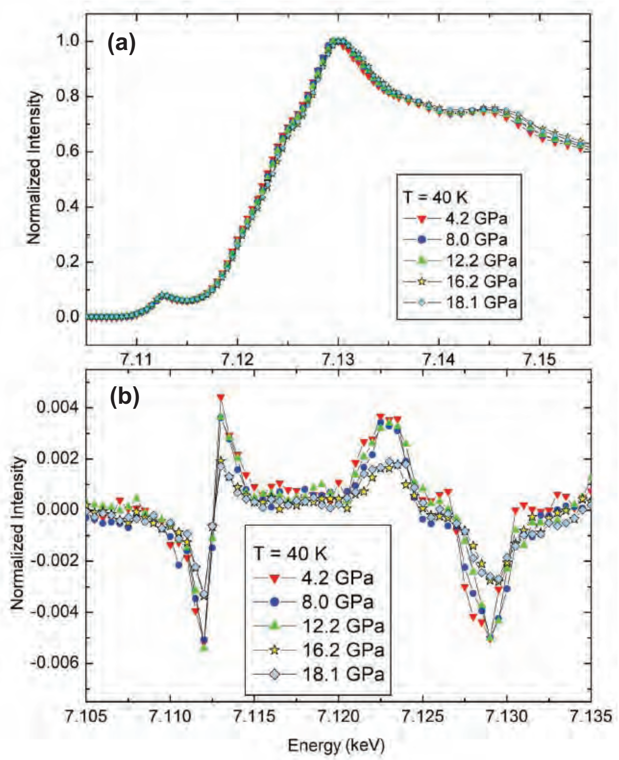


Fig. 1. (a) The normalized Fe K-edge x-ray absorption near edge structure (XANES) spectra of magnetite collected at 40K from 4.2 GPa to 18.1 GPa. (b) The corresponding normalized Fe K-edge x-ray magnetic circular dichroism spectra at the same P-T conditions.

A major ore of iron, magnetite (Fe_3O_4), was discovered more than 2,000 years ago by the Chinese and Greeks and was used as the first compass material for navigation. Magnetite plays vital roles in many natural phenomena, from the biological and geological sciences to materials science. Tiny crystals of magnetite are found in the skulls of migratory birds, which may explain how they use the Earth's magnetic field for navigation. Magnetotactic bacteria use tiny nanoparticles of magnetite to follow the geomagnetic field towards favorable oxygen-poor, nutrient-rich habitats in aquatic environments. Magnetite also has found its way into numerous modern-day technological applications such as magnetic recording media and ferrofluids used in magneto-rheological applications.

Despite being known and studied for a few thousands of years, magnetite remains at the forefront of condensed matter research because the intense interplay between charge, spin, and orbital degrees of freedom displayed by magnetite's electrons in this strongly correlated electron system makes the derivation of a microscopic picture of its coupled electrical, magnetic, and structural properties a rather difficult task.

Using a novel approach aimed at unraveling the secrets of magnetite, a collaboration of researchers from the Carnegie Institution of Washington, Argonne National Laboratory, and the Kirensky Institute of Physics combined diamond anvil cell techniques with high-brilliance, circularly-polarized x-rays to study the intricate coupling between electronic structure and magnetism in magnetite. Using special instrumentation recently developed at XOR beamline 4-ID-D at the APS, the researchers probed the magnetic state of magnetite up to applied pressures of 20 GPa (200,000 atm). While it was known that high pressure modifies the overlap of electronic wavefunctions and affects electron mobility in an unusual manner, the presence or absence of correlated magnetic effects and their impact on such electrical anomalies was unknown up to now, due to the difficulty in directly probing magnetic ordering under such extreme conditions. The researchers used a specialized diamond anvil cell featuring perforated diamond anvils to allow transmission of the relatively low-energy x-rays needed for measurements of the x-ray magnetic circular dichroism at the Fe K^{-} absorption edge (1s electron excitation at 7.112 keV).

The measurements revealed the presence of a sharp magnetic transition in the same pressure range where electrical anomalies occur in magnetite, providing unambiguous evidence of a strong interplay between the electronic and magnetic degrees of freedom. Furthermore, by combining the dichroism results with x-ray emission data taken at the HP-CAT beamline 16-ID-D at the APS (Fig.1), and theoretical cluster calculations, the researchers were able to pinpoint the origin of the magneto-electrical anomaly to changes in the electronic configuration of octahedrally-coordinated iron sites.

Their results clearly demonstrate that electron mobility is strongly tied to the precise electronic orbital- and spin-configuration in this strongly correlated electron system. By squeezing electronic orbitals together they were able to trigger electronic transitions that provided an understanding of the relevant interactions in magnetite.

The group thinks that this new ability to directly probe magnetic ordering at extreme pressure conditions will prove to be a very valuable tool for the materials and geological sciences alike. While other powerful techniques are available, including x-ray emission and Mossbauer spectroscopies, the x-ray magnetic circular dichroism technique is readily applied to most magnetic materials without the need for isotope enrichment, and provides a true measure of long-range magnetic order. — *Daniel Haskel & Richard Fenner*

See: Yang Ding[1]**, Daniel Haskel[2]*, Sergei G. Ovchinnikov[3,4], Yuan-Chieh Tseng[2], Yuri S. Orlov[4], Jonathan C. Lang[2], and Ho-kwang Mao[1], "Novel Pressure-Induced Magnetic Transition in Magnetite (Fe_3O_4)," Phys. Rev. Lett. **100**, 045508 (2008). DOI:10.1103/PhysRevLett.100.045508

Author affiliations: [1]Carnegie Institution of Washington, [2]Argonne National Laboratory, [3]Kirensky Institute of Physics, [4]Siberian Federal University

Correspondence:
*haskel@aps.anl.gov and
*yangding@aps.anl.gov

Use of the HP-CAT facility was supported by DOE-BES, DOENNSA (CDAC), NSF, and the W.M. Keck Foundation. Theoretical calculations were supported by RFBR Grant No. 07-02-00226 and by the Presidium of Russian Academy of Science Program ''Quantum Macrophysics.'. Use of the APS was supported by DOE-BES, under Contract No. DE-AC-02-06CH11357.

ANTIFERROMAGNET CHROMIUM REVEALS ITS ELECTRICAL PROPERTIES

Manipulating regions of *aligned* magnetic spins (domains) within ferromagnets, along with the interfaces separating them (walls), allows for the modification of electrical properties of magnetized materials. Such domain-structure modification happens often—through application of an external magnetic field and more recently by flowing current—to control charge transport within spintronic systems, such as the magnetic read heads within hard drives. Fewer manipulations, however, have been performed on the domain structures of antiferromagnets (AFM). The structures of antiferromagnets, in contrast to ferromagnets, possess *opposed* magnetic spins for neighboring electrons. Because of this difference, antiferromagnets do not possess a net magnetic field and, therefore, are more difficult to modify and control. Researchers using two APS beamlines studied whether electrical properties of AFM chromium, the only element known to be an antiferromagnet, depend on the spin configuration in a way similar to ferromagnets. Their work may lead to new applications of antiferromagnets in such areas as advanced magnetic recording materials and technologies. As the physical and chemical nature of antiferromagnetic materials is better understood, the technological potential of antiferromagnets can be more fully applied within nanometer-scale devices in computing and communications.

Two distinct spin-related electrical effects were observed in chromium—shown as thermal hysteresis in the longitudinal and Hall resistivity—one caused by quantization of spin-density waves (SDW) due to finite film thickness in thin films, and another caused by magnetic domain-wall scattering of electrons in thick films. Because such chromium spin-effects are as large as in ferromagnets, their work reveals tunable electrical effects as a function of film thickness.

The researchers grew chromium films of various thicknesses by using magnetron sputtering on magnesium oxide substrates. X-ray diffraction was used to measure the films as both single-crystal and epitaxial. The longitudinal and Hall resistivity were measured for various thicknesses (3,500 Å, 506 Å, 430 Å, and 175 Å) of the chromium films. The researchers used the Quantum Design Physical Property Measurement System, along with a 9-T superconducting magnet, to perform electrical measurements. The charge-density wave measurements were performed at the XOR 4-ID-D beamline and the XOR/UNI 33-BM beamline, both at the APS.

The researchers found, as expected, that the electrical resistivity of chromium drops with decreasing temperature. They also uncovered a decrease in the carrier density at the Néel temperatures of between 280K (lower Néel temperature for films) and 311K (bulk Néel temperature).

Film disorder lessened the resistivity anomaly at the Néel temperature associated with the loss of carriers. The disorder also affected the lower-temperature Hall coefficient. Changes to the flat regions of the Fermi surface caused by Fermi surface nesting appeared most evident in the Hall coefficient and somewhat evident in the resistivity, but to almost no extent in the Hall conductivity. When passing the thermal phase transition at the Néel temperatures, a constant value for the Hall conductivity was observed. The researchers concluded that antiferromagnetic order affects primarily the flat regions of the Fermi surface.

The investigators discovered that chromium electrical behavior differs during heating and cooling. This difference indicates that the metal possesses a slight but distinct internal rearrangement of electrons and their spins. For all samples below the Néel temperature, the longitudinal resistivity and Hall coefficient are larger during cooling than during warming. The result counters the assumption that antiferromagnetic order is the single cause of hysteresis.

The researchers also found that as film thickness decreases, only a certain allowed number of SDW nodes occur. Moreover, as temperature decreases, SDW node numbers abruptly increase by one (Fig. 1). Because an energy barrier is present, the temperature at which the SDW node increases by one is lower upon cooling than warming, which leads to thermal hysteresis in the node numbers. By employing synchrotron x-ray diffraction, the researchers

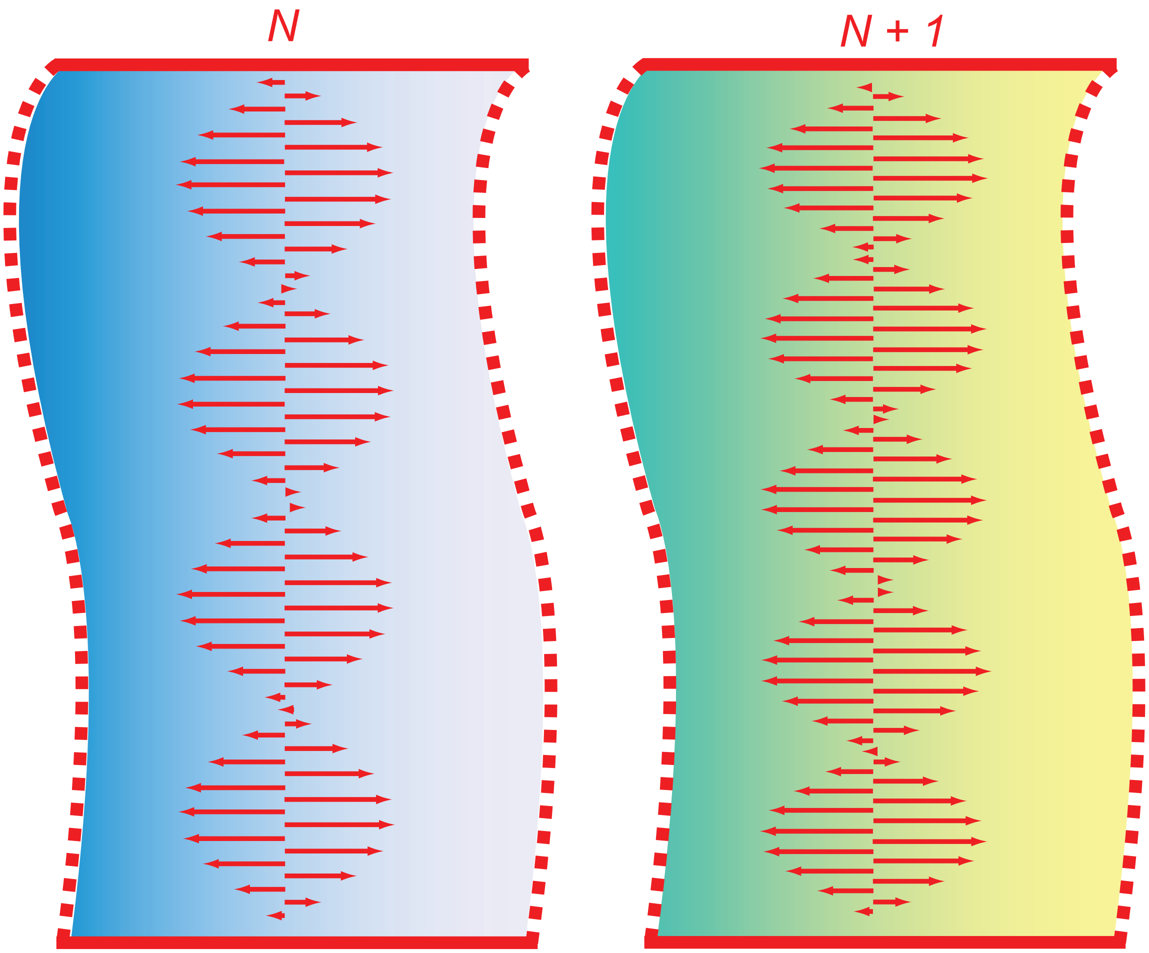


Fig. 1. Schematic diagram of change in the number of SDW nodes. The horizontal boundaries indicate the film surfaces, which impose boundary conditions on the charge density wave such as a node (as shown in the diagram) or an antinode.

verified that SDW node changes produce spikes in the resistivity.

As warming progressed at certain temperature windows in regions of hysteresis, a larger charge carrier density appeared compared to that of cooling. This finding implies that an increase in SDW node results in a greater free-carrier density due to a reduction in the amplitude of the SDW. Computer simulations confirmed the dependence of SDW amplitude upon film thickness (with increased node numbers).

The researchers found that electron scattering by neighboring domain walls had an impact on both resistivity and hysteresis for thick films. Because they found hysteresis is not dependent on the applied field (as measured up to 9 T), they concluded that directionally dependent resistance is probably not the dominant cause of hysteresis. As the domains freeze at low temperature, so does thermal hysteresis.

In summary, varying the film thickness allows for a controllable range of reactions—from quantized density wave predominant (thin film) to domain wall predominant (thick film).

— William Arthur Atkins and Patricia E. Panatier

See: Ravi K. Kummamuru[1,‡] and Yeong-Ah Soh[1*], "Electrical effects of spin density wave quantization and magnetic domain walls in chromium," Nature **452**(17), 859 (April 2008). DOI: 10.1038/nature06826

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33-BM • XOR/UNI • Materials science, physics, chemistry • Anomalous and resonant scattering (hard x-ray), diffuse x-ray scattering, powder diffraction, x-ray reflectivity, general diffraction, grazing incidence diffraction • Bending magnet • Accepting general users

4-ID-D • XOR • Physics, materials science • Anomalous and resonant scattering (hard x-ray), magnetic x-ray scattering, magnetic circular dichroism (hard x-ray) • 3.5-cm undulator • Accepting general users

Is Graphene a New Paradigm for Electronic Circuits?

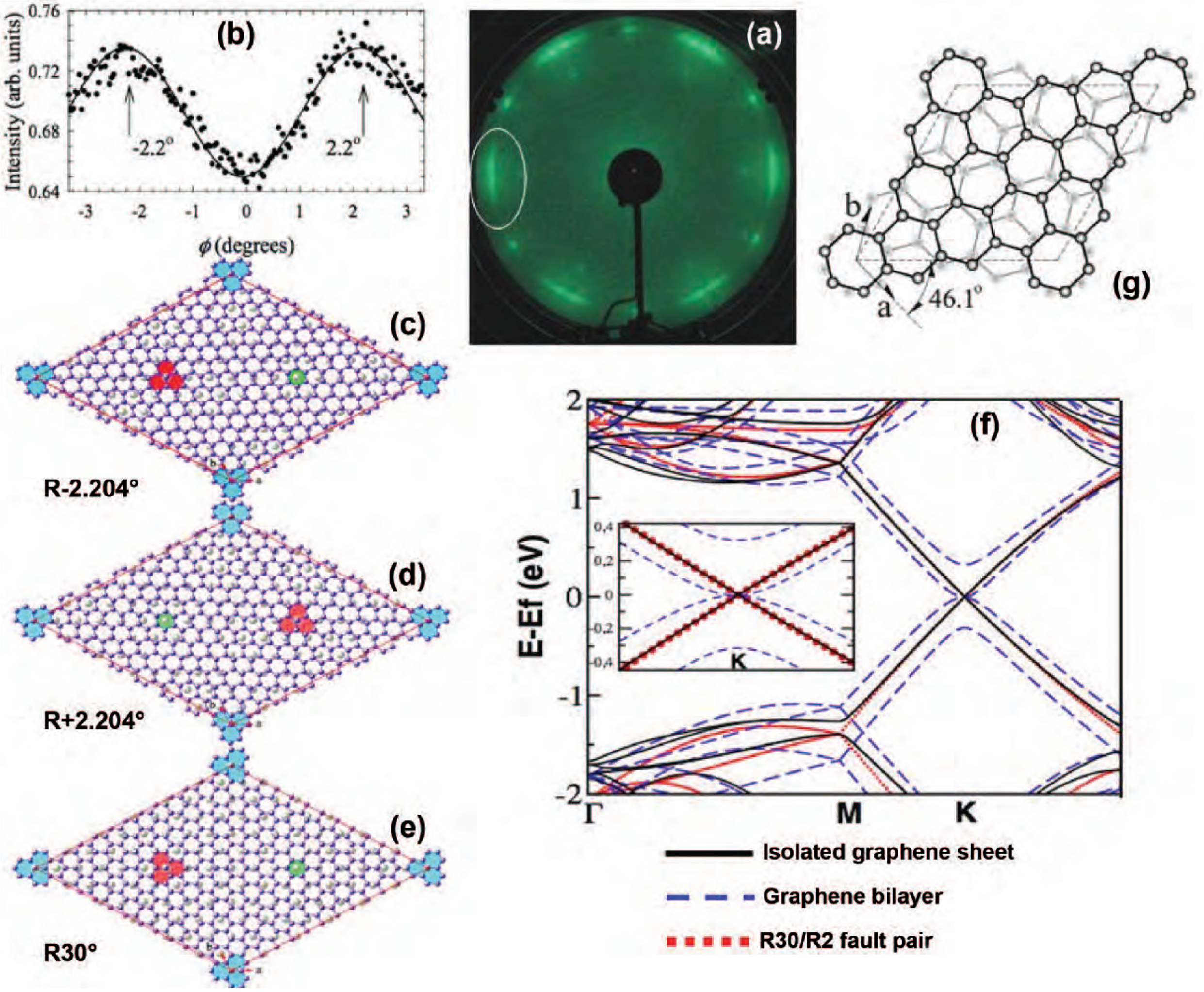

Fig. 1. (a) A low-energy electron diffraction (LEED) pattern from a 10-graphene-layer film grown on the C-face of SiC. The diffuse rings at the graphene radius are due to rotational stacking faults. (b) An x-ray azimuthal scan over the portion of the ring circled in the LEED image in (a). The intensity is peaked at ±2.2°. These rotational angles are the two additional ways (other than a 30° rotation) that a $\sqrt{13} \times \sqrt{13}$ graphene sheet can be commensurate with the SiC surface. These commensurate structures are shown in (c), (d), and (e). Making a stacking fault with the either of the two R±2.2° graphene orientations on top of the R30 structure leads to a new graphene/graphene commensurate structure (g). This structure behaves electronically like an isolated graphene sheet, as demonstrated by the calculated band structure shown in (f).

A recent experimental study suggests it may be possible to use an all-graphene system as a new archetype for electronic circuits. The question, explored by a group of researchers from the Georgia Institute of Technology and the Institut Néel in Grenoble, France, was whether graphene sheets could be lithographically cleaved into ribbons that could then be used to make gates and wires. With the aid of the MU/XOR 6-ID-B and -C beamlines at the APS, The group discovered that nature provides a stacking sequence in C-face-grown films that has the electronic symmetry of an isolated, single-layer graphene sheet. The research also points to an explanation as to why magnetotransport and infrared magnetotransmission measurements on C-face-grown graphene give the same results as those obtained from an isolated graphene sheet. Furthermore, it provides an explanation for prior experimental results that showed single-layer electronic properties, even for epitaxial graphene films tens of layers thick.

The trick, it turned out, was to successfully grow wafer-scale graphene on a substrate while preserving the electronic properties of an isolated graphene sheet. This was done using epitaxial graphene on an SiC(000$\bar{1}$) substrate, where typically 5- to 10-graphene-layer films are obtained. These films are characterized by having high charge carrier mobility similar to highly doped graphene single layers. However, this was surprising given that graphitic stacking would tend to break the equivalency of the sub-lattice atoms in the graphene sheet, and therefore the multilayers should not exhibit the electronic properties observed. The challenge, then, was to identify the source of the single-layer electronic properties, in both the transport region and the undoped multilayer.

C-face epitaxial graphene can grow with layers rotated in three different forms: (R30), and (R2±). The group prepared all the 4H-SiC(000$\bar{1}$) substrates and performed the surface x-ray diffraction (SXRD) at the 6-ID-B and -C beamlines at 16.2-eV of beam energy.

In the past, C-face graphene was thought to be highly disordered azimuthally due to streaking present on low-energy electron diffraction images. However, upon closer inspection of the diffraction data the group found that the streaks were not due to random rotational disorder. Instead, they found that while it was well known graphene only grows epitaxially in the R30 phase, an SXRD azimuthal scan taken at the radial position of the rod showed intensity peaks at ±2.2°. The stacking of these three rotational phases is crucial to understanding the electronic properties of the films, and their key discovery using surface reconstruction measurements by scanning tunneling microscopy was that the R30 and the R2± sheets are interleaved in a multilayer graphene film, giving rise to a high density of R30/R2± fault pairs, instead of the expected AB stacked R30 or R2± isolated domains. This high density of fault pairs is apparently due to the fact that the graphene-SiC interaction makes the production of these faults more ubiquitous, and it is expected that at least one rotational fault pair must exist near the graphene surface; further SXRD measurements confirmed the fault pairs were present throughout the film.

The electronic properties of the graphene films are expected to change significantly in areas where the fault density is high, because only two atoms per sheet out of the 52 in the faulted cell are in positions of high symmetry (one over the other), and therefore the interplanar interactions will be weaker at the locations of the fault. To gain a better understanding of this, density functional theory detailed calculations of the band structure of an R30/ R2± fault pair were carried out. It was found that the main difference in the electronic structures of the three graphene forms appeared near the K-points of the dispersion curves. While the band structure of the isolated graphene sheets showed gapless linear Dirac dispersion of the π bands at the K-point, the A-B stacked layers lifted the sublattice symmetry, thereby splitting the π bands and giving rise to parabolic bands, as shown in Fig. 1. This implies that in the rotated layers, the atoms on the A and B sublattices can be thought to be identical, and therefore the linear character of the dispersion at the K-point will hold for infinite stacks of graphene fault pairs.

This important study may also explain why magnetotransport and infrared magnetotransmission measurements on C-face-grown graphene give the same results as those obtained from an isolated graphene sheet, and it has provided an explanation to prior experimental results that showed single-layer electronic properties, even for epitaxial graphene films tens of layers thick. — *Luis Nasser*

See: J. Hass[1], F. Varchon[2], J.E. Millán-Otoya[1], M. Sprinkle[1], N. Sharma[1], W. A. de Heer[1], C. Berger[1,2], P.N. First[1], L. Magaud[2], and E.H. Conrad[1]*, "Why Multilayer Graphene on 4*H*-SiC000$\bar{1}$ Behaves Like a Single Sheet of Graphene," Phys. Rev. Lett. **100**, 125504 (28 March 2008).
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6-ID-B,C • MU/XOR • Physics, materials science • Anomalous and resonant scattering (hard x-ray), liquid scattering, magnetic x-ray scattering, powder diffraction, general diffraction, grazing incidence diffraction, surface diffraction (UHV) • 3.3-cm Undulator A • Accepting general users

STRONG ELECTRIC FIELDS DISTORT FERROELECTRICS AND STRETCH THEORY

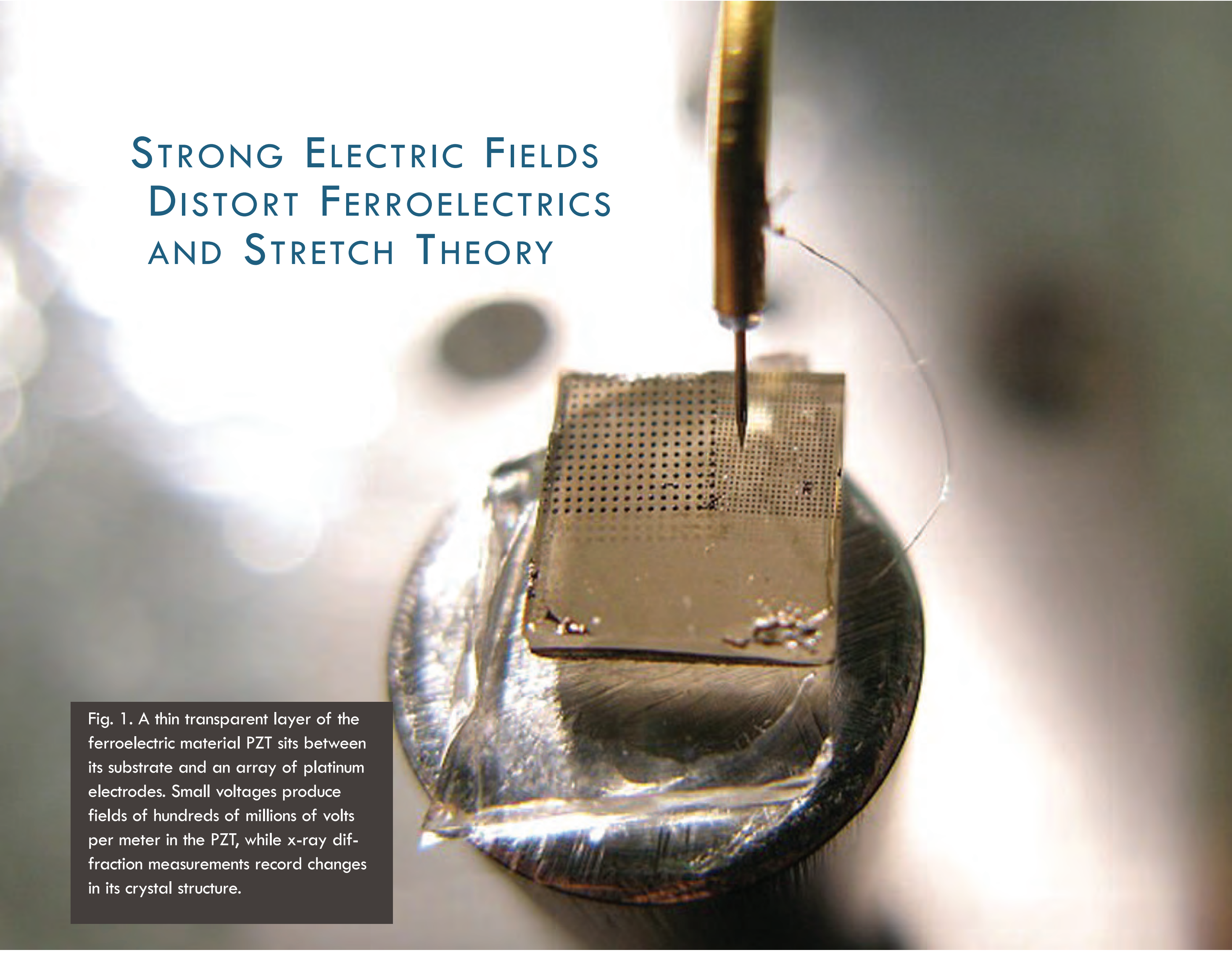

Fig. 1. A thin transparent layer of the ferroelectric material PZT sits between its substrate and an array of platinum electrodes. Small voltages produce fields of hundreds of millions of volts per meter in the PZT, while x-ray diffraction measurements record changes in its crystal structure.

Modest voltages applied across the small distances occurring in nanoscale structures can produce electric fields as high as hundreds of millions of volts per meter. Fields of this strength can significantly alter the properties of many materials and even modify their crystal structure. Working at XOR beamline 7-ID at the APS, researchers have used time-resolved x-ray diffraction to measure changes in the piezoelectric response of thin films of a ferroelectric material at high electric fields. Their findings should help refine the theoretical understanding of these materials and also promote practical applications by characterizing their behavior in a new regime.

Just as ferromagnets exhibit spontaneous magnetization, ferroelectrics possess a spontaneous electric polarization. They are also piezoelectric, so that strain changes their polarization, and an applied electric field distorts their crystal lattice. In the case of lead titanate ($PbTiO_3$), a model ferroelectric, theoretical arguments suggest two contrasting effects at high electric fields. One prediction is that larger polarization within the material will make the lattice more rigid and steadily decrease the dielectric coefficient, the response of the material to the applied field, as the field strengthens. According to this prediction, the dielectric coefficient should fall significantly at a field strength of 100 MV/m. The other prediction, however, is that at

***"Fields"** continued on page 18*

PROBING DYNAMIC CHANGES IN SOLIDS

A phonon is a collection of vibrations that moves through a crystal lattice. Acoustic phonons have been extensively studied, using ultra-short laser pulses and time-resolved x-ray diffraction (TRXD). But these phonons tended to have low-wave vectors, which could be detected using standard light-scattering techniques. Researchers using the APS have found a way to directly detect high-wave vector phonons by looking at the sidebands from synchrotron-based TRXD. Their work extends science's ability to use acoustic phonons as probes to investigate heat transport and other important characteristics of bulk materials.

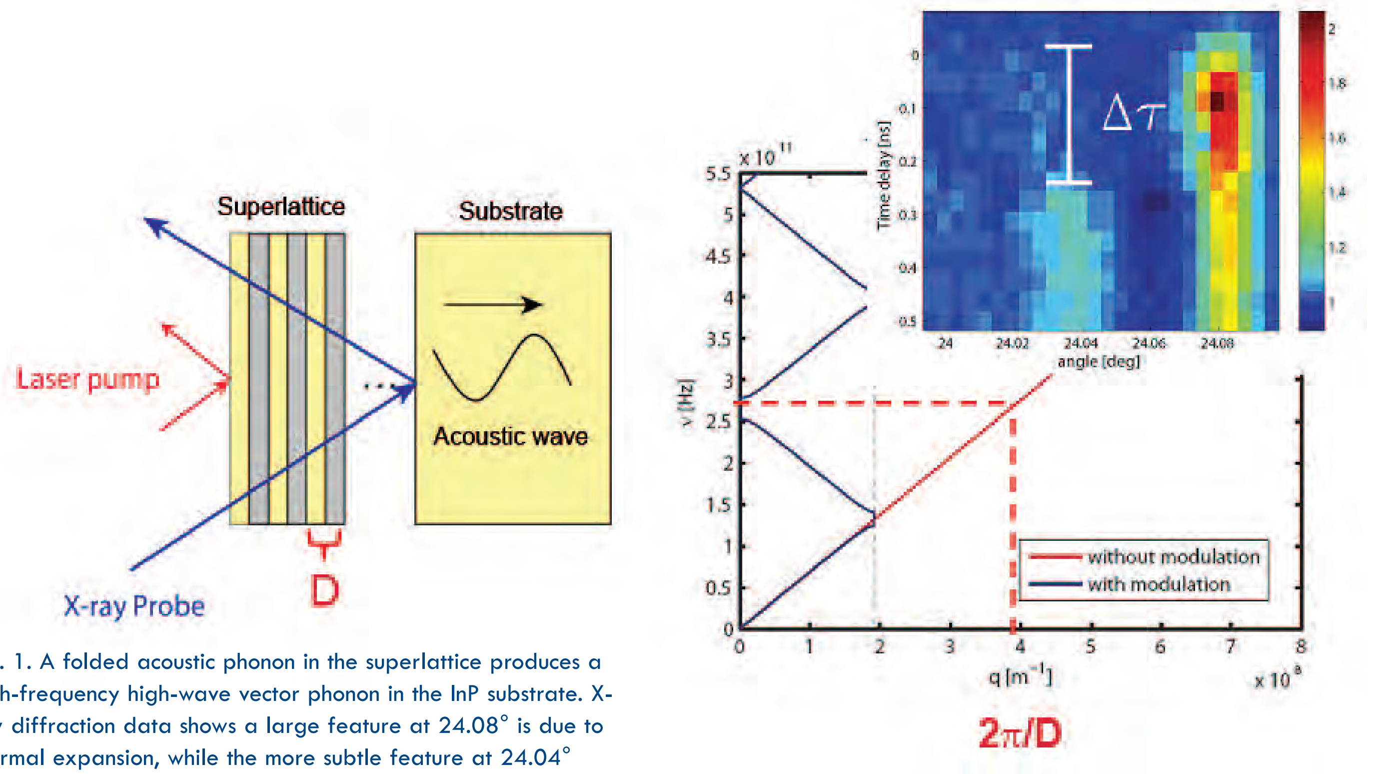

Fig. 1. A folded acoustic phonon in the superlattice produces a high-frequency high-wave vector phonon in the InP substrate. X-ray diffraction data shows a large feature at 24.08° is due to thermal expansion, while the more subtle feature at 24.04° results from unfolded phonons in the substrate.

No material is a perfect insulator. In solids that are thermal insulators, heat travels via vibrations that can be modeled as high-frequency acoustic phonons. Because these phonons have short wavelengths, researchers have used them to probe tiny structures with features smaller than a micron, and because they have lower energies than photons at comparable wavelengths, phonon probes are far less likely to damage the material. In addition to probing very small structures, this approach also revealed what goes on at the interface between two materials.

Researchers know how to make acoustic phonons by focusing ultrafast laser pulses onto a material. But to achieve the high-wave vector phonons, researchers from the University of Michigan and Argonne used a trick: First, the laser pulses were absorbed by a thin-film superlattice to excite high-frequency modes through the folding of the acoustic branches. Then the folded phonon was transferred across the interface into the bulk material, producing a high-frequency phonon in the bulk material. In this case, the group shot 50-fs-long pulses of near-infrared light from a titanium-doped sapphire laser at a superlattice made of 60 pairs of GaInAs and AlInAs layers, grown on an indium phosphide substrate.

To detect acoustic phonons, researchers often use light scattering or TRXD. High-wave vector phonons are inaccessible to light-scattering methods in the bulk because of the long wavelength of the light compared with the wavelength of these phonons. Therefore, the use of TRXD was crucial. This method has been used in other studies as a sensitive probe of the ultrafast atomic motion associated with coherent phonons, and other researchers have used it to study

"Dynamic" continued on page 18

“Dynamic” *from page 17*

phonons in superlattices.

The Michigan/Argonne team used synchrotron-based TRXD to detect propagating bulk modes with high-wave vector that originated as zone-folded modes in a superlattice. As the phonon moved through the solid, the atoms shifted (like the surface of water rising and falling as waves pass), but detecting the displacement of atoms directly required very short x-ray pulses. (The Linac Coherent Light Source, scheduled to come online in 2009, will be able to provide x-ray pulses short enough to directly detect these photons.) Without a good source for direct detection, the researchers instead looked for indirect evidence of the phonon, which appeared as a sideband to the x-ray diffraction peak. The hard x-ray probe pulses came from the XOR 7-ID beamline at the APS, and had an energy of 10.3 keV, which is below the absorption edge of gallium.

In the future, these researchers plan to continue with the acoustic phonon work. They want to detect phonons from the entire Brillouin zone, which could potentially provide complete information on the forces between the atoms at all lengths scales with ultrafast time resolution.

–Yvonne Carts-Powell

See: M. Trigo[1],* Y.M. Sheu[1], D.A. Arms[2], J. Chen[1], S. Ghimire[1], R.S. Goldman[1], E. Landahl[2,‡], R. Merlin[1], E. Peterson[1], M. Reason[3], and D.A. Reis[1], “Probing Unfolded Acoustic Phonons with X Rays,” Phys. Rev. Lett. **101**, 025505 (11 July 2008).
DOI: 10.1103/PhysRevLett.101.025505

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7-ID • XOR • Materials science, atomic physics, chemistry • Time-resolved x-ray scattering, radiography, time-resolved x-ray absorption fine structure • 3.3-cm Undulator A • Accepting general users

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“Fields” *from page 16*

some still larger field strength, the lattice will abruptly distort, increasing the length ratio of one side of the unit cell with respect to another and resulting in a larger dielectric coefficient.

To test these predictions, researchers from the University of Wisconsin-Madison, Oak Ridge National Laboratory, and Argonne National Laboratory probed 35-nm-thick films of $PbZr_{0.2}Ti_{0.8}O_3$ (PZT) on a substrate of strontium titanate, with a thin electrode layer sandwiched underneath the PZT and platinum electrodes attached to the top (Fig. 1). They used PZT rather than pure lead titanate because it has superior electrical and mechanical properties for these experiments.

Because sustained strong fields would destroy the thin PZT film, the researchers applied electric pulses lasting 35 to 50 nsec to create fields with strengths up to about 500 MV/m. To observe the resulting strain on the PZT lattice, bursts of 10-keV x-rays for diffraction measurements were synchronized with the electric pulses. The maximum strain observed in this way was 2.7%, extremely large for any ferroelectric.

Contrary to the first prediction, the piezoelectric response remained linear for fields up to almost 200 MV/m. From 200 MV/m to about 400 MV/m, diffraction measurements indicated a lattice distortion consistent with the second prediction, and the dielectric coefficient grew to as much as 10% above its low-field value. But at still higher field strengths, it decreased again.

The apparent disagreement with theory is not alarming, the researchers say, because predictions for bulk $PbTiO_3$ do not straightforwardly apply to a thin film of PZT. Not only is the material different, but attachment to a substrate places constraints on the way its lattice can move. The researchers are planning further experiments to go to higher field strengths and characterize more precisely the lattice distortions that are created.

Understanding the nonlinear behavior that occurs in PZT and related materials could help designers aiming to build tunable nanoscale components for electronic devices. The nonlinearities seen in PZT so far are modest, the researchers say, but other ferroelectrics may display bigger changes in their properties in large electric fields. — *David Lindley*

See: Alexei Grigoriev[1], Rebecca Sichel[1], Ho Nyung Lee[2], Eric C. Landahl[3], Bernhard Adams[3], Eric M. Dufresne[3], and Paul G. Evans[1]*, “Nonlinear Piezoelectricity in Epitaxial Ferroelectrics at High Electric Fields,” Phys. Rev. Lett. **100**, 027604 (18 January 2008).
DOI: 10.1103/PhysRevLett.100.027604

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SUPERCONDUCTIVITY IN SILANE

As science seeks to find efficient superconducting wires and metals at inexpensively-achieved temperatures, the possibility of turning hydrogen into a superconductor has remained out of reach, requiring pressures a third again as high as what is possible in the lab. With the help of an x-ray beamline at the APS, scientists have, for the first time, created a superconductor out of a hydrogen-dominant material: a hydride called silane, which is normally a gas at room temperature. The silane entered a metallic phase with a close-packed, hexagonal atomic structure at the relatively low pressure of 50 GPa, and at a temperature of 17K. These results could be a step toward the goal of more affordable superconducting materials.

The researchers, from the Max Planck Institute for Chemistry and the University of Saskatchewan, carried out their synchrotron x-ray research on the GSECARS 13-ID beamline at the APS. Their work followed on theoretical predictions in 2006 of similar structure of metallic silane; however, the original work predicted metallization at much higher pressures, i.e., greater than 250 GPa. There is little previous experimental data on these hydrogen-rich compounds at high pressures.

The team studied ten samples of silane at pressures up to nearly 200 GPa, using Raman scattering, electrical resistance measurements, optical absorption and x-ray powder diffraction. Electrical resistance dropped sharply between 50 and 65 GPa, and upon cooling the sample became superconducting at 7K. That temperature went up, however, as the pressure went up, suggesting that even higher superconducting temperatures are achievable.

Because the metallization pressures were lower than predicted, the team also closely studied the silane’s structure. X-ray diffraction could provide exact positions of the silicon atoms, but not those of hydrogen. However, the close-packed arrangement of the silicon atoms—in four tight tetrahedrons and two larger octohedral cages—required a unique set of positions of the eight hydrogen atoms in each unit. Four hydrogen atoms lie at the tetrahedral interstices and two each are inside the octahedrons.

Under pressures greater than 120 GPa at room temperature, the sample entered a transparent or insulating phase. This transformation from metal to insulator is very unusual, if not unique, as the sequence is normally opposite: going from insulator to metal under high pressures.

Because bringing hydrogen into the superconducting range would require pressures upwards of 400 GPa—substantially higher than the 300 GPa currently achievable in the lab—the metallization of hydrogen-dominant silane opens

“Silane” *continued on page 22*

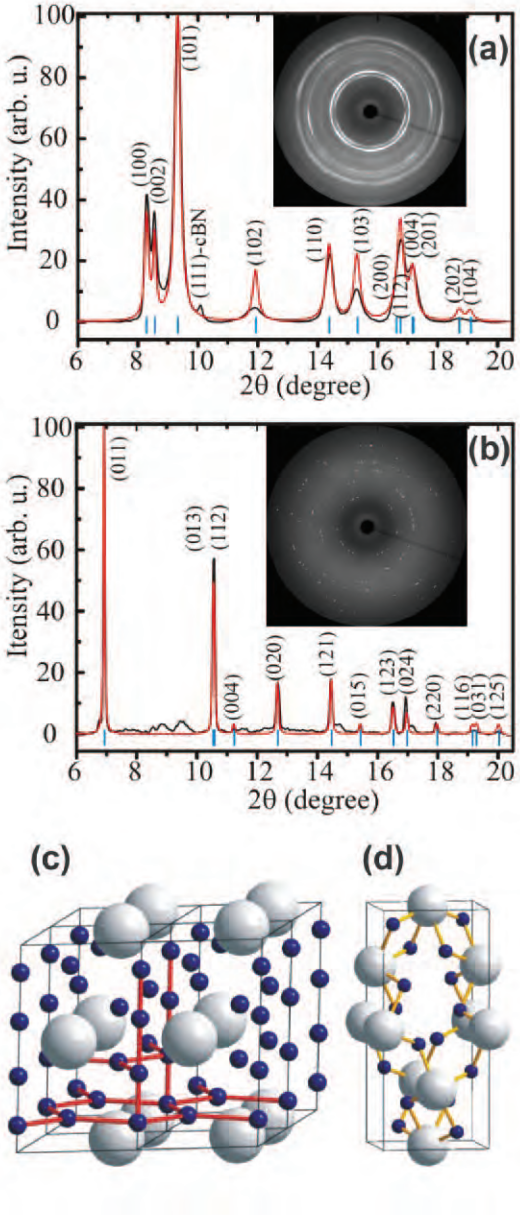

Fig. 1. X-ray diffraction patterns of metallic (a) and transparent (b) phases of SiH_4 at 113 GPa and 160 GPa, respectively. The black solid lines are experimental profiles, while red solid lines are calculated for the P63 structure. The experimental integrated diffraction pattern is on panel (b). Asterisks on (c) indicate features from metallic phase coexisting with I41/a phase. Gray spheres on (c) and (d) represent silicon atoms, and the blue spheres hydrogen atoms. The hydrogen sublattice in the metallic P63 structure is shown by red lines.

PRESSING THE SUPERCONDUCTING ISSUE IN CUPRATES

High-temperature superconductivity (high T_c) is still a mysterious phenomenon in many ways, yet its vast potential makes it one of the busiest and most exciting areas of research in condensed matter physics. But that potential won't be fully realized until a much better understanding of the underlying mechanisms can be achieved, and this remains one of the great unresolved questions of physics. Research at an APS beamline has pinpointed a pressure at which dramatic changes are induced in a sample superconducting material, opening the potential for a host of new research into high-T_c phase transitions.

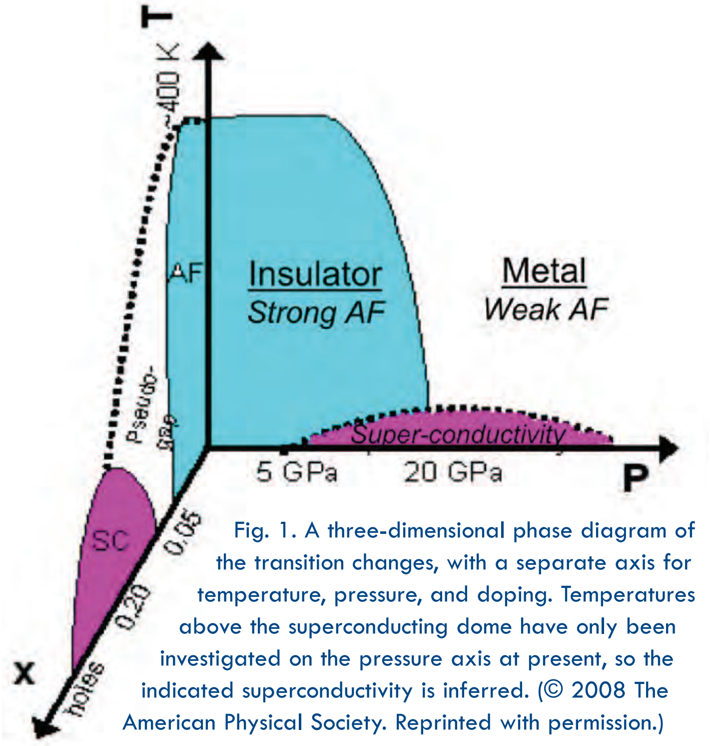

Fig. 1. A three-dimensional phase diagram of the transition changes, with a separate axis for temperature, pressure, and doping. Temperatures above the superconducting dome have only been investigated on the pressure axis at present, so the indicated superconductivity is inferred. (© 2008 The American Physical Society. Reprinted with permission.)

Part of the difficulty in understanding the underlying mechanisms of high-T_c superconductivity is that the crystalline structure of the materials that display high-T_c superconductivity tends to be highly complex and difficult to model, making the characterization of the nature and processes of the crucial T_c (the critical temperature below which superconductivity appears) transition quite challenging.

Generally, as with semiconductors, the particular capacities of the usual high-temperature superconducting compounds such as the cuprates are controlled via doping. But that's an impractical and awkward method for studying transitions in the laboratory. Another way to examine and tune the electronic structure and transitions in a high-T_C compound is by subjecting it to another variable that can be more readily controlled in the laboratory, such as pressure.

Using this strategy, re-searchers from Stanford University, the Carnegie Institution of Washington, the University of Waterloo, and the National Institute of Advanced Industrial Science and Technology subjected a common high-T_c compound, a form of BSCCO (bismuth strontium calcium copper oxide) and also a Mott insulator, to pressures of up to 35 GPa using Raman spectroscopy and x-ray diffraction. They induced and observed changes that are strongly similar to those associated with optimal doping.

Working at the HP-CAT 16-ID-B beamline at the APS, the team examined single crystals of $Bi_{1.98}Sr_{2.06}Y_{0.68}CU_2O_{8+\delta}$ in a diamond anvil cell and obtained Raman spectra and x-ray diffraction data. Because Raman spectroscopy requires no direct physical contact, it avoids the limitations of other techniques (that use a probe tip in contact with the sample under study) in examining the critical point of a specimen under pressure in a DAC experimental setup.

The team observed a pressure-driven electronic transition at ~21 GPa that featured a sudden increase in electron-phonon coupling and a linear electronic background. The Raman spectra showed a decided weight shift from high to low frequencies, with a softening in phonon and magnon activity. The linear incompressibility of the c-axis also showed a break in continuity at the ~21 GPa pressure.

The fact that so many related physical quantities abruptly change at this pressure clearly indicates that they are driven by a single low-energy feature, such as a change of topology in the Fermi surface. The group concludes that a continuous second-order transition, probably a Lifshitz type, is the most likely explanation. Such a topological change in the Fermi surface accompanied by an increase in mobile charge carriers has been seen in cuprates across optimal doping with Hall effect measurements. They

"Cuprates" *continued on page 22*

THE ROLE OF HO IN THE MAGNETISM WITHIN MULTIFERROIC HOMNO$_3$

In a magnetoelectric multiferroic compound, both electric polarization and magnetic order can be controlled with the use of an applied magnetic field. The ability to control magnetic properties by external electric fields, and vice versa, offers an extra degree of freedom in the design of actuators, sensors, and data storage devices. (Applying an electric field is particularly easy and fast for nonvolatile memory devices.) Single-crystalline HoMnO$_3$ (holmium manganite) has been proposed as a material with such dual effects. However, detailed studies have not been performed regarding the role of the magnetic holmium ions (Ho^{3+}) in the magnetic response and ordering. So researchers used two APS beamlines to study the Ho^{3+} magnetism in HoMnO$_3$ with respect to the magnetic order without field and to the response on a magnetic or electric field. Their results show that an applied electric field does not couple to the Ho magnetism.

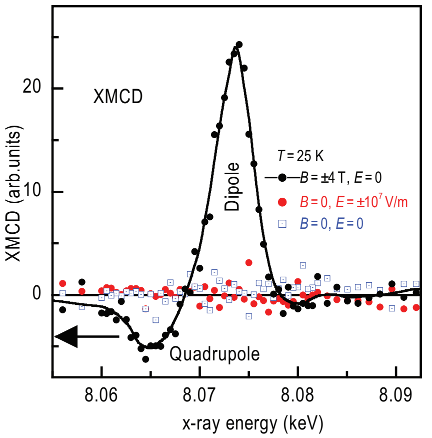

Fig. 1. XMCD spectra at the Ho L$_{III}$ absorption edge measured with and without electric (*E*) and magnetic (*B*) fields.

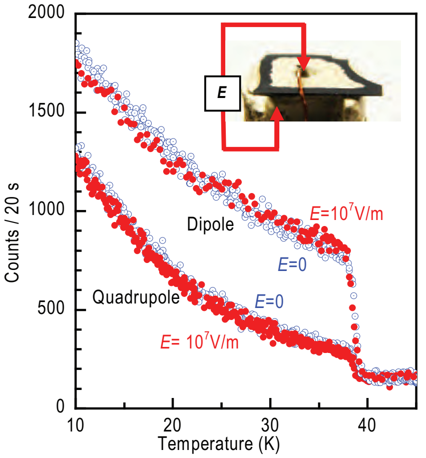

Fig. 2. Effect of an applied electric field (*E*) on the (0 0 9) magnetic peak. Inset shows the sample (dark/black) coated with silver (white) on top and bottom as electrodes, to apply the electric field.

The researchers, from Ames Laboratory at Iowa State University and Argonne, employed element-specific x-ray magnetic circular dichroism (XMCD) and x-ray resonant magnetic scattering (XRMS) techniques at low temperatures to separate the Ho^{3+} from the Mn^{3+} magnetism. Below a temperature of 40K (-388° F or -233° C), the Ho^{3+} moments order antiferromagnetically. They also undergo a transition to another antiferromagnetic structure at temperatures below 4.5K (-451.6° F or -268.7° C). When a magnetic field was applied, a ferromagnetic response of the Ho^{3+} moments could be observed, whereas in the presence of an electric field with a value of 1 × 10^7 volts/meter (V/m), no ferromagnetic response from Ho^{3+} ions could be detected (Fig. 1). In addition, the antiferromagnetic structure remains unchanged in an applied field. Therefore, the researchers conclude that Ho^{3+} ions do not play a role in the ferromagnetic response of HoMnO$_3$ within an applied electric field. Hence, the proposed mechanism behind the control of magnetism by an external electric field should be revisited.

The researchers used a floating-zone method to produce the single crystal of HoMnO$_3$. The crystal, with a polished surface perpendicular to the hexagonal **c** direction, was mounted in a cryostat to reach low temperatures. The researchers analyzed the magnetic resonance at the Ho L$_{III}$ absorption edge in their XMCD experiment by using the XOR beamline 4-ID-D at the APS, and in the XRMS experiment by using the XOR beamline 6-ID-B, also at the APS. Below a temperature (T) of 40K, the magnetic Ho^{3+} moments cause a first resonance peak at the quadrupole energy just below the Ho L$_{III}$ absorption edge, and a second one at the dipole energy just above the Ho L$_{III}$ edge (Fig. 1). When the researchers applied a magnetic field, the resonant peaks in the XMCD spectrum flipped signs, indicating a ferromagnetic response of the Ho^{3+} moments to the applied magnetic field. In contrast, an applied electric field did not change the XMCD spectrum at all.

A similar behavior was observed in the detailed study of the magnetic structure using the XRMS technique. In the absence of a field, and below a temperature of 40K, the Ho^{3+} moments are aligned in the hexagonal **c** direction, with opposite directions between the nearest neighbors in the **c** direction as well as in the (**ab**) plane. In addition, they undergo a transition to another antiferromagnetic structure when the temperature is below 4.5K.

Specifically, just below 40K, the diffraction peak intensities of the dipole and quadrupole resonances increase abruptly; this is followed by a much more gradual increase in both intensities down to a temperature of 4.5K. In

“Magnetism” continued on page 22

***“Silane”** from page 19*

doors to investigation of a heretofore relatively unstudied new superconducting material. The researchers hope that the new insights they find will help to create superconductors that can operate at higher temperatures.

— *Karen Fox*

See: M.I. Eremets[1]*, I.A. Trojan[1], S.A. Medvedev[1], J.S. Tse[2], and Y. Yao[2], “Superconductivity in Hydrogen Dominant Materials: Silane,” Science **319**, 1506 (14 March 2008).
DOI: 10.1126/science.1153282
Author affiliations: [1]Max Planck Institute für Chemie, [2]University of Saskatchewan
Correspondence: *eremets@mpch-mainz.mpg.de

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13-ID • GSECARS • Geoscience, environmental science • Microfluorescence (hard x-ray), x-ray absorption fine structure (XAFS), microdiffraction, micro-XAFS, high-pressure diamond anvil cell, high-pressure multianvil press, inelastic x-ray scattering • 3.3-cm Undulator A • Accepting general users

***“Cuprates”** from page 20*

believe that this is similar to the abrupt increase in Raman background and electron-phonon coupling seen here.

This transition and its accompanying phenomena also strongly resemble the critical point during optimal doping of the cuprate compound, as the Raman spectroscopy data show. But because the pressure environment can be controlled and tuned more precisely than a doping process in the laboratory, the present technique allows the transition changes at the critical point T_c to be studied and characterized to a much finer degree than previously possible. The work thus demonstrates the great possibilities of extending such pressure-tuned techniques to a wide range of other condensed-matter studies of the high-T_c phase transition.

— *Mark Wolverton*

See: T. Cuk[1]*, V.V. Struzhkin[2], T.P. Devereaux[3], A.F. Goncharov[2], C.A. Kendziora[4], H. Eisaki[5], H.-k. Mao[2], and Z.-X. Shen[1], “Uncovering a Pressure-Tuned Electronic Transition in $Bi_{1.98}Sr_{2.06}Y_{0.68}\ CU_2O_{8+\delta}$ using Raman Scattering and X-Ray Diffraction,” Phys. Rev. Lett. **100**, 217003 (30 May 2008).
DOI: 10.1103/PhysRevLett.100.217003
Author affiliations: [1]Stanford University, [2]Carnegie Institution of Washington, [3]University of Waterloo, [4]Naval Research Laboratory, [5]National Institute of Advanced Industrial Science and Technology
Correspondence: *cukster@gmail.com

The work at Carnegie was supported by DOE/NNSA and DOE/BES Grant No. DE-FG02-02ER45955 and No. DE-FC03-03NA00144. A. F.G. and V.V. S. acknowledge the financial support of the Carnegie Canada Foundation. The Stanford work was supported by DOE Office of Science, Division of Materials Science, with contract No. DE-FG03-01ER45929-A001. T. P. D. acknowledges support from NSERC, CFI, and the Alexander von Humboldt Foundation. C. A. K. acknowledges support from the NRL/ONR. Use of the HP-CAT facility was supported by DOE-BES, DOE-NNSA (CDAC), NSF, DOD-TACOM, and the W. M. Keck Foundation.Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

16-ID-B • HP-CAT • Materials science, geoscience • Microdiffraction, powder diffraction, single-crystal diffraction, high-pressure diamond anvil cell • 3.3-cm Undulator A • Accepting general users

***“Magnetism”** from page 21*

addition, a change in the magnetic ordering of the Ho^{3+} ions was seen as the peak intensities changed at 4.5K. Above 40K, however, magnetic peaks did not occur.

Concerning the antiferromagnetic structure in an applied electric field, the researchers compared the temperature dependence of both dipole and quadrupole resonances without a field and with electric fields of up to a value of 1×10^7 V/m, obtained when a voltage of up to 1,500 V was applied (Fig. 2). The curves are identical and prove that the antiferromagnetic structure is not changed by an applied electric field.

Based on these results, and together with the absence of a ferromagnetic signal in the XMCD experiment, the researchers conclude that an applied electric field does not couple to the Ho magnetism.

— *William Arthur Atkins and Patricia E. Panatier*

See: S. Nandi[1]*, A. Kreyssig[1], L. Tan[1], J.W. Kim[1], J.Q. Yan[1], J.C. Lang[2], D. Haskel[2], R.J. McQueeney[1], and A.I. Goldman[1], “Nature of Ho Magnetism in Multiferroic $HoMnO_3$,” Phys. Rev. Lett. **100**, 217201 (30 May 2008).
DOI: 10.1103/PhysRevLett.100.217201
Author affiliations: [1]Ames Laboratory and Iowa State University, [2]Argonne National Laboratory
Correspondence: *nandi@iastate.edu

The work at Ames Laboratory and use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

4-ID-D • XOR • Physics, materials science • Anomalous and resonant scattering (hard x-ray), magnetic x-ray scattering, magnetic circular dichroism (XMCD hard x-ray) • 3.5-cm undulator • Accepting General Users

6-ID-B,C • MU/XOR • Physics, materials science, anomalous and resonant scattering (hard x-ray), liquid scattering, magnetic x-ray scattering, general diffraction, grazing incidence diffraction, surface diffraction (UHV), 3.3-cm Undulator A • Accepting General Users

“SCIENCE CAREERS IN SEARCH OF WOMEN”

Every year, the Argonne Women in Science and Technology program, with support from the Argonne Division of Educational Programs, organizes a day-long conference at the Laboratory entitled “Science Careers in Search of Women” for female high school students (mainly sophomores and juniors) from the greater Chicago, IL, area. One of the day’s events is a tour of a facility at Argonne. The 350 to 400 young women who attend can choose from among about a dozen tours, one of which is at the APS.

On the 2008 APS tour, the students and some of their teachers were given an overview of the facility and learned what a light source is, the types of research that are carried out at the facility, and how that research benefits society. They also learned some of the technical aspects of producing x-ray beams for researchers. After being divided into smaller groups, the students were given a closer look at insertion devices, the main control room, vacuum technology, and strong permanent magnets. The students also visited an x-ray beamline for a glimpse of research being carried out. Throughout the tour, the students were encouraged to ask questions.

Advanced Photon Source personnel who participate in giving the tour each year work in a variety of different capacities, including engineering, physics, x-ray science, computers, and design/drafting, and serve as an interface between users and the APS facility. This gives the young women an opportunity to see some of the many fields of specialization that contribute to the building and running of a facility such as the APS, and to hear about some of the fun and exciting challenges in scientific, engineering, and technological careers from female and male role models. *Contact Liz Moog (moog@aps.anl.gov)*

Above: Magnetic Devices Group Leader Liz Moog (foreground, Accelerator Systems Division) provides students with an overview of the APS experiment hall.

Left: Beamline scientist Dean Haeffner (X-ray Science Division) explains a research station on the APS experiment hall floor.

Below: Accelerator physicist Marion White (Accelerator Systems Division) demonstrates different types of magnets and their effects.

LOOKING FOR PIEZOELECTRICITY IN ITS PUREST FORM

Piezoelectricity is where you find it. First discovered in naturally-occurring minerals in the 19th century, it is the property of certain materials to polarize or generate an electrical voltage under strain. It has proven to be one of nature's most useful and handy gifts to humanity, and is used to create everything from microphones to cigarette lighters, to name a couple of its more mundane applications. But a more sophisticated use of the phenomenon in complex devices requires the precise engineering of custom-made piezoelectric materials structured in various ways at the atomic level. Researchers using an APS x-ray beamline have developed a technique that has the potential for creating less expensive, more versatile piezoelectric materials for use in a wide range of sophisticated applications.

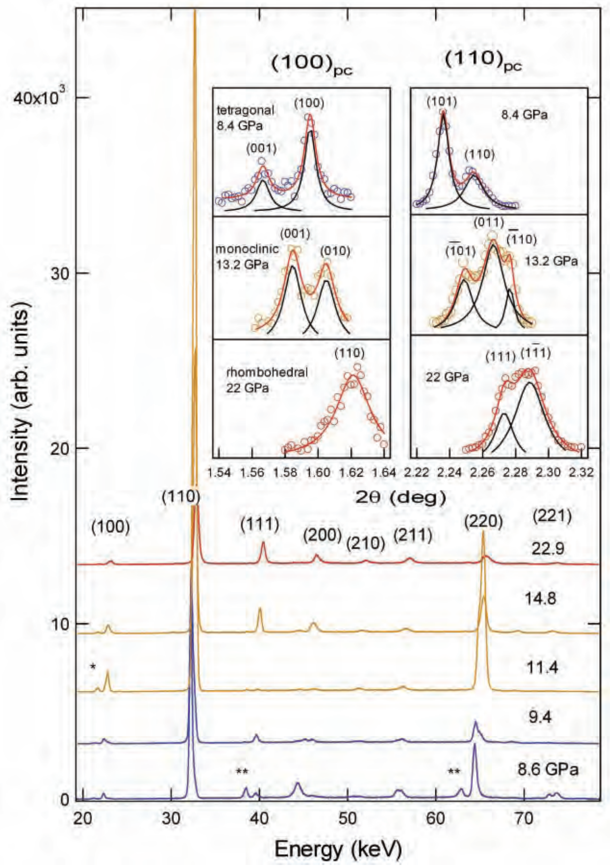

Fig. 1. Pressure dependence of energy dispersive and high-resolution angle-dispersive x-ray diffraction spectra at selected pressures at 10K. The energy dispersive results shown are insufficient for identifying the phases. The single asterisk represents the ghost peak and the double asterisks represent the Au peaks. The major reflection lines were indexed with a pseudocubic symmetry (pc). For instance, the pseudocubic (110) reflection splits into a doublet in the tetragonal phase and a quadruplet in the monoclinic phase. The inset shows high-resolution diffraction data at different pressures: the left panels show the pseudocubic (100) reflection at 8.4 GPa (tetragonal phase), at 13.2 GPa (monoclinic phase, the (100) reflection is missing) and at 22 GPa (rhombohedral phase); the right panels show the pseudocubic (110) reflection at 8.4 GPa (tetragonal phase), at 13.2 GPa (monoclinic phase, the (101) reflection is missing), and at 22 GPa (rhombohedral phase). (© 2008 Nature Publishing Group)

These more complex materials generally manifest their high electromechanical coupling through the formation of morphotropic phase boundaries (MPBs), regions where rhombohedral symmetry is separated from tetragonal symmetry and where the phase transition permits the rotation of polarization characteristic of piezoelectricity.

> This technique has the potential for creating less expensive, more versatile piezoelectric materials for use in a wide range of sophisticated applications

The more complex the material, the more expensive and difficult it is to produce. While one of the most commonly used piezoelectric materials, lead zirconate titanate, can be made in different compositions depending on its intended application, it cannot be made in single crystals, a fact that limits its application. New high-coupling piezoelectric single crystals such as lead magnesium niobate-lead titanate melt incongruently, and thus form zoned single crystals. If the development of a

"Looking" continued on page 26

A NEW COLLECTIVE EXCITATION DISCOVERED IN SUPERCONDUCTORS

Condensation of pairs of electrons into a single macroscopic quantum state is thought to be responsible for all superconductivity. In many superconducting materials, the electron pairs have a fully symmetric, or *s*-wave, internal symmetry, which is a natural consequence of phonon-mediated pairing. But in cuprate high-transition-temperature (high-T_c) superconductors, the condensed pairs have a *d*-wave symmetry, which indicates an unconventional mechanism. Many models have been proposed in which the “glue” that binds the carriers consists of something other than phonons. But there is no agreement about what that glue might be, nor even a consensus as to the simplest “effective Hamiltonian” (which is a shorthand description of the motions and interactions of the valence electrons) needed to account for cuprate superconductivity. Experimental study of electronic excitations in cuprates promises to help identify the effective Hamiltonian, and it has become clear that investigations of the mid-infrared (mid-IR) energy regime are essential in this regard. Experimenters have made a significant contribution to this growing body of research with studies carried out at the APS.

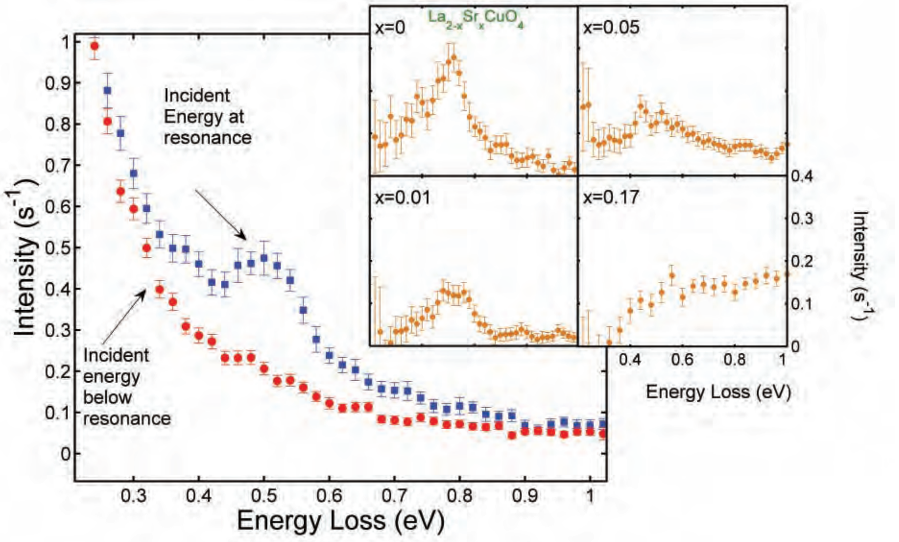

Fig. 1. Inelastic x-ray scattering in La_2CuO_4 observed at the (π, 0) point. The incident energy on resonance (blue) was 8992.5 eV, while the off-resonance data (red) were taken with E_i = 8980 eV. Doping dependence of the 500-meV feature for $La_{2-x}Sr_xCuO_4$ is shown in the inset. Data were taken at (π, 0) and have the off-resonance background subtracted.

The researchers in this study, from Brookhaven National Laboratory, the University of Oxford, Bell Laboratories, the University of Toronto, Central Research Institute of Electric Power Industry, the University of Maryland, and Argonne, carried out a resonant inelastic x-ray scattering (RIXS) study of the mid-IR region involving a series of superconducting $La_{2-x}Sr_xCuO_4$ samples and the related cuprate Nd_2CuO_4. This technique, which probes the electronic excitations associated with the copper site, provides momentum-resolved bulk information and is therefore an ideal probe for the investigation of electron dynamics in cuprates. The experiments were performed at the XOR/CMC 9-ID beamline at the APS.

In the undoped parent compound (x = 0), the researchers discovered a previously unobserved excitation peaked around the (π, 0) point in reciprocal space (q space) at 500 meV (Fig. 1). The excitation was seen to soften and broaden on moving away from the (π, 0) position, and it was not observed at either the zone center (0, 0) or the antiferromagnetic point (π, π). The new mode was rapidly suppressed with increased Sr doping and was entirely absent at x = 0.17, where it was replaced by a continuum of excitations due to the compound’s metallic electronic structure. The mode was found to have a strong dependence on photon polarization, as it was observed only when the incident x-ray polarization was normal to the CuO planes.

The researchers rule out the possibilities that (1) the new mode is directly related to the mid-IR peaks seen in the optical conductivity, (2) the peak arises from charge excitations associated with electronic inhomogeneity of the doped carriers, and (3) the peak results from transitions to impurity-derived midgap states. This leaves two plausible origins for this new mode—as a *d–d* excitation and as a multi-magnon excitation. In investigating the first possibility, the researchers carried out a study involv-

“Collective” continued on page 26

“Collective” from page 25

ing Nd_2CuO_4. The results for Nd_2CuO_4, showed a weak peak at 500 meV, just as in La_2CuO_4, leading the researchers to conclude that the *d–d* excitation interpretation is unlikely, although it could not be ruled out completely.

Investigating the multimagnon hypothesis also led to difficulties, leading the researchers to suggest that the preponderance of evidence perhaps favors an (interlayer) x-ray-induced spin exchange process, with the definitive identification of this mode having to await further experimental and theoretical investigations, which will potentially provide new insights into the correct effective Hamiltonian. — *Vic Comello*

See: J.P. Hill[1,2], G. Blumberg[3], Young-June Kim[4]*, D.S. Ellis[4], S. Wakimoto[4], R.J. Birgeneau[4], Seiki Komiya[5], Yoichi Ando[5], B. Liang[6], R.L. Greene[6], D. Casa[7], and T. Gog[7], “Observation of a 500 meV Collective Mode in $La_{2-x}Sr_xCuO_4$ and Nd_2CuO_4 Using Resonant Inelastic X-Ray Scattering,” Phys. Rev. Lett. **100**, 097001 (2008).
DOI: 10.1103/PhysRevLett.100.097001

Author affiliations: [1]Brookhaven National Laboratory; [2]University of Oxford; [3]Bell Laboratories; [4]University of Toronto; [5]Central Research Institute of Electric Power Industry; [6]University of Maryland; [7]Argonne National Laboratory

Correspondence: *yjkim@physics.utoronto.ca

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9-ID • XOR/CMC • Physics, materials science • Liquid scattering, inelastic x-ray scattering, resonant inelastic x-ray scattering • 3.3-cm Undulator A • Accepting general users

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“Looking” from page 24

morphotropic phase boundary could be demonstrated in a pure compound without a complex microstructure or composition, the door would be opened for the development of much more powerful and less expensive high-coupling piezoelectrics.

A team of researchers from Argonne National Laboratory; the Carnegie Institution of Washington; and the University of California, Berkeley has found just such a thing in the common piezoelectric substance lead titanate. They observed that an MPB could definitely form in pure lead titanate under pressure at low temperatures, raising the possibility that the same might be possible at room temperature and pressure for use in practical devices.

The experimenters conducted synchrotron x-ray diffraction and Raman scattering studies of powder samples of lead titanate at the HP-CAT 16-BM-D and XOR/BESSRC 11-ID-C beamlines at the APS at high pressures and cryogenic temperatures. This revealed the formation of a morphotropic phase boundary between 10 and 20 GPa, with a phase transition from tetragonal to monoclinic at 10 GPa, monoclinic MC to monoclinic MA at 15 GPa, and monoclinic to rhombohedral at 20 GPa (Fig. 1). (The two monoclinic phases represent differences in the direction of polarization.) Lead titanate is a classic ferroelectric, which has been thought since the 1950s to have only a single simple phase transition, from tetragonal to cubic perovskite.

The team found a much higher degree of electromechanical coupling than expected resulting from this MPB, without the necessity of nanodomains, compositional or structural heterogeneity, or other such phenomena seen in other ferroelectrics. They conclude that the high coupling seen in ferroelectric solid solutions containing lead titanate is simply a result of tuning this high-pressure MPB to the ambient pressure.

Changing this pressure in some way, then, might prove a handy means of producing more efficient and better-performing ferroelectric materials. The researchers suggest the possibility of using chemical pressure, a technique that involves injecting smaller atoms (such as tin) into the lattice of the material, causing enough electromechanical pressure to induce the MPB phase transition. The possibilities are numerous and very promising, pointing the way to inexpensive and versatile piezoelectric substances for everything from our most mundane devices to our most sophisticated, continuing the process of taking an interesting curiosity of nature and making it even more useful.

— *Mark Wolverton*

See: Muhtar Ahart[1], Maddury Somayazulu[1], R.E. Cohen[1]*, P. Ganesh[1], Przemyslaw Dera[1], Ho-kwang Mao[1], Russell J. Hemley[1], Yang Ren[2], Peter Liermann[1] and Zhigang Wu[3], “Origin of morphotropic phase boundaries in ferroelectrics,” Nature **451**, 545 (2008).
DOI: 10.1038/nature06459

Author affiliations: [1]Carnegie Institution of Washington, [2]Argonne National Laboratory, [3]University of California, Berkeley

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11-ID-C • XOR/BESSRC • Materials science, geoscience, physics, chemistry • Diffuse x-ray scattering, high-energy x-ray diffraction, pair-distribution function • 2.3-cm undulator • Accepting general users

16-BM-D • HP-CAT • Materials science, geoscience • Powder diffraction, single-crystal diffraction • Bending Magnet • Accepting general users

TAKING THE FaST TRACK TO SYNCHROTRON X-RAY SCIENCE

From Roentgen's discovery of x-rays in 1895 to the present, his invisible light has afforded an opportunity to visualize the unseen. For Maude Johnson, her experience with x-rays from the APS allowed her to see herself in a new light.

"This facility has let me view myself as a scientist, and realize the potential I have for improving the well-being of the environment and society," said Johnson, one of three Southern University and A&M College (Louisiana) undergraduate students who, under the tutelage of Southern U. Assistant Professor Riyadh Al-Raoush, spent the summer of 2008 doing research at the APS. Al-Raoush, Johnson, and her student colleagues Lindsey Thomas and Meagan Pinkney embarked on a 10-week research project carried out at the GSECARS Sector 13 beamlines at the APS. Their stay was sponsored by the Faculty and Student Teams (FaST) Program, a cooperative effort between the U.S. Department of Energy's (DOE's) Office of Science and the National Science Foundation that "provides hands-on research opportunities in DOE national laboratories during the summer for faculty and students from colleges and universities with limited research facilities, and those institutions serving populations, women, and minorities under represented in the fields of science [and] engineering..." The SBC-CAT beamlines at APS Sector 19 also hosted FaST students. The program at Argonne is administered by the Division of Educational Programs under Director Harold Myron.

"The research we're doing at GSECARS is focused on the use of tomography to investigate microscale processes in permeable media, such as flow, mass transport, and pressure–saturation relations," said Al-Raoush. "The data being obtained at Argonne will enable us to develop and verify numerical and theoretical models. There is a wide range of applications to this research, including water resources engineering, environmental remediation, and enhanced oil recovery.


The Southern University and A&M College FaST contingent readies their experiment sample inside the GSECARS 13-BM-C enclosure. Left to right are Maude Johnson, Riyadh Al-Raoush, Lindsey Thomas, and Meagan Pinkney.

"The purpose of this visit is focused on education and research; I am trying to integrate both components. This is a great opportunity for my students to think outside the classroom, to utilize state-of-the-art tools to tackle a research problem, and to interact with scientists."

Lindsey Thomas, a mechanical engineering student entering her third year in 2008 at Southern U., noted that, "Having the chance to do research at the APS and GSECARS and to be exposed to the research world is a huge opportunity for me. The research that I have done is a little out of my area of expertise because it's more of an environmentally focused project, so it has been a great way to broaden my horizons." Thomas plans on going to graduate school after graduation, "so having this experience will be a positive for my future."

Maude Johnson's career objective after graduation with a Bachelors of Science in Civil Engineering "is to continue my education in a Ph.D. program in Hydrology and Fluid Dynamics. I would love to gain a fellowship with Argonne and conduct my research at the Lab during Graduate School, and also as a postdoc."

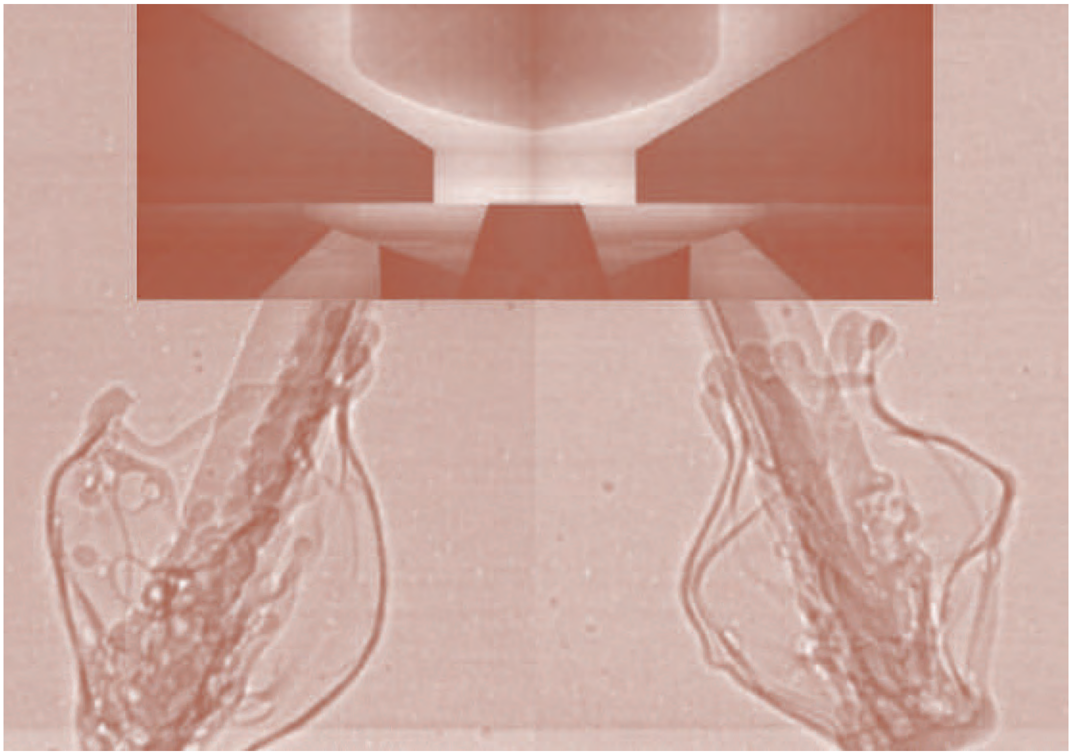
After graduation, Meagan Pinkney plans to "enter industry and move up the corporate ladder. I also plan to obtain a Master's Degree in Business Administration in the near future, and working at Argonne this summer will accelerate my chances of gaining this degree. My ultimate goal is to open my own engineering company."

GSECARs is one of four sectors at the APS managed by the University of Chicago's Center for Advanced Radiation Sources (CARS); the others are BioCARS (Sector 14), ChemMatCARS (Sector 15), and IMCA-CAT (Sector 17).

"This is GSECARS' first experience with the FaST program," said Mark Rivers, Associate Director of CARS, "and it has been very positive. The group brought a variety of skills to the project, including engineering design, so they were really able to design the experiment from the ground up. We provided the x-ray beam and tomographic expertise, and Dr. Al-Raoush had the ideas for the science they wanted to accomplish. It was a successful collaboration, and we look forward to participating in the program again in the future."

Contact Harold Myron (hmyron@dep.anl.gov)

GOING WITH (AND SEEING INSIDE) THE FLOW OF LIQUID JETS



Sometimes the most common things are also the hardest to understand. That is definitely the case with liquid jets and sprays. They are examples of multiphase flow, and they are encountered every day when we turn on a faucet, squeeze a spray bottle, or watch a rainfall. While those examples occur at relatively low speeds, the same phenomena at much higher speeds occur in other important places, such as the engine of your car. Obviously, this is a phenomenon that is of more than passing interest, and understanding the dynamics of this common occurrence is a valuable goal from both theoretical and practical standpoints. Researchers used the APS to aid in developing a new way of probing the dynamic structure and velocities of dense liquid sprays with a spatial and temporal resolution never before achieved. This new ability to see the previously unseeable will aid in the design of better fuel injection systems and other industrial tools, and find application in physiology, meteorology, and even geology.

This new ability to see the previously unseeable will aid in the design of better fuel injection systems and other industrial tools

Not only is high-speed multiphase flow essential to many industrial and natural processes (multiphase flow is happens inside the heart every second, as blood courses throughout the body), the fuel injection system of a car could not function without it.

Many basic questions about multiphase flow remain unanswered: How does a high-speed jet or spray break up? Does the process begin inside the nozzle or after? How is the mechanism affected by the shape or size of the nozzle? The answers have important implications for the design of more efficient fuel injection systems, among other applications. A group of scientists from Argonne National Laboratory, the Visteon Corporation, and the Mayo Clinic developed a new way of probing the dynamic structure and velocities of dense liquid sprays with a spatial and temporal resolution never before achieved.

Seeing into these phenomena inside, at, and near the nozzle, before the flow breaks up and scatters apart, has traditionally been a challenge, not only because of the inherent speed of the liquid and the transience of the flow, but also because optical effects make peering into the dense spray of hurtling liquid almost impossible. It is all but opaque to visible light, so attempts to see inside with lasers and other techniques have been largely unsuccessful. Instead of penetrating into the moving fluid, light tends to be absorbed, scattered, or reflected, and when a jet or spray breaks up in air or another gas, the complex morphology that results only complicates the problems. One trick that has been attempted is the use of tracer particles to see and track the internal fluid flows and speeds, but this tactic is invasive; the shape, size, and other properties of the particles themselves can affect the very phenomena they are trying to study. Describing high-speed multiphase flow through computer models can only provide a highly simplified and not very accurate solution because of a lack of hard experimental data to back up the assumptions of the computer simulations.

< Fig. 1. The liquid breakup of a high-density stream from a fuel injector as imaged with ultrafast synchrotron x-ray full-field phase contrast imaging.

Working at the XOR 32-ID beamline at the APS, the research team took a different approach to the dilemma, using ultrafast pulses of synchrotron x-rays to do full-field phase-contrast imaging. Single and double snapshot images, less than half a μsec long, were obtained using a fast mechanical shutter coupled with a charge-coupled device camera. The team examined high-speed jets of a simulated gasoline formed by a gasoline direct injection system using a number of different nozzles: single hole, dual-hole, and even a nine-hole nozzle plate. Earlier techniques were unable to directly visualize the effects of nozzle structure on the breakup or slowing of the spray, and such effects could only be inferred by analysis of the downstream spray, the only part that could be fully imaged in visible light. But the present technique actually provides the same advantages of using tracer particles: the ability to delineate velocity fields and jets of different densities and refractive properties while avoiding the disadvantages of that method, such as the possible modification of or interference with flow dynamics by the particles. The image contrast features that reveal the inner workings of the flow are a natural by-product of the ultrafast-pulsed x-ray strategy.

The team's observations clearly demonstrate that while the high-speed jet through the single-hole nozzle is fairly uncomplicated, the structure of the multiple-hole nozzles creates eddies and turbulence that result in a complex breakup of the spray as it exits, where it is dominated by a membrane-like internal structure. The experimental technique is also able to differentiate velocities from different parts of the spray, providing a much more complete picture of the entire process of the formation, evolution, and breakup of the high-speed flow.

This newly developed ability to see and study high-speed liquid jets and sprays will prove useful in much more than its obvious application of designing better fuel injection systems and other industrial tools. Because of the commonplace nature of multiphase flow, a better understanding of the phenomenon promises to resonate far beyond its immediate applications and into diverse realms such as physiology, meteorology, and even geology.

— *Mark Wolverton*

See: Yujie Wang[1], Xin Liu[2], Kyoung-Su Im[1], Wah-Keat Lee[1], Jin Wang[1], Kamel Fezzaa[1]*, David L.S. Hung[3], and James R. Winkelman[3], "Ultrafast X-ray study of dense-liquid-jet flow dynamics using structure-tracking velocimetry," Nat. Phys. **4**, 305 (April 2008). DOI: 10.1038/nphys840

Author affiliations: [1]Argonne National Laboratory, [2]Mayo Clinic, [3]Visteon Corporation

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Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

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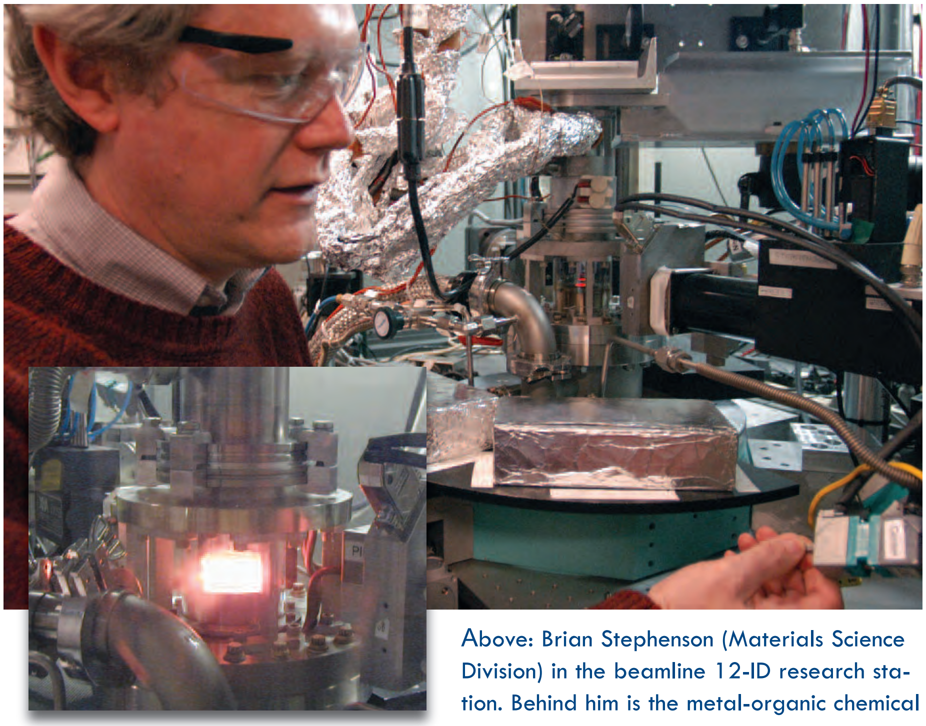
Riding the Waves of InN Formation

Patterns and cycles are everywhere in nature, and much of science involves discovering, studying, and understanding them. Sometimes they show up where we expect, as in the regular and predictable structure of a crystal or in routine chemical reactions. Most chemical reactions happen in a straightforward manner, one step following another until an equilibrium state is reached and the reaction ends. But oscillating chemical reactions can sometimes occur, usually only in particular molecules in solution or on surfaces, or in biological systems such as microbe colonies or cardiac muscle. Now, researchers using the APS have seen an oscillating chemical reaction in a very unexpected place: during the creation of a semiconductor material. This discovery promises to open new pathways for studies in fundamental nonlinear dynamics and in semiconducting materials for advanced applications.



Above: Brian Stephenson (Materials Science Division) in the beamline 12-ID research station. Behind him is the metal-organic chemical vapor deposition chamber mounted on a z-axis surface diffractometer. Inset at left: a closeup of the chamber with a sample heated to 1200K.

Researchers from Argonne, Philips Lumileds Lighting Corporation, Northern Illinois University, and Oakland University have discovered a self-sustaining oscillatory chemical reaction involving phase transitions in bulk materials. Using synchrotron x-ray diffraction and fluorescence at the XOR/BESSRC 12-ID beamline of the APS to observe metal-organic chemical vapor deposition (MOCVD) of indium nitride (InN) onto gallium nitride (GaN) films on a sapphire substrate, the experimenters found that a repeating oscillatory reaction develops.

Indium nitride is an advanced semiconductor with very promising optoelectronic qualities, including the smallest bandgap of the group III nitrides, but it has proven difficult to manufacture in high-quality form. Metal-organic chemical vapor deposition using ammonia (NH_3) as a nitrogen source and trimethylindium (TMI) as an In source is one technique for growing InN, although its precise workings are still under study, and a better understanding of the mechanisms involved could allow greater and more precise control of InN synthesis.

With that objective in mind, the experimenters studied the growth of InN onto GaN under constant pressure. They noted that after the initial period of InN nucleation and growth on the GaN substrate, self-sustaining oscillations began to occur. The cycle involved the following steps: After the initial crystalline islands of InN formation grew to a certain point, they suddenly all transformed into elemental In liquid droplets, which then began to evaporate and expose more surface area of the GaN substrate. This allowed InN islands to begin growing again, at first from the conversion of the remaining In droplets and then deriving In from the incoming TMI gas. The oscillating process continued as long as the supply of NH_3 and TMI remained constant and pressure remained unchanged, without any continued accumulation of InN or In.

X-ray studies showed that the oscillations manifested as regular changes in both fluorescence and diffraction, with the diffraction signal rising to a maximum and then sharply dropping off, corresponding with maximum In fluorescence (Fig. 1). The highest diffraction signal corresponded to the greatest amount of crystalline InN on the GaN surface, and the most intense fluorescence was seen when the highest amounts of InN and elemental In were present. Imaging with visible light revealed that the oscillations were due to waveforms of various geometries—including linear, circular, and spiral—traveling on the surface. The spatial period of these waves depended on the TMI pressure, producing faster oscillations at higher TMI pressures.

The oscillations were seen under the entire regime in which InN initially

“InN” continued on page 32

SEEING THE STRAINS IN DEFORMED METALS

Since their discovery 75 years ago, dislocations in materials have been studied extensively to learn more about their collective behavior. Dislocations are crystallographic irregularities in a crystalline material that determine the mechanical behavior of that material. Plastic deformation of metals causes individual dislocations to assemble into ordered groupings (dislocation structures), which consist of regions with a reduced number of dislocations—called subgrains—separated by regions having a higher density of dislocations, or dislocation walls. The resulting deformation structures possess a length scale that is much smaller than the original grain size. Two techniques used to analyze the dynamics of dislocation structures are transmission electron microscopy and x-ray line profile analysis. Unfortunately, the applicability of both techniques is limited. Researchers from Risø National Laboratory and Argonne developed a new synchrotron x-ray diffraction-based technique and applied it at the APS to non-destructively study the volume, strain, and orientation of deeply embedded single subgrains within single bulk grains in polycrystalline samples. This technique promises to help science gain a better understanding of the mechanical properties of deformed materials and how to develop stronger, lighter materials for applications from construction to medical implants.

The team's new technique, high-angular-resolution three-dimensional x-ray diffraction (3DXRD), is a combination of 3-D x-ray diffraction and peak shape analysis. The technique provides a 3-D, high-resolution, reciprocal-space map of the broadened reflections from an individual deformed grain in the bulk of a macroscopic specimen. Such a map reveals bright sharp peaks (Fig. 1), which represent individual regions of reduced dislocation density, superimposed on a diffuse cloud of enhanced intensity representing regions of dense dislocation walls. Their technique allows them to identify dislocation-free regions within a grain in the bulk of a tensile, deformed copper sample.

The researchers investigated a single bulk grain in a 99.99% pure oxygen-free, high-conductivity polycrystalline copper sample with an average grain size of 36 μm. The experiment was performed at the XOR 1-ID beamline at the APS.

A low-divergence, high-flux x-ray beam of 52-keV energy impinged upon a copper sample. The incident beam was focused on a sample that was deformed in tension to 2% strain. A 3-D reciprocal-space map of a 400 reflection with a resolution of 0.007° for the orientation and 0.01% for the elastic strain was obtained by rotating the sample in many intervals at a constant speed around an axis perpendicular to the scattering plane.

Confirming earlier observations, the projection of the 3-D distribution onto the direction of the scattering vector (the integrated radial profile) was found to be asymmetric, with a slower decay on one side of the peak than on the other side, and differing positions for the maximum intensity and the average intensity (Fig. 2).

The research team discovered that the intensity distribution contained a distinct structure consisting of a large, structureless cloud of enhanced intensity on which sharp, bright peaks were superimposed. Detailed analysis of all possible radial profiles from the 3-D reciprocal-space map showed a strong correlation between the value of the maximum intensity and the position of the maxima along the radial profile (Fig. 2). That is, high-intensity maxima were found at large scattering angles and at more negative strains with respect to the mean strain in the grain. Low-intensity maxima were found at low scattering angles corresponding to positive strains.

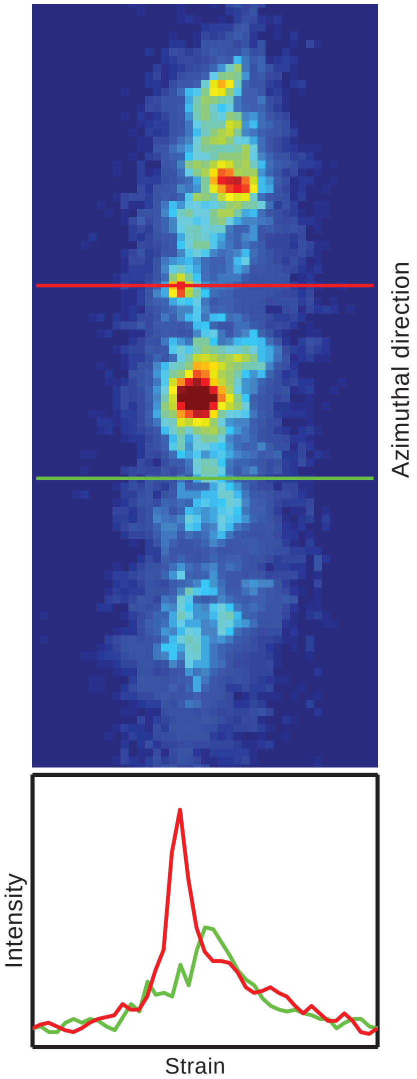


Fig. 1. Illustration of raw data. Top part shows a detector image, with clearly visible sharp peaks on top of a cloud of enhanced intensity. The bottom part shows two cuts (along the lines shown in the top panel) through the intensity distribution in the radial direction. From these radial profiles, strain differences between cloud and peak are clearly seen.

The bright peaks corresponding to the high-intensity maxima show that the subgrains are subject to backward stresses and strains, which lends support to previously obtained data from other scientific studies. In addition, the enhanced intensity cloud corresponding to the low-intensity maxima reveals that the material associated

"Strains" continued on page 32

"InN" from page 30

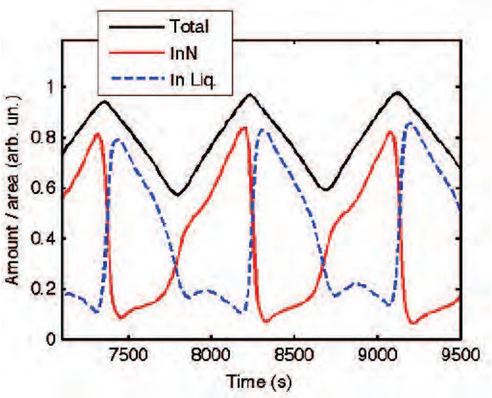


Fig. 1. Self-sustaining oscillations during metal-organic chemical vapor deposition of InN. Total (InN + In Liquid) and InN curves are normalized x-ray fluorescence and diffraction intensities; In Liquid curve is the difference.

condensed and in which elemental In evaporated. If MOCVD was performed directly onto the sapphire substrates without overlying GaN films, the oscillatory phenomenon did not develop, although some initial InN condensation was sometimes observed. This indicates that the type of substrate is an important factor in the oscillatory chemical reaction.

Although the oscillations observed in this experiment resemble those seen in other types of systems, the differences provide vital clues to the mechanisms involved in InN formation. In the MOCVD scenario, the oscillatory behavior depends on the catalytic decomposition of ammonia from NH_3 to N_2 at the film surface, along with the type of surface area exposed, confirming that this is a vital part of the process.

The observation of this sort of oscillatory chemical reaction for the first time in a system involving reactions and phase transformations between bulk materials opens new and intriguing avenues of basic study in fundamental nonlinear dynamics. But on a more direct, practical level, this work also points the way toward a greater understanding, and ultimately better and more exacting control of the processes involved in growing and tailoring these important semiconducting materials for advanced applications.

— Mark Wolverton

See: F. Jiang[1‡], A. Munkholm[2], R.-V. Wang[1†], S.K. Streiffer[1], Carol Thompson[3], P.H. Fuoss[1], K. Latifi[3], K.R. Elder[4], and G.B. Stephenson[1]*, "Spontaneous Oscillations and Waves during Chemical Vapor Deposition of InN," Phys. Rev. Lett. **101,** 086102 (22 August 2008). DOI:10.1103/PhysRevLett.101.086102

Author affiliations: [1]Argonne National Laboratory, [2]Philips Lumileds Lighting Company, [3]Northern Illinois University, [4]Oakland University ‡Present address: Ohio University; †Present address: Numonyx

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12-ID • XOR/BESSRC • Chemistry, physics, materials science • Small-angle x-ray scattering, wide-angle x-ray scattering, grazing incidence small-angle scattering, surface scattering • 3.3-cm Undulator A • Accepting general users

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"Strains" from page 31

with the dislocation walls is acted upon by forward stresses and strains, which substantiates the interpretation put forth in previous experimental studies by these researchers.

This work brings new insight to the process of plastic deformation of materials and their mechanical properties. This research strengthens the ability of scientists to study the self-organization of dislocations, the emergence of ordered dislocation structures, and the establishing of materials length scales below the grain level. The latter becomes essential for strengthening materials and developing light, strong materials for construction, aviation, transport, and implants and other medical applications.

— William Arthur Atkins
& Patricia E. Panatier

See: B. Jakobsen[1,2]*, U. Lienert[3], J. Almer[3], H.F. Poulsen[1], W. Pantleon[1], "Direct observation of strain in bulk subgrains and dislocation walls by high angular resolution three-dimensional X-ray diffraction," Mat. Sci. Eng. A-Struct. **483-484**, 641 (2008). DOI: 10.1016/j.msea.2006.12.168

Author affiliations: [1]Risø National Laboratory, [2]Roskilde University, [3]Argonne National Laboratory

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This work was supported by the Danish National Research Foundation and the Danish Natural Science Research Council. Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

1-ID • XOR • Materials science, physics, chemistry • High-energy x-ray diffraction • 3.3-cm Undulator A • Accepting general users

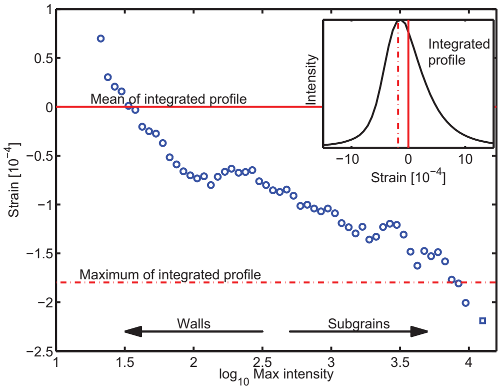
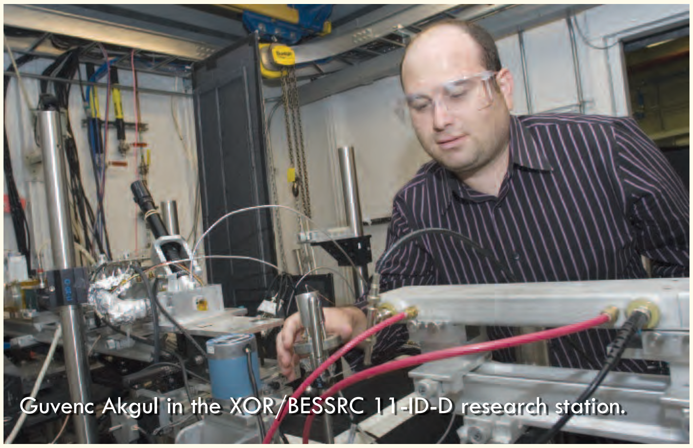


Fig. 2. Main panel shows the average strain at the maximum intensity in dependence on the maximum intensity along radial profiles. High-intensity regions have a negative strain and low-intensity regions have a positive strain. The insert shows the asymmetric integrated radial profile. These observations are in agreement with the interpretation of the peaks as coming from individual subgrains and the low-intensity cloud as coming from the walls.

Opening Doors Helps the Light Shine In

As Guvenc Akgul went about learning the finer points of x-ray spectroscopy from his colleagues at the APS, he represented a bridge between countries separated by culture, distance, and/or regional factionalism, but with a common ground in science. In 2008, Akgul, who hails from Adana in Turkey, worked toward his Ph.D. by gaining knowledge that will help in the development of SESAME, the Synchrotron-light for Experimental Science and Applications in the Middle East light source facility that is under construction in Jordan, bringing together scientists from several Middle Eastern countries.

The idea of an international synchrotron light source in the Middle East was first proposed in 1997 by Herman Winick of the SLAC National Accelerator Laboratory, and Gustaf-Adolf Voss of the German Synchrotron Deutsches Elektronen Synchrotron. Their main motivation for proposing SESAME was to help create a project in which people could work constructively and collectively. Now, in a collaboration that Winick characterized as “reasonably unusual,” Baharanian, Cypriot, Egyptian, Iranian, Israeli, Jordanian, Pakistani, Palestinian, and Turkish scientists are working together to make SESAME a reality.



Guvenc Akgul in the XOR/BESSRC 11-ID-D research station.

Akgul‘s studies centered on extended x-ray absorption fine structure experiments and how to apply that technique to the study of materials related to the development of new detectors for experimental physics at synchrotron x-ray facilities such as the APS and SESAME. He was funded at the APS by the Turkish government; the APS, which is supported by the U.S. Department of Energy (DOE) Office of Basic Energy Sciences; and SLAC, with funds from the DOE Cooperative Research Program for SESAME.

“The SESAME project has motivated me to get involved with x-rays, and many others will follow,” Akgul said. “SESAME is very important for Turkey and the Middle East. Turkey and SESAME will be in collaboration in the future, and this collaboration will give young researchers a big opportunity, like the one I am enjoying now. The APS is a great place to learn how to do research using x-rays: great people, a friendly atmosphere, an excellent opportunity to learn and practice science.” *Contact Klaus Attenkofer (klaus.attenkofer@anl.gov)*

AAAS Science Education Winner Visits the APS

Diane Riendeau, winner of the 2008 American Association for the Advancement of Science (AAAS) Leadership in Science Education Prize for High School Teachers, visited the APS on October 1, 2008. Riendeau, who teaches physics at Deerfield High School in Deerfield, IL, was the guest of Murray Gibson, Argonne Associate Laboratory Director for Photon Sciences; and Harold Myron, Director of the Argonne Division of Educational Programs. Riendeau met with Myron to discuss potential science education collaborations with the Laboratory and receive a tour of the APS from Gibson.

According to the AAAS, Riendeau’s "Make It, Take It, Teach It" program’s “combination of hands-on learning and teaching by the students—along with positive feedback from their families—has raised physics comprehension and interest, according to data collected on the program.” The number of physics survey classes at Deerfield High School has doubled under Riendeau’s stewardship.

Left to right: Harold Myron, Diane Riendeau, and Murray Gibson.

The Leadership in Science Education Prize includes a teaching visit to the Shanghai International Forum on Science Literacy of Pre-college Students. Riendeau, a 20-year teaching veteran and active member of the American Association of Physics Teachers, has already conducted a teachers’ training workshop in Africa, and in Puerto Rico as part of the first Materials World Modules Workshop at the University of Puerto Rico.

An article on "Make It, Take It, Teach It" that appeared in the March 2007 issue of Physics Education can be found here.

ALLAYING STRUCTURAL-ALLOY CORROSION

The search for ways to conserve energy is leading scientists to explore unexpected but important avenues, such as technologies that make extensive use of alloys that are subject to corrosion, which can result in significant energy inefficiency. Researchers using three DOE facilities at Argonne National Laboratory—including an APS beamline—and a variety of experimental techniques, have studied the phase composition of the oxide scale that protects alloys. Their research indicates that a change in the phase composition of the oxide scale on alloy surfaces could save over $1 billion per year in lost energy for the U.S. hydrogen industry alone.

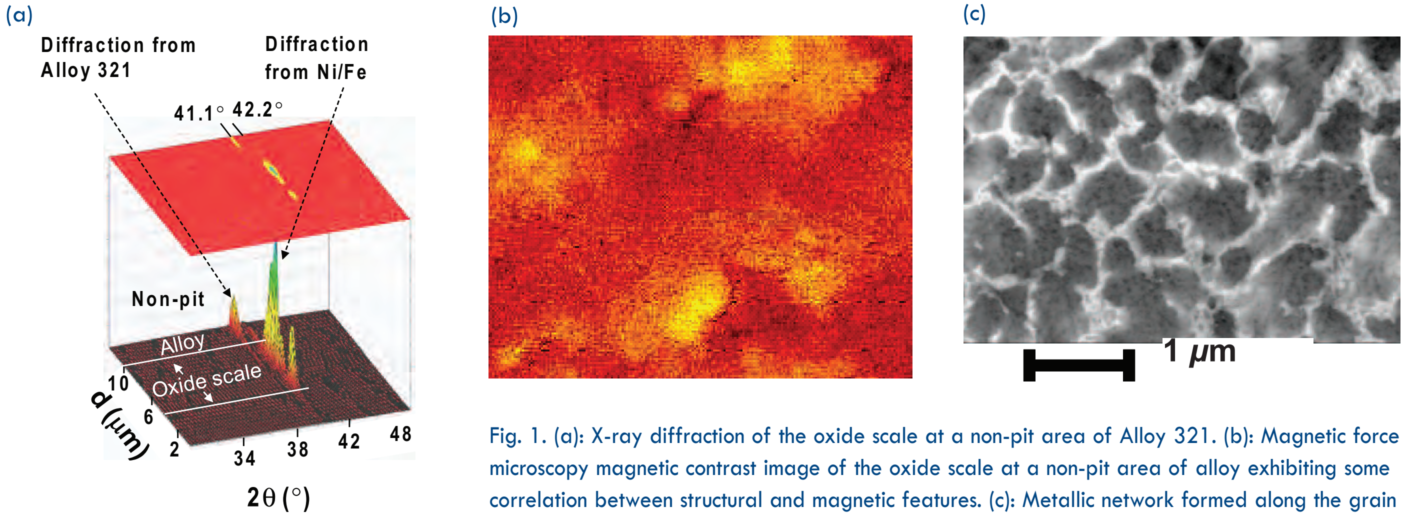


Fig. 1. (a): X-ray diffraction of the oxide scale at a non-pit area of Alloy 321. (b): Magnetic force microscopy magnetic contrast image of the oxide scale at a non-pit area of alloy exhibiting some correlation between structural and magnetic features. (c): Metallic network formed along the grain boundary of oxides, enabling diffusion of carbon through oxide scales.

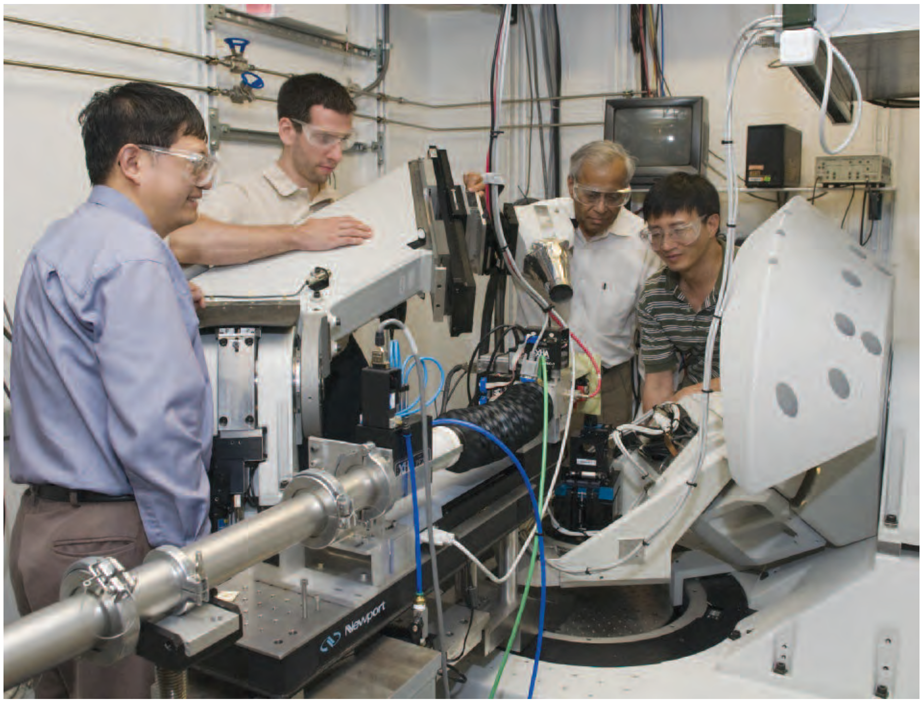
Approximately 137 quadrillion Joules of energy are lost annually due to high-temperature degradation (basically, corrosion) of structural alloys used in the manufacture of myriad technologies, including energy conversion and production systems such as ethylene furnaces and hydrogen reformer plants (see sidebar, next page).

Corrosion occurs when the integrity of a material is compromised by an intruder substance (such as the carbon generated at elevated temperatures), which causes scale breakdown and degrades the underlying alloy, forcing the impacted facilities to shut down. The degradation can be slowed by maintaining a system temperature below 400° C, so industries combat this detrimental effect by quickly quenching to below 400° C the chemical products formed at high temperatures, leading to a huge loss of (heat) energy.

Structural alloys are generally protected from extensive corrosion by oxide scales that develop on the alloy surface at high temperatures. The diffusion rate of carbon in oxides, such as those expected to comprise the majority of these scale layers, is negligible. Despite this, carbon often diffuses into alloys and leads to brittleness and even pitting corrosion. Carbon transport through the oxide scale is usually considered to involve the diffusion of carbon-bearing molecules such as CO and/or CO_2 through pores or cracks in the scales. But this mechanism has several fundamental flaws that suggest an alternative mechanism must be at work.

The Argonne research team devised an alternate explanation for the corrosion mechanism. It is well known that, unlike in oxides, carbon can dissolve in and diffuse through nickel and iron metals. Therefore, if metal particles are present in oxide scale, a new path for carbon atom transport is available that does not involve defects in the scale. The Argonne team probed oxide scales using nanobeam x-ray analysis at XOR beamline 2-ID-D at the APS, magnetic force microscopy at the Argonne Center for Nanoscale Materials (CNM), and scanning electron microscopy at the Argonne Electron Microscopy Center for Materials Research. Their results show that metal nanoparticles are indeed present in the scale. These metal nanoparticles join to form continuous channels for carbon transfer from the exposure environment to the substrate alloy.

Traditional x-ray beams are too



The authors at the goniometer in the XOR beamline 2-ID-D enclosure. Left to right: Zuotao Zeng, Seth Darling, Ken Natesan, and Zhonghou Cai.

large for analysis of the cross section of oxide scales that are only a few micrometers in thickness. Further complicating the problem, some alloys develop scales with several sublayers. Local phases could be analyzed by transmission electron microscopy (TEM), but it is difficult to prepare samples for this technique that allow us to study the regions of interest. Moreover, such preparations could also induce decomposition of oxides to metal.

These technical problems are some of the reasons that the local chemistry of oxide scales on alloy surfaces has not been carefully studied to date. In contrast with TEM, the nanobeam x-rays from the APS and the tip of the CNM magnetic force microscope can easily scan through the whole oxide scale for study of the phases and oxidation state of elements (Fig. 1).

It is projected that these new Argonne alloys could be used to build facilities that can recycle the wasted high-temperature heat and save more than $1 billion in lost energy for the U.S. hydrogen industry alone, based on the current cost of the natural gas needed to produce an amount of energy equivalent to that lost during hydrogen production.

This study may have a broad influence on not only metal dusting and carburization, but also in other research areas such as alloy development and surface coatings for high-temperature fuel cell applications.

See: Z. Zeng, K. Natesan*, Z. Cai, and S.B. Darling, “The role of metal nanoparticles and nanonetworks in alloy degradation,” Nat. Mater. **7**, 641 (2008). DOI:10.1038/nmat2227

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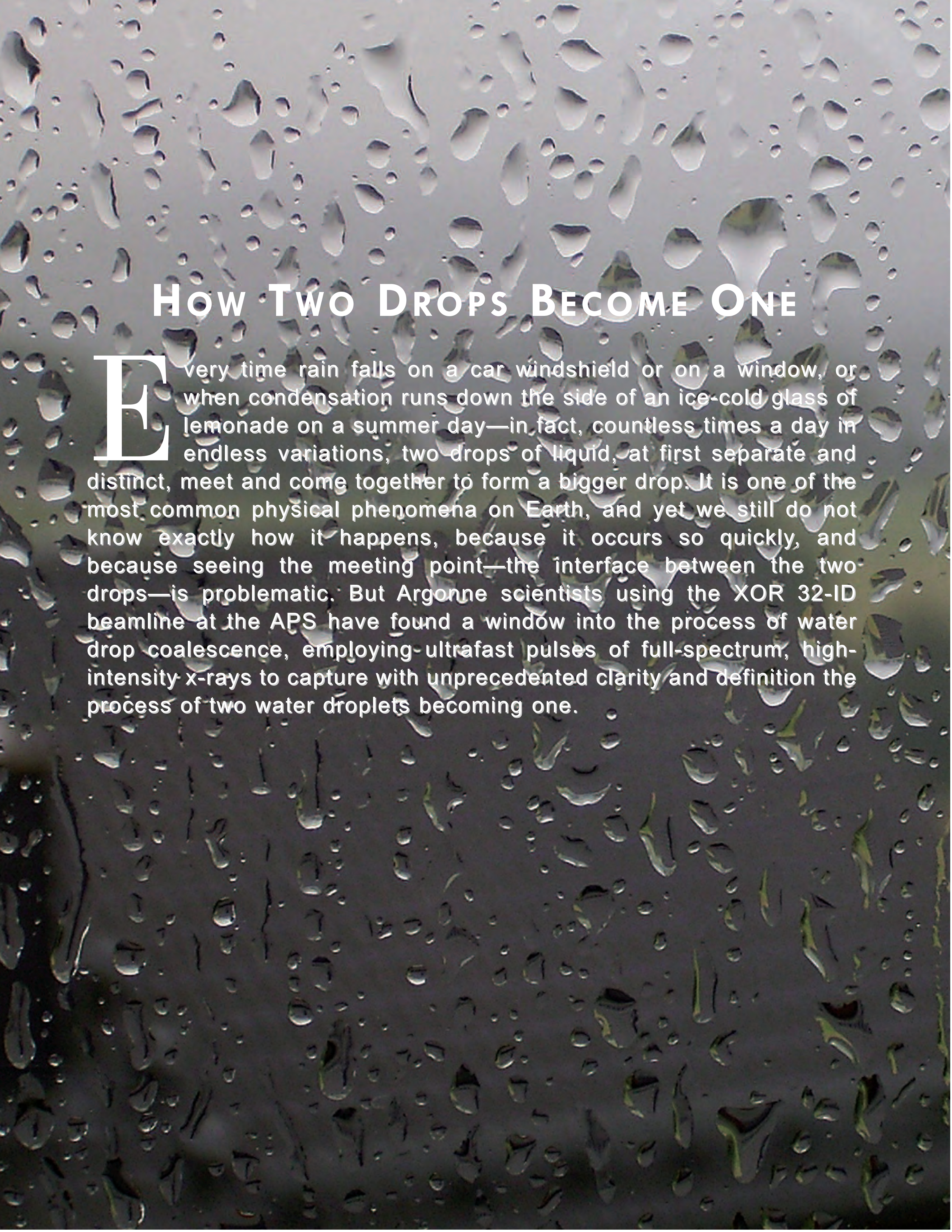
2-ID-D • XOR • Life science, materials science, environmental science • Microfluorescence (hard x-ray), microdiffraction, micro-x-ray absorption fine structure • 3.3-cm Undulator A • Accepting general users

The High Cost of Hydrogen

Hydrogen could be produced more efficiently if the issue of metal dusting was better understood and materials were available to resist this type of degradation in the temperature range of 400° C to 800° C. Current technology generally avoids the use of metals or alloys in that temperature range and only recovers the heat at 400° C and lower. This results in an energy loss of 4,414 BTU for the production of every standard cubic meter of hydrogen (scmh). Without metal dusting corrosion, the heat above 400° C could be utilized directly in hydrogen plants. In the year 2000, the U.S. produced 107.6 million scmh every day, and lost 173 trillion BTU annually in the hydrogen industry alone. That much energy was produced from 4.9 billion scm of natural gas. Based on current natural gas prices, $1.04-$2.77 billion could be saved in the hydrogen industry alone if the metal dusting corrosion can be avoided.

The gas to liquids (GTL) for methanol production is in its infancy with one operating plant producing about 21,000 barrels of product per day (bpd) from 160 million standard cubic feet per day (MMscfd) of natural gas. Some estimates suggest that six 100,000-bpd plants will be built in the next 10 years. This translates into 4,570 MMscfd of natural gas usage in year number 10. Calculations show that a plant designed for high-temperature heat transfer can realize a 6% natural gas saving. This amounts to 274 MMscfd at the tenth year. The average over 10 years would be a natural gas savings of about 137 MMscfd, or 3.9 million cubic meters in 10 years. The cost of the natural gas increases as energy demand increases. There are known reserves that will only come to the market if GTL becomes viable. What is known, however, is that overcoming the metal dusting problem would reduce the cost of a typical 100,000-bpd plant from $50 to $133 million per year.



HOW TWO DROPS BECOME ONE

Every time rain falls on a car windshield or on a window, or when condensation runs down the side of an ice-cold glass of lemonade on a summer day—in fact, countless times a day in endless variations, two drops of liquid, at first separate and distinct, meet and come together to form a bigger drop. It is one of the most common physical phenomena on Earth, and yet we still do not know exactly how it happens, because it occurs so quickly, and because seeing the meeting point—the interface between the two drops—is problematic. But Argonne scientists using the XOR 32-ID beamline at the APS have found a window into the process of water drop coalescence, employing ultrafast pulses of full-spectrum, high-intensity x-rays to capture with unprecedented clarity and definition the process of two water droplets becoming one.

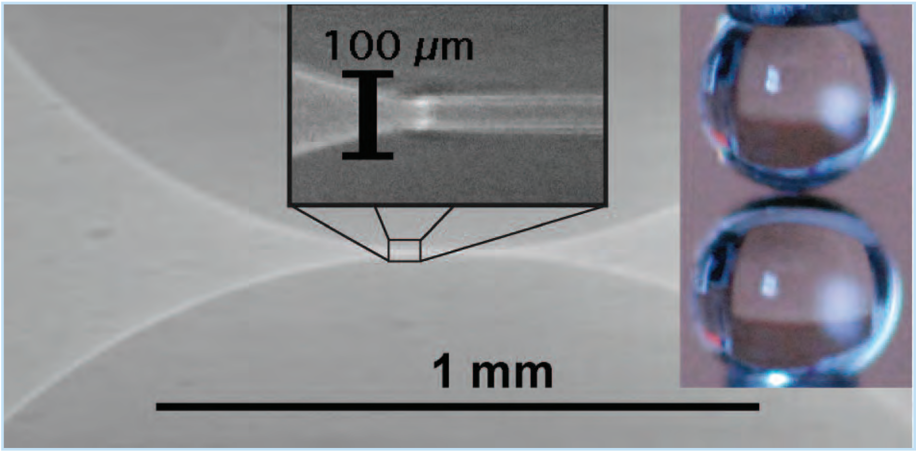


Fig. 1. A phase-contrast, ultrafast x-ray image taken 26 μs after the start of coalescence, with an enlarged view of the meniscus between the droplets. For comparison, the inset photo was taken in visible light, showing the obscuring effects of shadowing and refraction.

The problem of coalescence between two drops of liquid has generated a great deal of theoretical work and speculation that has been difficult to support by actual experiment. The Argonne researchers were interested in this particular problem because there are discrepancies in the literature about the initial contact between two drops: just when does it really start? With visible light one has a very unsatisfactory viewing angle for this type of phenomena because of shadowing and refraction. But the greatly enhanced resolution and penetrating power of the ultrafast white x-ray pulse from the APS offered a way to settle some of the arguments.

In the experiment, two syringes in precise alignment, one above the other, were connected to a water tank located slightly above the merging plane, so that one droplet from above and one from below would be brought together by a natural siphoning effect. The water was made slightly saline to enhance its electrical conductivity, to complete a circuit upon droplet coalescence and thus serve to trigger the high-speed charge-coupled device camera that captured the merging of the drops. With the camera synchronized to an x-ray pulse with a duration of 472 nsec, a series of stroboscopic images of the coalescence event could be obtained. Using this technique, the experimenters could resolve details as tiny as 5 μm (Fig. 1).

That 5-μm resolution is important, as it turns out to be the smallest height of the liquid bridge between the water drops that could be seen during the experiment. As the drops continue to merge and the bridge between them increases in size, a toroidal bubble of trapped air temporarily forms. A bubble, or bulging, was visible inside the bridge between the two drops (Fig. 1). This bulge was actually predicted with some models, but had never been seen.

Both the formation of the bubble and the bridge—or meniscus—between the coalescing drops follow a power law scaling just as predicted by theory. Still elusive is what happens at “time zero,” i.e., the precise moment of first contact between the two drops. The scaling laws and power laws in this case are slightly different depending on when one sets the zero time. The researchers went approximately 5 μsec closer to the actual time zero. But still, what really happens exactly at time zero is beyond current experimental techniques. Peering into that “time zero” realm may be possible with other indirect approaches or the use of even faster x-ray pulses in the sub-nanosecond range with a higher spatial resolution, which the team considers a most exciting prospect.

For now, the researchers have demonstrated how very bright, very short x-ray pulses can capture extremely fast phenomena that cannot be seen with other methods. They have already used the technique to study the formation and breakup of a jet of liquid from a nozzle, and it can be used to probe subjects that move at hundreds of meters per second. The next step is to apply it for subjects that move even faster. Possibilities include the practical study of fuel-spray dynamics, flow singularities, the propagation of microscopic cracks in metals and other solids, and ballistic or explosive phenomena.

Even with this new ability to study what physicists call a hydrodynamic singularity, the essential, simple beauty of what our eyes see in visible light—two water drops joining together—remains unchanged.

— *Mark Wolverton*

See: Kamel Fezzaa** and Yujie Wang*, “Ultrafast X-Ray Phase-Contrast Imaging of the Initial Coalescence Phase of Two Water Droplets," Phys. Rev. Lett. **100**, 104501 (2008).
DOI: 10.1103/PhysRevLett.100.104501
Author affiliation: Argonne National Laboratory
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Use of the APS supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

Rain photo courtesy of Frank Vincentz (http://commons.wikimedia.org/wiki/Image:Rain_drops_on_window_01_ies.jpg)

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SEEKING A DEPLETION LAYER AT

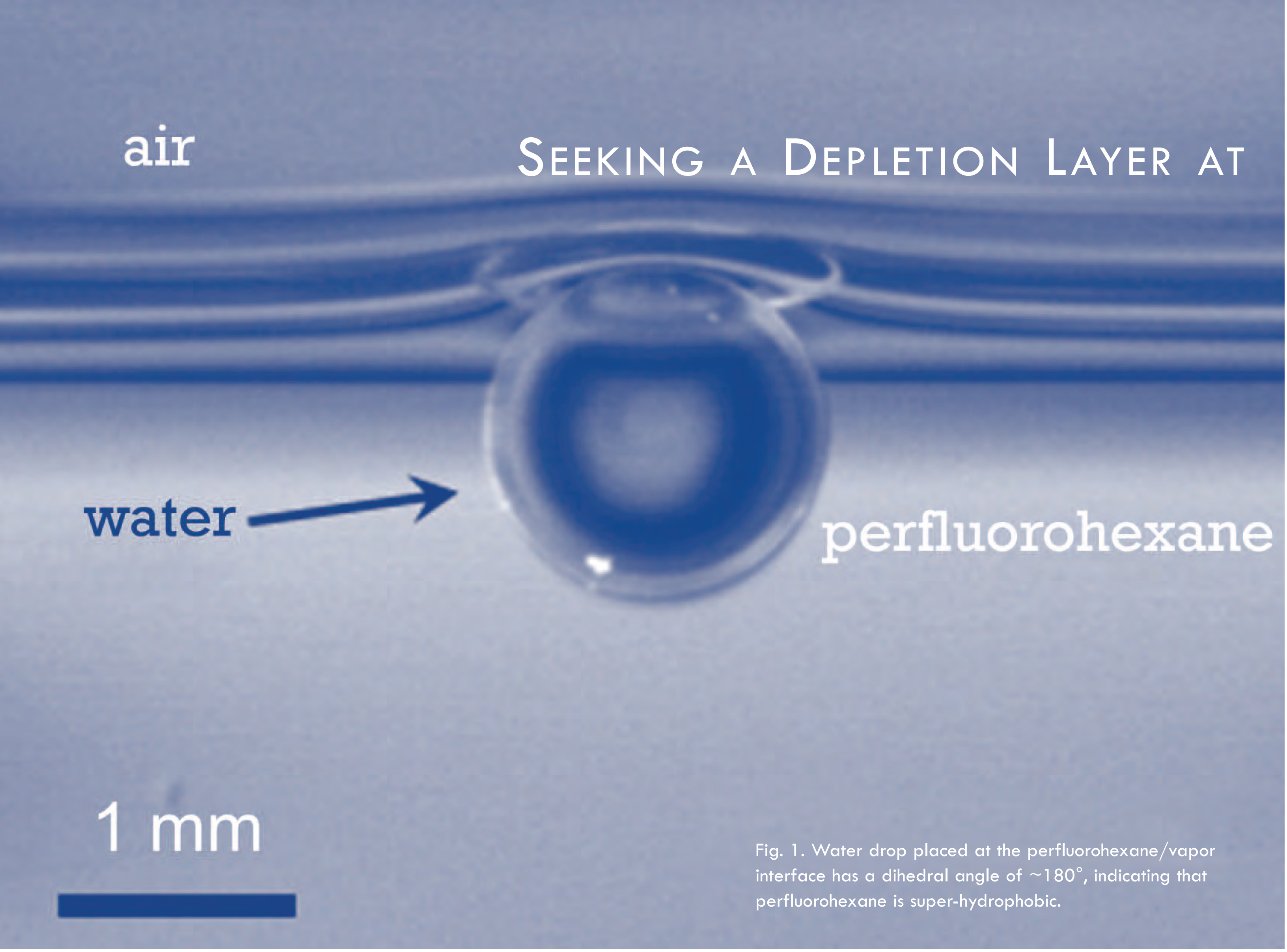

Fig. 1. Water drop placed at the perfluorohexane/vapor interface has a dihedral angle of ~180°, indicating that perfluorohexane is super-hydrophobic.

Theory predicts the occurrence of a vapor-like depletion layer at the interface between hydrophobic substances (those, such as oil, that repel water or cannot be completely dissolved in water) and an aqueous solution. However, recent experimental studies do not decisively agree as to whether such depletion layers exist or not. For example, recent evidence from x-ray and neutron scattering from the interface between hydrophobic solids and water indicates the presence of a depletion layer with a thickness of a few angstroms, though conflicting reports persist. Because of the importance of hydrophobic/aqueous interfaces to biological, chemical, and environmental processes, a group of researchers decided to experiment on the structure of two soft hydrophobic/aqueous interfaces. X-ray experiments at the APS and the National Synchrotron Light Source produced data that are consistent with the nearness of water to soft hydrophobic materials under a length of a fraction of an angstrom. The researchers contend that a depletion layer does not exist at these soft interfaces. Such conclusions are important for further advances in hydrophobic/aqueous applications for many environmentally and industrially important surfaces.

SOFT HYDROPHOBIC/AQUEOUS INTERFACES

The experiment carried out by researchers from the University of Illinois at Chicago, The University of Chicago, and Kyushu University, involved the use of x-ray reflectometry to characterize electron density variation with respect to interfacial depth of two oil/water interfaces: fluorocarbon (perfluorohexane) and water, and hydrocarbon (heptane) and water. The presence of a depletion layer of even a fraction of an angstrom thickness would have altered the electron density variation in such a way as to produce a measurable change in the reflectivity.

Perfluorohexane, a fully fluorinated alkane chain with six carbon atoms, is very difficult to wet (a super-hydrophobic material) and so provides a decisive test for the presence of a depletion layer (Fig. 1). The researchers measured the x-ray reflectivity of the perfluorohexane/water interface using the ChemMatCARS 15-ID beamline at the APS.

Though not as hydrophobic as perfluorohexane, heptane is a seven-carbon hydrocarbon chain that is used to model biomolecular hydrophobicity. Beamline X19C, at the National Synchrotron Light Source at Brookhaven National Laboratory, was used to measure the x-ray reflectivity of the heptane/water interface.

Distillation of the perfluorohexane and alumina column purification of the heptane hydrophobic materials increased the purity to acceptable levels for the experiment as tested by the methods of tensiometry and gas-liquid chromatography. Thereafter, the scientists measured the interfacial tension of the perfluorohexane/water interface with the pendant drop method, and measured the interfacial tension of the heptane/water interface with the Wilhelmy plate method.

Capillary waves at the perfluorohexane/water interface caused the measured x-ray reflectivity to be less than the calculated Fresnel reflectivity. However, further small deviations of the data from that expected for a simple interface roughened by capillary waves led the scientists to suggest that their data implies weak intrinsic molecular ordering at the interface. Their data are consistent with the presence of two to three layers at the interface, though the maximum density of these perfluorohexane layers is only 3% greater than the bulk liquid perfluorohexane density. Thus, the reflectivity results describe deviations that are not explainable by a depletion layer.

Results from the heptane/water interface are fully consistent with that of a simple interface fluctuating with capillary waves. Again, a depletion layer is absent. In this case, small deviations from the calculated reflectivity curve did not show up as they did with the perfluorohexane/water interface. The scientists suggest that the flexibility of heptane molecules, as opposed to the rigidity of perfluorohexane, is responsible for this difference. This is consistent with their measurements of interfacial excess entropy, which indicate that aqueous interfaces with small hydrocarbons, such as the hexane/water interface, are slightly more disordered than the perfluorohexane/water interface.

Such conclusions are important to scientists as they learn more about the biomolecular interactions of hydrophobic regions exposed briefly to water, along with the wetting of aqueous solutions, as they pertain to environmental and industrial surface applications. — *William Arthur Atkins & Patricia E. Panatier*

See: Kaoru Kashimoto[1,2], Jaesung Yoon[1], Binyang Hou[1], Chiu-hao Chen[1], Binhua Lin[3], Makoto Aratono[2], Takanori Takiue[2], and Mark L. Schlossman[1]*, “Structure and Depletion at Fluorocarbon and Hydrocarbon/Water Liquid/Liquid Interfaces,” Phys. Rev. Lett. **101**, 076102 (2008).
DOI:10.1103/PhysRevLett.101.076102

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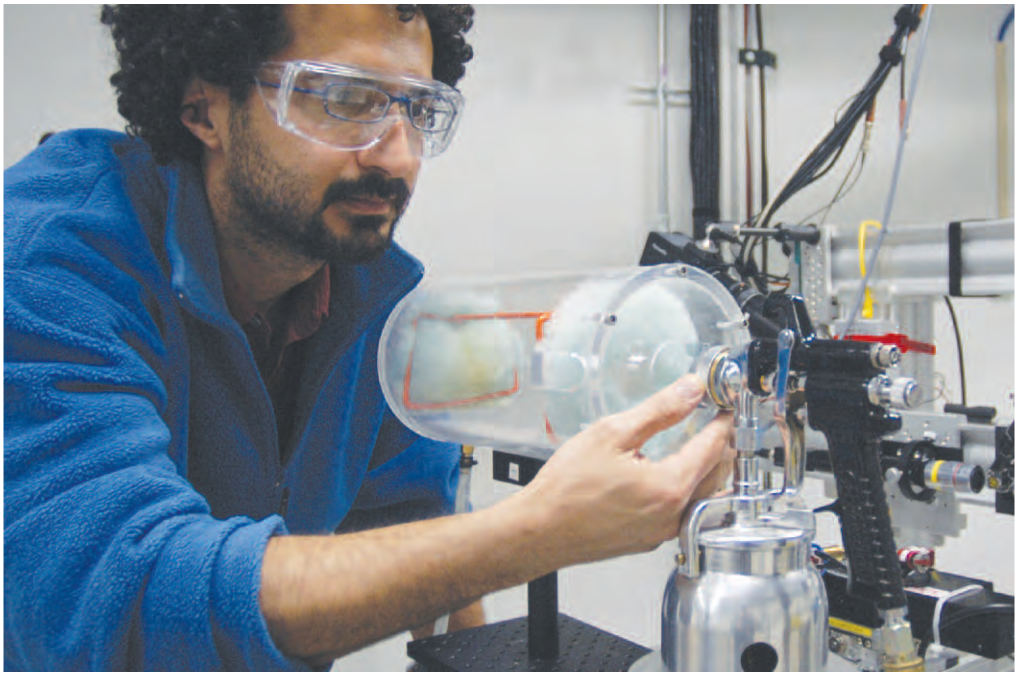
15-ID • ChemMatCARS • Materi-als science, chemistry • Anomalous and resonant scattering (hard x-ray), liquid scattering, microdiffraction, single-crystal diffraction, small-angle x-ray scattering, surface diffraction, wide-angle x-ray scattering • 3.3-cm Undulator A • Accepting general users

PROBING AIR-ASSISTED LIQUID-JET BREAKUP MECHANISMS

Scientific and practical applications for liquid-jet atomization abound. In liquid-propellant rocket engines, for example, a large number of coaxial atomizers supply the fuel and oxidizing agent for combustion, with the central liquid-oxygen jet in each atomizer becoming atomized by the higher-speed coaxial annular stream of hydrogen gas that surrounds it. Although the physics of high-speed liquid-jet atomization is not well understood because of its complexity and transient nature, scientists generally believe that atomization begins with surface undulations that cause small masses of liquid to leave the jet and subsequently break up into tiny droplets. These two distinctive subprocesses are conventionally termed the primary and secondary breakup, respectively. Results from experiments carried out at the APS are a significant step toward forming a clearer picture of the liquid-jet atomization process.

Fig. 1. X-ray phase-contrast image showing membranes entrained by the streaming air (at 90 m/sec) and separating from the main water jet. The exposure time is 472 nsec, and the image size is 1.4 × 1.7 mm^2.



Kamel Fezzaa (X-ray Science Division) demonstrates the elegantly simple apparatus employed for the liquid-jet breakup experiment. Fezzaa is adjusting the nozzle of a commercial paint spray gun utilized to generate a coaxial air-assisted water spray that is imaged within the first 10-20 mm of the nozzle exit. Windows (holes) in the acrylic cylinder behind his hand let the x-ray beam pass without going through the plastic. The cylinder contains the water and is designed to minimize back splashing and air returns that would corrupt or bias the measurements. Fezzaa notes that this experiment, and the problem of how two droplets of liquid coalesce to form one drop, are examples of relatively old questions that are being answered with the use of fairly simple apparatus linked to a complex, sophisticated source of synchrotron light such as the APS. For more on droplet coalescing, see "How Two Drops Become One" on page 36.

Argonne scientists studied the primary breakup process of a coaxial air-assisted, fixed-flow-speed water jet over a wide range of air speeds by using an ultrafast x-ray phase-contrast imaging technique at the XOR 32-ID beamline of the APS. By exploiting the unprecedented spatial and temporal resolutions offered by this new technique, the scientists quantitatively established similarities between the primary and secondary breakup processes, and among primary breakups on different length scales. A commercial paint spray-gun was used to generate the coaxial air-assisted water spray. The x-rays transmitted and diffracted through the jet were converted to visible light by a scintillating crystal and imaged with optical lenses onto a fast charge-coupled-device camera. The breakup process was studied by using a combination of single-exposure and multiple-exposure imaging schemes.

Surface undulations along the liquid jet developed earlier and with bigger amplitudes as the air speed increased. Only when the air speed was higher than 42 m/sec did the surface undulations begin to cause liquid masses to become caught up in the airstream. Below that speed, the water jet broke up as a whole as a result of the Rayleigh-Plateau instability, which explains the breakup of a falling stream of fluid into smaller packets of equal volume but less surface area.

As the air speed continued to increase, the surface undulations became amplified as they moved downstream, and formed rod-like structures protruding into the airstream, which broke away from the jet when the air speed reached 50.9 m/sec. When air speeds were further increased, the surface rods became stretched to form long ligaments that subsequently broke up. The scientists noted that the transition from rod-like breakup to ligament breakup greatly resembled the dripping-to-jetting transition in low-speed jet breakups.

The jet breakup changed drastically when the air speed rose above 60 m/sec. Instead of forming ligaments, the surface undulations became blown into two-dimensional membrane structures with thick rims (Fig. 1). The membrane structures continued to expand in the airstream and eventually burst. At even higher air speeds, breakups happened more chaotically, making them more difficult to study. However, membranes with much thinner rims could still be seen.

The group established quantitative relationships among the ligament- and membrane-mediated breakups and the rod-like breakups in the high-speed airstream. Their results imply that the phenomena have intrinsic connections, in that the breakups are controlled by a competition between aerodynamic forces and the surface tension of the liquid.

The complexity of jet breakup has been a daunting obstacle to research progress. The numerous similarities the researchers found among various aspects of the breakup phenomenology promise to provide a foothold to further insights into the processes involved.

— *Vic Comello*

See: Yujie Wang, Kyoung-Su Im, and Kamel Fezzaa*, "Similarity between the Primary and Secondary Air-Assisted Liquid Jet Breakup Mechanisms," Phys. Rev. Lett. **100**, 154502 (2008).
DOI: 10.1103/PhysRevLett.100.154502

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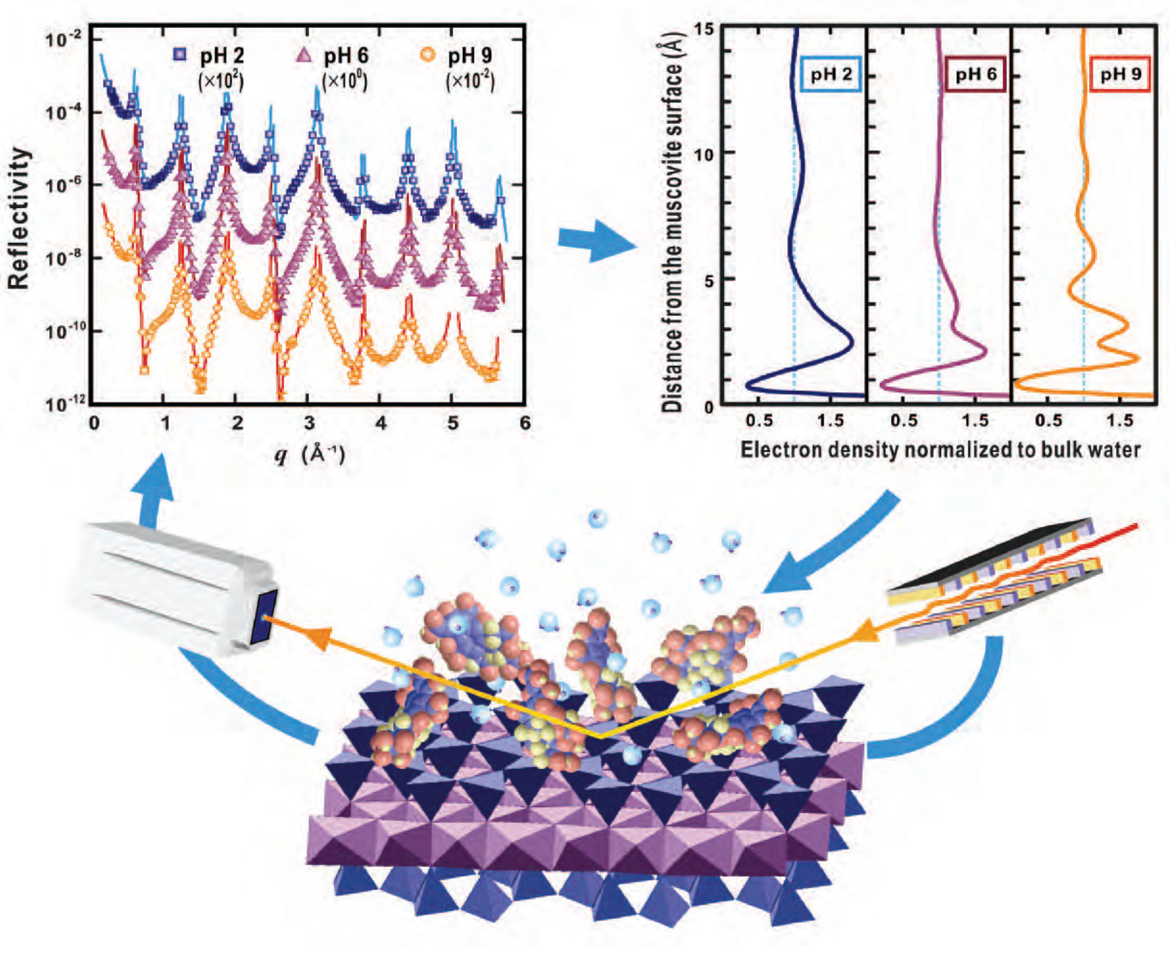
This research and the use of the Advanced Photon Source were supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

32-ID • XOR • Materials science, life science • Phase-contrast imaging, ultra-small-angle x-ray scattering, radiography • 3.3-cm Undulator A • Accepting general users

NATURAL ORGANIC MATTER AND THE MINERAL-WATER INTERFACE

Given the urgency to better understand the possible causes of and solutions for global warming, there is increasing interest in how natural organic matter (NOM), one of the largest global carbon sources, *adsorbs to* and *desorbs from* mineral surfaces. These processes strongly affect the diffusive flux of dissolved organic carbon, which can potentially transform to greenhouse gases. A salient feature of NOM-coated soil particles is their propensity to aggregate, which in turn improves both soil quality and its long-term agricultural sustainability. The organic coating can also change the reactive properties of mineral surfaces and influence the environmental distribution, speciation, and bioavailability of metals and organic pollutants. A team of researchers used an x-ray beamline at the APS to measure the *in situ* specular x-ray reflectivity of NOM-coated mineral surfaces. Their results reveal new information about the extent to which adsorbed NOM can affect the reactivity of mineral-water interfaces in more complicated solutions representing natural waters, and ultimately how organic matter is cycled between the lithosphere and hydrosphere at the Earth's surface.



Direct demonstration of sorption mechanisms is challenging because NOM has supramolecular organic structures containing various macromolecules, each having a different size and chemical composition, and different concentrations of reactive functional groups. Atomic force microscopy techniques have been used to observe the morphology of NOM adsorbed on mineral surfaces. But soft organic matter is often difficult to image when wet, and drying may alter the original structure of organic molecules adsorbed on a surface.

X-ray reflectivity, however, is an attractive method for overcoming this difficulty because it is non-invasive and can be applied in solution, making it a good choice for *in situ* investigations of soft organic films adsorbed on mineral surfaces. The researchers from the University of Illinois at Chicago and Argonne measured the *in situ* specular x-ray reflectivity of NOM-coated mineral surfaces at XOR beamline 11-1D-D. The team looked at the muscovite mica (001) surface in solutions of soil fulvic acid (FA) tailored to mimic the typical range of pH values found in nature. The acidic to neutral pH values (i.e., those ranging from 2 to 6) correspond to those found in freshwater wetlands or fast-flowing pore waters in shallow soils where background electrolyte concentrations are expected to be low, while the alkaline systems (pH > 8.5) represent organic-rich estuarine environments or shallow groundwaters in contact with mafic or ultramafic rocks.

Interpreting the x-ray reflectivity data was challenging because of the macromolecular nature of the FA. The team developed a new model to extract the electron density distribution at the interface from the reflectivity data. The model contained three components: (1) ideal muscovite substrate lattice; (2) interfacial species, including relaxed muscovite surface layers and any additional layers of surface adsorbed species; and (3) bulk water above the surface. Adsorbed simple ions and water near the muscovite surface were described by a Gaussian distribution, whereas the layer of FA molecules sorbed on the muscovite surface was characterized by using a composite electron-density distribution that included a near-surface Gaussian peak, representing FA fractions condensed near the surface during sorption. This was followed by a broad profile obtained from the summation of multiple, overlapping Gaussian peaks that diminished in electron density as the distance to the surface increased.

The study revealed that a thin film of FA (having a thickness between 6 and 12 Å) adsorbed on the muscovite surface in solutions at acidic to near neutral pH, while the layer decreased in both thickness and electron density until it disappeared in alkaline solutions (pH above 8.5). Disappearance above pH 8.5 likely occurred because of electrostatic repulsion between the negatively charged muscovite surface and the FA molecules, which become negatively charged at alkaline pH. At pH 3.7, the amount of FA that adsorbed in direct contact with the muscovite surface increased with increasing reaction time and became stabilized after approximately 10 h. However, the electron density within the entire film varied continuously over 500 h, perhaps as a result of the relatively slow condensation and fractionation of the sorbed FA molecules during the reaction.

Overall, *in situ* x-ray reflectivity was proven to be a highly useful method for determining the thickness and structural characteristics of adsorbed films of NOM on mineral surfaces. These results will help increase our understanding of the extent to which adsorbed NOM can affect the reactivity of mineral-water interfaces in more complicated solutions representing natural waters and, ultimately, of how organic matter is cycled between the lithosphere and hydrosphere at Earth's surface. — *Luis Nasser*

< Fig. 1. Schematic showing the sequence of steps used to determine the interfacial structure from measured x-ray reflectivity data. The x-ray photon beam from a synchrotron insertion device (bottom, right) strikes a muscovite basal surface in a fulvic acid solution represented by the molecular scale model (bottom, middle) and is reflected to a charge-coupled device area detector (bottom, left). Reflected intensities are measured as a function of momentum transfer, q (top left), and the curves are transformed into electron-density profiles as a function of height above the muscovite surface (top right). The electron-density profiles show that the sorbed fulvic acid forms a 6-Å- to 12-Å-thick film (bottom, middle) at pH 2 to 6, whereas the film disappears at pH ≥ 8.5.

See: Sang Soo Lee[1]*, Paul Fenter[2], Changyong Park[2], and Kathryn L. Nagy[1], "Fulvic Acid Sorption on Muscovite Mica as a Function of pH and Time Using *In Situ* X-ray Reflectivity," Langmuir **24**, 7817 (2008).
DOI: 10.1021/la703456t

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11-ID-D • XOR/BESSRC • Chemistry, geoscience, materials science • X-ray absorption fine structure (XAFS), general diffraction, time-resolved XAFS • 3.3-cm Undulator A • Accepting general users

GLASS DOES A DOUBLE-TAKE

Scientific mysteries aren't always found in exotic, out-of-the-way places. Take glass, for instance. Glass is an odd substance: definitely not gaseous, not quite solid, not quite liquid, but something in between. How and why glass forms remains a scientific mystery. Common wisdom has it that a liquid has to be cooled to turn into a glass. But recent experiments by scientists from Yale University and Argonne, using an APS x-ray beamline, have shown that, sometimes, heating a liquid can also turn it into a glass. By confirming predictions from recent theories about the transition of liquids to glass, their work might make glass a bit less mysterious.

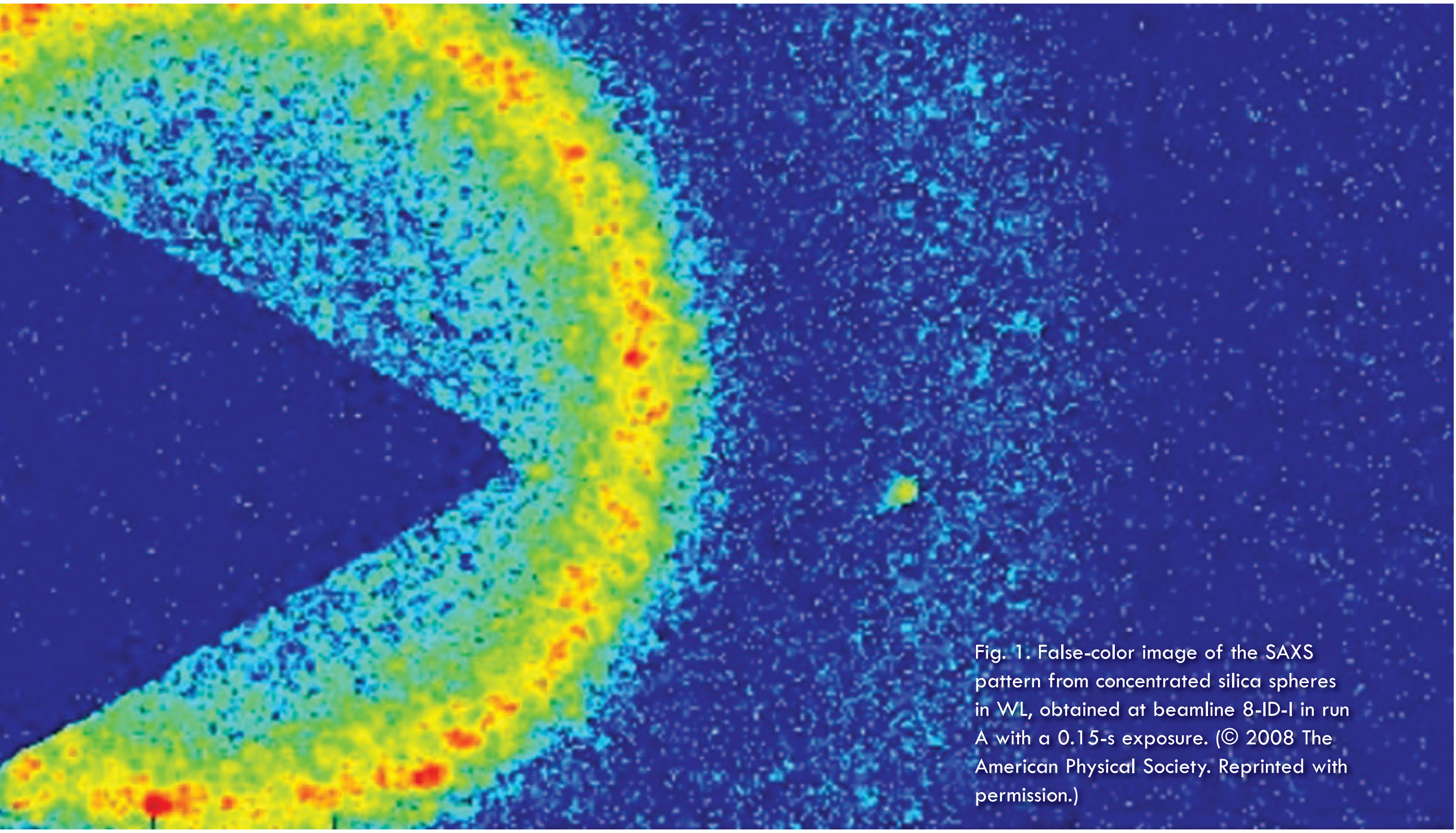

Fig. 1. False-color image of the SAXS pattern from concentrated silica spheres in WL, obtained at beamline 8-ID-I in run A with a 0.15-s exposure. (© 2008 The American Physical Society. Reprinted with permission.)

The predictions come from mode coupling theory (MCT), which, among other things, can be used to describe glassy behavior. MCT predicts that under the right conditions—for dense enough particles with a short-range attractive interaction in addition to a hard-core repulsion—one could transition to a glass by heating the fluid.

In the experiments, the researchers used x-ray photon correlation spectroscopy at the XOR 8-ID-I beamline to collect data on the movement of silica particles in a binary fluid—a water-luditine mixture—under varying temperatures. A partially coherent x-ray beam scattered from the sample produced a speckle pattern, from which the behavior of particles in the sample could be inferred (Fig. 1). In contrast to ordinary small-angle x-ray scattering (SAXS), the method used by the group could characterize the time dependence of particle movement. Collecting sequential SAXS patterns provided a "movie" of particle behavior over time. Figure 2 shows the experimental setup.

As expected, the team found that, upon cooling, the mixture underwent a transition from liquid to what is called a "repulsion-dominated" glass, in which each particle is surrounded, or caged, by its neighbors. This is the odd, solid-but-not-quite crystalline structure of most glass. If the attrac-

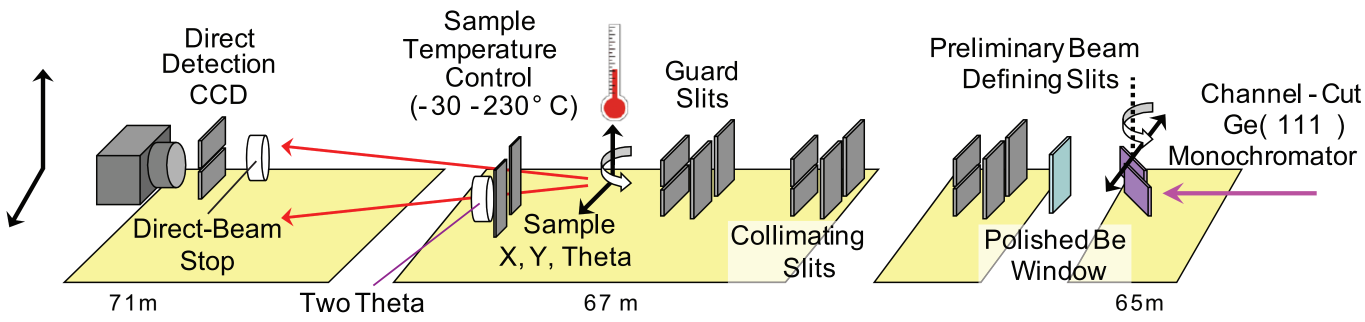

Fig. 2. Schematic of the experiment setup at 8-ID-I.

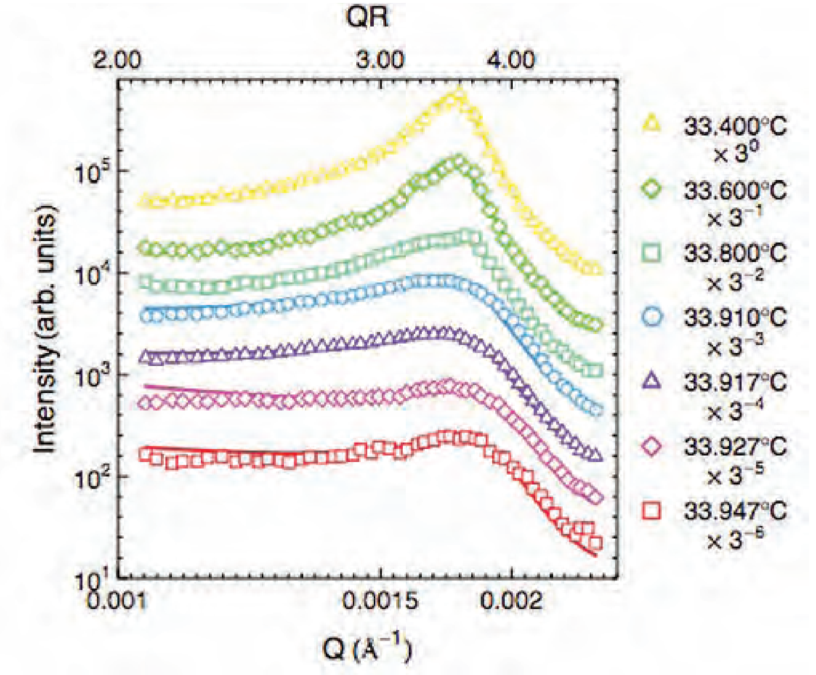

Fig. 3. Average SAXS intensity vs. wave vector offset values obtained for several temperatures on warming (run A). The lines are the best fits to the model. (© 2008 The American Physical Society. Reprinted with permission)

tion between the particles is increased by raising the temperature of the system, the glass once more becomes a liquid. As the caging particles attract each other, the trapped particles are released, and the structure breaks down.

But the experimenters found that if they raised the temperature still further, another glass transition took place—this one attraction-dominated rather than repulsion-dominated, just as MCT predicts (Fig. 3). Unlike the lower-temperature transition, in which particles are caged by one another—with everything keeping a respectful distance from everything else—in this new attraction-dominated structure, the particles are crunched together, squelching the free-motion characteristics of a liquid state. In between the two glass transitions, the intermediate liquid state obeys unusual logarithmic time dependence of the relaxations.

While other experiments using different techniques have shown similar phenomena, they required tedious procedures, such as precisely mixing samples, in order to alter the attraction strength. In the current work, the researchers did not have to do anything more complicated than turning up the heat. Simply by tuning the temperature, which changes the critical fluctuations in the binary fluid where the particles reside, they could change the strength of attraction between the particles. The team's work provides strong verification of the remarkable predictions of the behavior of such a model from MCT.

Aside from displaying a fascinating and unexpected behavior of certain physical systems, this experimental confirmation that a glass transition phase can occur by both heating and cooling may have practical implications. As scientists become more and more interested in controlling nanoparticles and nanoparticle structures, it is going to be very important for them to understand what sorts of nanoparticle phases can form. Such phenomena might interfere with the engineering and manufacture of nanoparticles and structures that make use of their unique qualities. It is also possible that materials scientists may find a way to turn this odd dual transition to their advantage in nanoprocessing or other applications.

— *Mark Wolverton*

See: Xinhui Lu[1], S.G.J. Mochrie[1]*, S. Narayanan[2], A.R. Sandy[2], and M. Sprung[2], "How a Liquid Becomes a Glass Both on Cooling and on Heating," Phys. Rev. Lett. **100**, 045701 (1 February 2008).

DOI: 10.1103/PhysRevLett.100.045701

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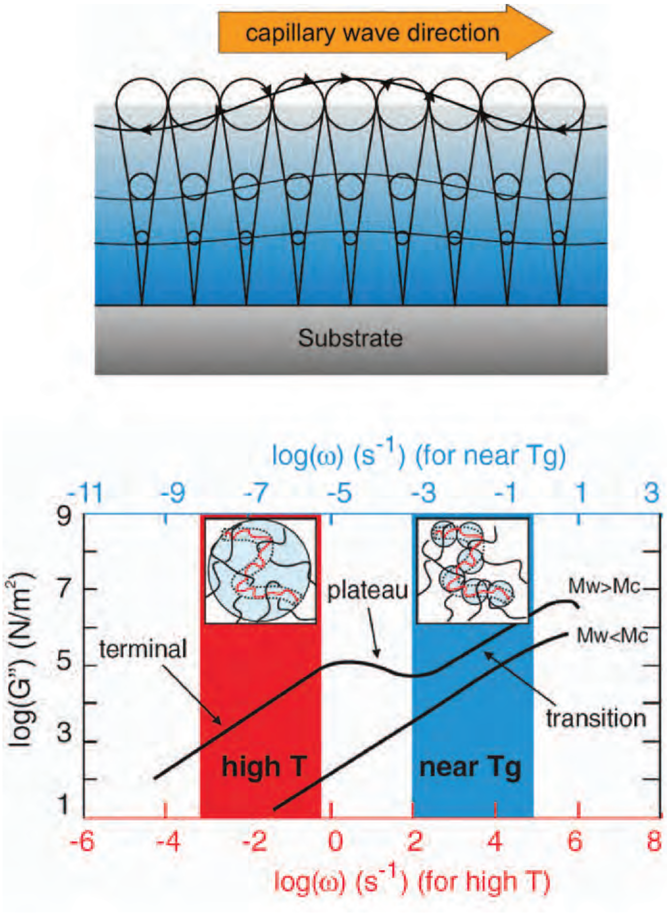
8-ID-I • XOR • Polymer science, materials science, physics • Intensity fluctuation spectroscopy, coherent x-ray scattering, small-angle x-ray scattering, x-ray photon correlation spectroscopy • 3.3-cm Undulator A • Accepting general users

RIDING THE WAVES TO PROBE LIQUID POLYMER FILMS

Capillary waves, which are fluctuations in the height of a liquid surface caused by hydrodynamic motion, are a natural and important phenomenon arising whenever air and water interface with each other. Capillary wave behavior can provide important clues about the dynamics, viscosity, kinetics, and other properties of the liquids in which they are seen. Just as waves can have important physical effects on the large scale (think: the ocean), their manifestation as capillary waves on the microscopic scale can have equally crucial impact. One example is liquid polymer films, where entanglement effects from polymer chains in the liquid can affect the dynamics of the capillary waves. This can serve as a vehicle for gathering new information about thin liquid polymer films, which are ubiquitous in our lives as coatings for slow-release fertilizer and timed-release medicines, photo prints, liquid-crystal TVs and computer monitors, and a host of other products and technologies. Researchers using an x-ray beamline at the APS have gained new information on how the motions of entangled polymer chains in a thin liquid film freeze as the film approaches the temperature at which the liquid goes into a glassy state.



Using surface x-ray photon correlation spectroscopy (XPCS) at the XOR 8-ID-I beamline at the APS, researchers from the University of California, San Diego; Northern Illinois University; Sogang University; and Argonne examined overdamped surface capillary wave relaxations on liquid polystyrene films of various molecular weights (M_W), thicknesses (d), and temperatures. X-ray photon correlation spectroscopy provides a noninvasive method for the study of both damping and propagation modes of capillary waves in molten polymer films as temperatures are adjusted. In highly viscous polymer films such as those examined in this study, all modes are essentially overdamped, so the researchers concentrated on observing relaxation times.

Studying the evolution of the intermediate scattering function (g2) to reveal film surface dynamics, they found that in films of $M_W > 30$ kg/mol, single exponential relaxation occurs at high temperatures, with multiple relaxation times with decreasing temperature. As temperature approaches the glass transition (T_g), single exponential relaxations are again seen. The capillary wave relaxation near the T_g temperature becomes independent of the molecular weight of the film. In films of $M_W < 30$ kg/mol, only single exponential relaxations are seen above the T_g temperature, and no g2 activity is seen at all below the T_g temperature.

The researchers explain this behavior by noting that at temperatures much higher than the T_g temperature, viscous flow in the surface films is in the low-frequency zone, and thus entangled polymer chains are able to diffuse according to the topological

"Waves" *continued on page 48*

< Fig. 1. Upper panel: Capillary waves on liquid surfaces. Lower panel: Frequency ranges of capillary wave measured by XPCS far above and near T_g.

HOW BINARY MIXTURES OF BLOCK COPOLYMER MICELLES FORM SUPERLATTICES

Block copolymers can work miracles when placed in the right solvents. The surfactants then self-assemble into aggregates called micelles, which have found many applications that today include drug delivery and design. At relatively high concentrations, micelles may self-assemble into larger, nanostructured lattices that can provide for a host of new application areas, such as templating agents in the production of molecular sieves and as separation media for DNA in capillary electrophoresis. Researchers from the University of Minnesota, using an APS beamline, explored the possibility that block copolymer micelles could be made to self-assemble into even larger structures, superlattices having unit cells whose dimensions are an order of magnitude greater than those of typical micelle lattices, thereby possibly taking micelle uses into a new realm, potentially including photonic applications.

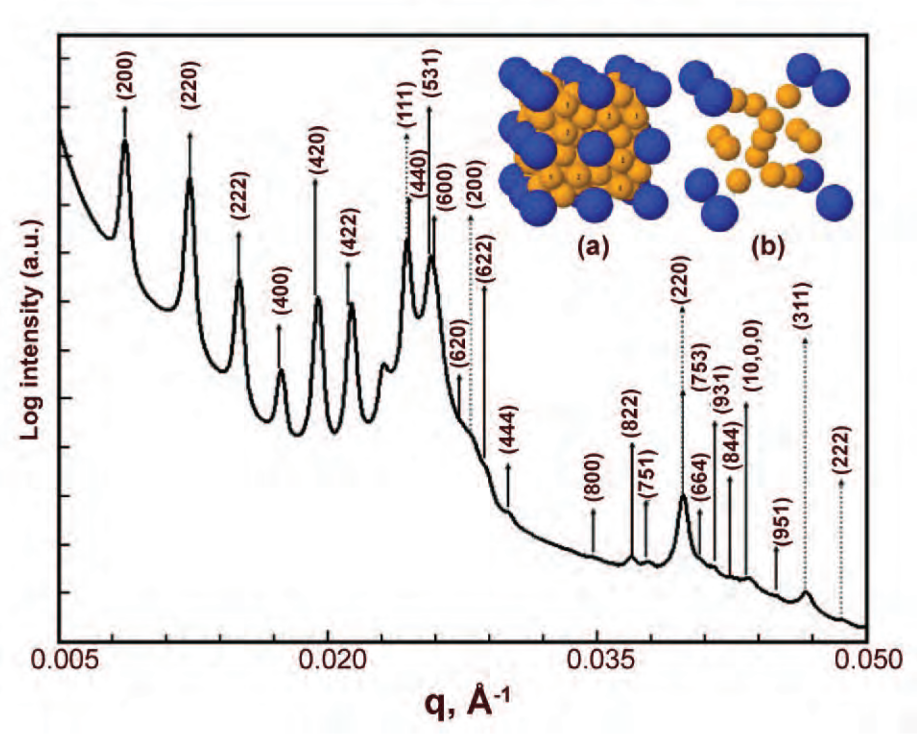


Fig. 1. One-dimensional scattering pattern from the sample 20% SD(16-9) + 4% SI(30-33) at room temperature. The peaks indexed by the solid lines correspond to the superlattice LS_{13}, whereas the dashed lines correspond to the coexisting FCC phase composed of small SD micelles. The inset (a) shows the full unit cell of the superlattice containing 104 small (S) spheres and 8 large (L) spheres. The structure can be simplified by considering 8 subcells. The structure of one such subcell is shown in inset (b). Twelve S spheres are located on the vertices of a regular icosahedron surrounding a sphere located at the center of the simple cube, whereas the large spheres occupy the corners of the cube. The icosahedron rotates by 90° between adjacent subcells in the unit cell shown in (a). The rotation is shown by labeling equivalent positions of two spheres (labeled “1” and “2”) within adjacent subcells.

The researchers’ basic approach was to mix two populations of AB and AC micelles in a solvent that is selective for the A block, in the hope that the two types of micelles would form a superlattice under the right conditions. The researchers adjusted the size and number ratios of the large and small micelles and the overall micelle volume fraction in solution. They also ensured that the B and C blocks were incompatible with one another and sufficiently different in electron density so that the two populations of micelles could be distinguished via cryogenic transmission electron microscopy (cryo-TEM) and small-angle x-ray scattering (SAXS). Additionally, the core blocks had to have glass transition temperatures that were below room temperature and molecular weights such that only spherical micelles of significantly different radii could exist in solution.

The diblock copolymers poly(styrene-*b*-isoprene) (SI) and poly(styrene-*b*-dimethylsiloxane) (SD) were selected and codissolved at various concentrations in the polystyrene-selective solvent diethyl phthalate. Dioxane, also a selective solvent for polystyrene, was chosen as the cosolvent. A cosolvent is required to codissolve the copolymers in dilute solutions, facilitating the formation of a binary mixture of micelles prior to ordering.

The researchers employed two SI diblocks and two SD diblocks. The size ratio of the smaller SD micelles (S) to the larger SI micelles (L) varied from approximately 0.5 to 0.6, based on hydrodynamic radii determined by dynamic light scattering. Due to the incompatibility between the polyisoprene and polydimethylsiloxane blocks, a binary mixture of distinct SI and SD micelles was formed in each mixed solution, as confirmed by cryo-TEM. When the total concentration of polymer was increased to 20-30%, the micelles adopted a superlattice structure, as revealed by SAXS. Small-

“Micelles” continued on page 48

"Micelles" from page 47

angle x-ray scattering showed the lattice to be the full LS_{13} superlattice (cubic, isomorphic to $NaZn_{13}$) in all cases, with unit cell dimensions in excess of 145 nm. A coexistent face-centered cubic phase composed of SD micelles was also observed when the number ratio of S to L micelles was large (Fig. 1). All x-ray scattering experiments were performed on the DND-CAT 5-ID beamline at the APS.

The results demonstrate conclusively that the full LS_{13} superlattice can be formed in binary mixtures of uncharged block copolymer micelles. When the concentration of L micelles is high, the superlattice is the dominant phase formed in samples having a size ratio that varied from 0.5 to 0.6. Samples with other size ratio values did not form superlattices. Theoretical studies have shown that entropy drives the formation of the superlattice structures. The driving force is greater in colloidal systems primarily because of the short-range, hard-sphere interparticle interactions. With micelles, the interactions are softer and the coronal chains are compressible, thereby providing the micelles with an additional degree of freedom. For example, when the number concentration of the particles is increased in solution, colloidal particles are forced to adopt superlattice structures to maximize the local free volume entropy; on the other hand, micelles can adjust their size by compressing coronal chains, thereby greatly reducing the entropic driving force to form superlattices.

Nonetheless, the formation of superlattices by micelles is seen as an important development, particularly because these results pave the way for creating new symmetries and larger lattice sizes using block copolymer micelles. — *Vic Comello*

See: S. Abbas and T.P. Lodge*, "Superlattice Formation in Binary Mixtures of Block Copolymer Micelles," Langmuir **24**, 6247 (2008). DOI: 10.1021/la8002367

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5-ID • DND-CAT • Materials science, polymer science • Powder diffraction, x-ray reflectivity, small-angle x-ray scattering, surface diffraction, wide-angle x-ray scattering, x-ray standing waves, x-ray optics development/techniques • 3.3-cm Undulator A • Accepting general users

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"Waves" from page 46

constraints of their immediate neighborhood, so a single relaxation is observed. When the temperature is lowered to near the glass transition, Rouse dynamics take over and "blobs" of entangled polymers form. Capillary waves show the overall effect of this as a terminal zone where M_W equals M_C (critical entanglement value). At intermediate temperatures, the formation and annihilation of the entanglement blobs of various lengths and times results in multiple modes and stretched relaxation times. To put it in other terms, the effective viscosity can be defined according to the particular measurement regime; at high temperatures, it is dominated by one value representing the diffusion of the entire polymer chain, and near the glass transition temperature by another single value that involves the diffusion of chain segments within the entanglement length. In between, the frequency dependence of the viscosity is more complex, as shown by the stretched exponential relaxation of the capillary waves.

The ability to fit the relaxation times at different film thicknesses, molecular weights, and temperatures onto a single universal curve has another useful byproduct: as long as entanglement hydrodynamics are taken into account, it allows scaling of the dynamics in various conditions, so that the behavior of the capillary waves can be used to probe the viscoelasticity of the liquid films. In effect, capillary waves can serve as a technique to peer into the viscoelastic and hydrodynamic behavior of these thin liquid polymer films. — *Mark Wolverton*

See: Zhang Jiang[1,2], Mrinmay K. Mukhopadhyay[1], Sanghoon Song[3], Suresh Narayanan[2], L.B. Lurio[4], Hyunjung Kim[3], and Sunil K. Sinha[1], "Entanglement Effects in Capillary Waves on Liquid Polymer Films," Phys. Rev. Lett. **101**, 246104 (2008). DOI: 10.1103/PhysRevLett.101.246104

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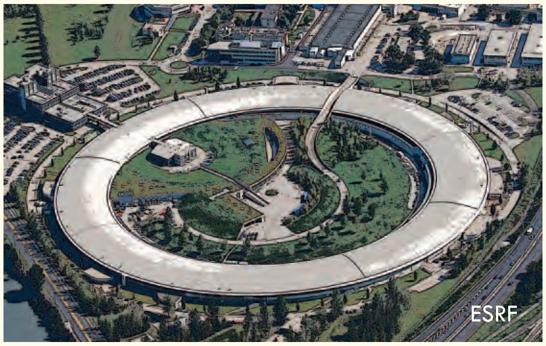
8-ID-I • XOR • Polymer science, materials science, physics • Intensity fluctuation spectroscopy, coherent x-ray scattering, small-angle x-ray scattering, x-ray photon correlation spectroscopy • 3.3-cm Undulator A • Accepting general users

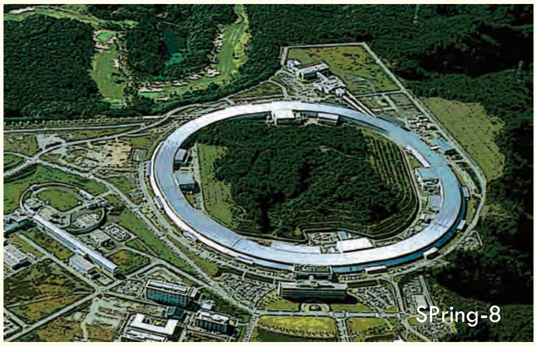
THE 2008 3-WAY MEETING

The 2008 3-Way Meeting participants in the atrium of the APS central lab/office building.

APS



ESRF



SPring-8

The 2008 Three-Way Meeting (3WM) between management and staff of the world's third-generation, hard x-ray synchrotron facilities was held at Argonne on March 18-19, 2008.

More than 20 representatives from each facility (the European Synchrotron Radiation Facility [ESRF] located in Grenoble, France; SPring-8, located at Harima Science Park City in Hyogo Prefecture, Japan; and the APS) were in attendance. Organizers of this year's meeting were Katherine Harkay (Argonne), Fabio Comin (ESRF), and Yoshiharu Sakurai (SPring-8).

Satellite workshops were held on March 17 on the topics "X-ray Optics," "Nanoscience with X-rays," and "User Services," and on March 19 on "Accelerator R&D."

Both the 3WM and the satellite workshops served as platforms for presentation and discussion of new developments that will positively impact the synchrotron radiation community well into the future and foster collaboration among the facilities.

The main meeting opened on March 18 with a welcome by Argonne Director Robert Rosner. He was followed by ESRF Director General William Stirling, who spoke on the current status of both the ESRF and the proposed upgrade program. Next, SPring-8 Director General Akira Kira delved into the "Socialization of SPring-8," followed by APS Director Murray Gibson on planning for the APS Renewal. Of particular interest in the discussions were the upgrade plans being proposed by each of the facilities. While different in detail, all three respond to the same science drivers – basically the realm of the ultra-small (<1 nm) and the ultra-fast (<1 ps).

There followed two very full days of presentations on topics of mutual interest to the three facilities. In the 3WM tradition, the directors' talks were followed by status reports on accelerator operation and stability, and on future accelerator development.

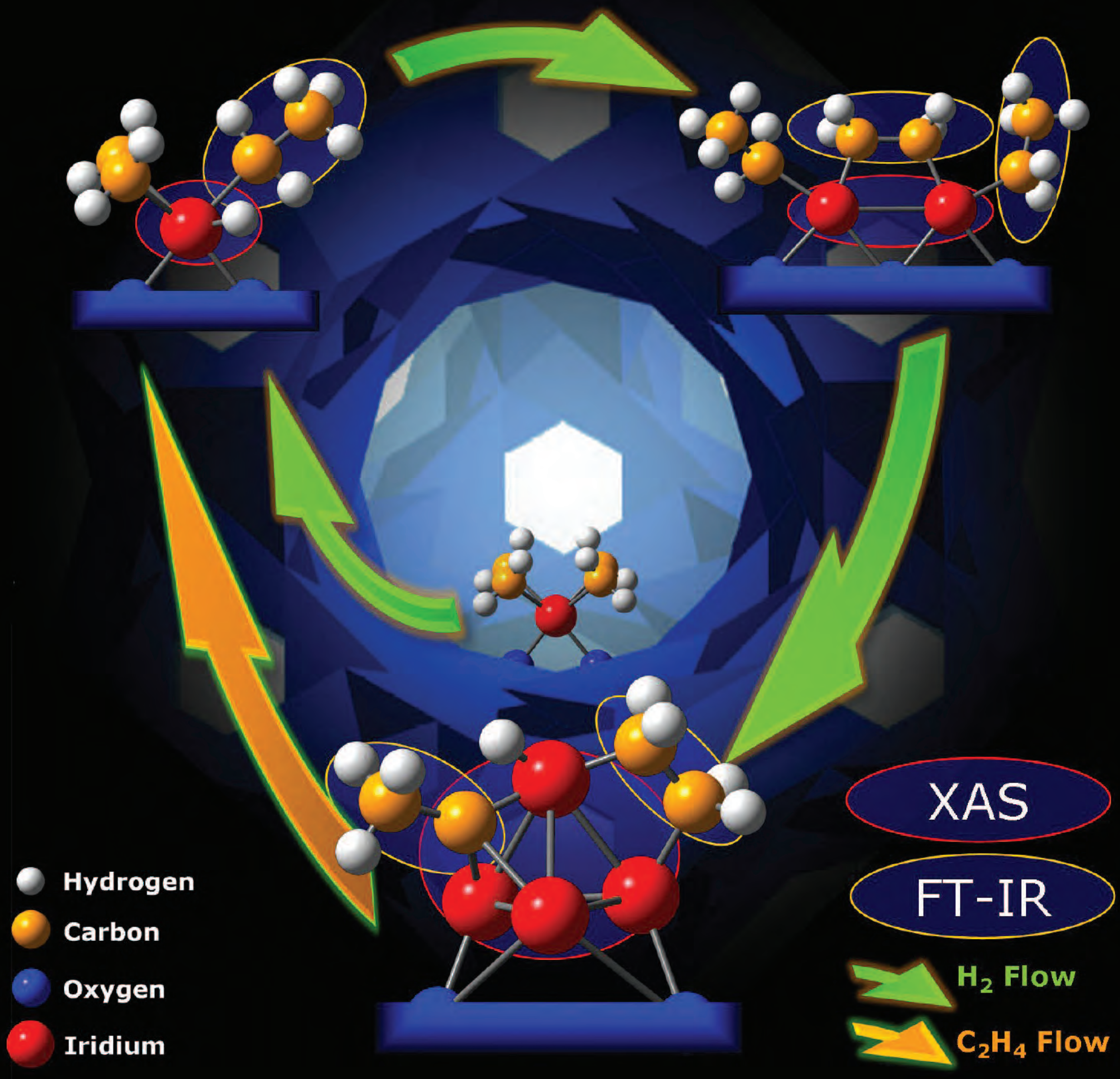
The rest of the meeting focused on beamlines and x-ray science, beginning with beamline strategic planning and including a discussion of scientific and economic regional links, and discussions of beamline enablers, including optics, detector development, and scientific data handling, with an emphasis on macromolecular crystallography.

Highlights of the meeting were presentations of exciting new scientific developments in nanoscience using x-rays, science with high-energy x-rays, dynamical single molecular observations of functional membrane proteins, polarization-dependent soft x-ray studies, advances in magnetism and soft condensed matter, and time-resolved science.

During the final session, the three facility directors reiterated the value of the 3WM and their support for future meetings. Interested visitors stayed on to participate in tours of the beamlines and the accelerator areas.

The 3WM Web site, with complete agenda, copies of the talks, and a photo gallery, can be found here.

SHIP-IN-A-BOTTLE CATALYSTS



Reversible formation and breakup of iridium clusters in a zeolite.
Illustration courtesy of Alper Uzun and Bruce Gates, UC Davis.

High-intensity x-rays from the APS are helping researchers from the University of California, Davis (UC Davis) investigate the properties of tiny clusters of metal that are constructed, ship-in-a-bottle-like, within the nanoscale pores of certain crystalline solids. This work is providing new information about the nature of the interface between metal clusters and a support material, and how this interface can be controlled and modified to improve industrial catalysts.

The researchers used compounds that contain both an organic and a metal component—organometallic precursors—to make structurally simple metal-oxide-supported and zeolite-supported metals, including single-metal-atom complexes, metal carbonyl clusters, and metal clusters.

They have shown that some of these compounds have catalytic properties for speeding up industrial chemical reactions. Like other solid catalysts, these offer the advantages of ease of separation from products of the reactions and lack of corrosion. Because they have uniform structures, they offer the prospect of selective conversions, with the added advantage of reducing the side products and overall energy demands of the chemical conversion.

The UC Davis team has experimented with so-called rhenium subcarbonyls supported on magnesium oxide, and with clusters containing 4 or 6 iridium atoms or 15 platinum atoms supported on alumina and in zeolites (crystalline aluminosilicates). The process of studying catalysts dissolved in liquids is usually obscured by the presence of solvent molecules, which bond to the metals and hide the details of their chemistry. When the metals are bonded to a support, they can be investigated in the absence of solvents, and the simplicity of the structures allows new insights into the structures and the chemistry. The understanding emerges from probing the structures with infrared spectroscopy and other techniques.

The researchers recently showed how to create well-defined clusters of the metal iridium, containing just four atoms of iridium in each cluster. They began by reacting an organometallic precursor containing iridium with the surface of the zeolite from which some of the aluminum had been removed. The dealumination process provided a set of isolated sites within the zeolite pores with which the precursor could react.

They used infrared spectroscopy to reveal the exact nature of the reaction between this precursor, $[Ir(C_2H_4)_2(acac)]$, and the zeolite. The spectra show that the zeolite's hydroxy (OH) groups are partially lost from the interior surface of the pores and the acac group (acetylacetone) splits off from the precursor. This dissociation process paves the way for the iridium atoms to anchor to the exposed reactive sites in the zeolite. The researchers used extended x-ray absorption fine structure (EXAFS) data, recorded at the MR-CAT 10-ID beamline at the APS, to show that, at this stage, only single, site-isolated iridium units were present in the zeolite pores.

The next step on the road to creating the well-defined iridium clusters was to initiate cluster formation by removing the ethylene groups that remained π-bonded to the iridium atoms by reaction with hydrogen gas; as a result, the bonds anchoring the iridium atoms to the zeolite were disrupted. The team followed the changes by continually checking via infrared spectroscopy and EXAFS spectroscopy. After just minutes, the spectral peaks associated with the attached ethylene ligands began to shrink and new peaks associated with ethyl groups replaced them; these peaks, in turn, disappeared as ethane gas formed and flowed out of the zeolite.

More critically, however, new weak spectroscopic bands indicative of a different type of group formed from ethylene emerged, bands that could only exist if more than two metal atoms were close together, thus hinting at the onset of iridium cluster formation. At this stage, EXAFS was unable to see these sparse fledgling clusters.

Heating the material in a flow of hydrogen gas and monitoring with x-ray absorption near edge spectroscopy and EXAFS spectroscopy proved that Ir-Ir bonds were forming. This process involved continuous breaking of bonds between carbon atoms and iridium, and the migration of individual iridium atoms within the pores of the zeolite.

The researchers emphasize that, strictly speaking, the notion of a ship-in-a-bottle catalyst remains unexplained. What is known is that the zeolite pores are like tiny cages linked by windows. The team's clusters formed within the cages and when they became larger than the diameter of the windows, they could no longer escape and were potentially stabilized like ships in bottles.

This work is leading to new insights about the nature of the interface between metal clusters and a support material, and how this interface can be controlled and modified to improve catalysts. — *David Bradley*

See: Alper Uzun and Bruce C. Gates*, "Real-Time Characterization of Formation and Breakup of Iridium Clusters in Highly Dealuminated Zeolite Y," Angew. Chem. Int. Ed. 2008 **47**, 9245 (2008).
DOI: 10.1002/anie.200802140

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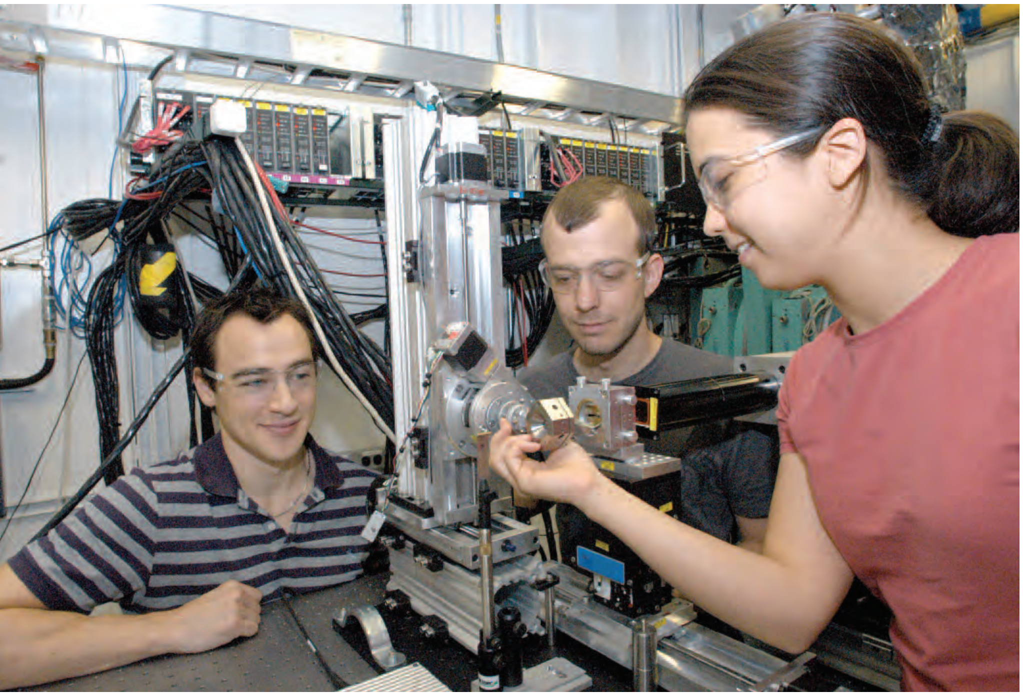
10-ID • MR-CAT • Materials science, environmental science, chemistry • Microfluorescence (hard x-ray), x-ray absorption fine structure (XAFS), diffraction anomalous fine structure, micro-XAFS • 3.3-cm undulator A • Accepting general users

PUTTING THE PRESSURE ON MOFS

Sometimes, it's not what is on the outside that matters, but what happens inside, in the spaces in between. That is certainly the case with metal-organic framework (MOF) materials, which are crystalline constructs made up of metallic ions connected to organic molecules, put together in such a way that "guest" molecules can find temporary havens within spaces and cavities inside the MOF structure. It's a handy attribute with a wide range of possible applications, from filtering, capturing, or detecting molecules such as carbon dioxide, to storing large amounts of hydrogen in a very small space for use in fuel cells for cars. But before such practical uses can be fully realized, we need a better understanding of how MOFs react to real-world conditions outside of the controlled conditions of the laboratory. A group of Argonne National Laboratory researchers using an APS beamline investigated the behavior of a classic MOF structure under high pressures, including its compressibility characteristics, changes in morphology, and the permeability and diffusion of guest molecules. This study has important implications for the ways MOFs might be used for gas storage and other vital applications.



Left to right: Gregory J. Halder (Materials Science Division), Peter J. Chupas (X-ray Science Division), and Karena W. Chapman (X-ray Science Division) with a portable *in situ* diffraction assembly set-up in the XOR 1-BM research station.

The Argonne experimenters studied a pulverized sample of Cu-btc [Cu_3 (1,3,5-benzenetricarboxylate)$_2$(H_2O)$_3$], subjected to various pressures from 0 to 8 GPa inside a diamond anvil cell (DAC), both without and with several different types of pressure-transmitting fluid. Monochromatic x-rays from the XOR 1-BM beamline at the APS provided high-pressure diffraction data to probe the behavior of the MOF lattice (Fig. 1).

As a MOF system containing guest molecules is compressed, additional guest molecules from the pressure-transmitting fluid are forced into the accessible cavities inside the MOF. At low pressures, where both the pressure within the DAC and within the cavities increase in parallel, the MOF structure largely holds up against the pressure. But as pressures inside the DAC increased, the experimenters observed a sharp transition from this "hard" regime to a "soft" regime, in which the Cu-btc framework rapidly compresses under the pressure.

The threshold pressure for this hard-to-soft transition depended on which pressure-transmitting fluid was used within the DAC, and occurred at higher pressures in methanol-ethanol-water (MEW) than in isopropyl alcohol. The transition pressure also varied according to the rate at which pressure was applied, beginning at higher pressure under slow compression compared to rapid compression. In the experiments , either without any pressure-transmitting fluid or with the use of Fluorinert (a large-molecule organic liquid), no hard-to-soft transition occurs.

This difference in the observed MOF behavior is due to the presence of smaller molecules in the alcohol-based pressure-dependent fluid that can permeate into the Cu-btc cavities. (The Fluorinert molecules are too large to enter the pores of the Cu-btc framework.) The Cu-btc MOF is able to admit a large number of these extra "guests" into the pore network of its structure to create a hypersaturated state. The

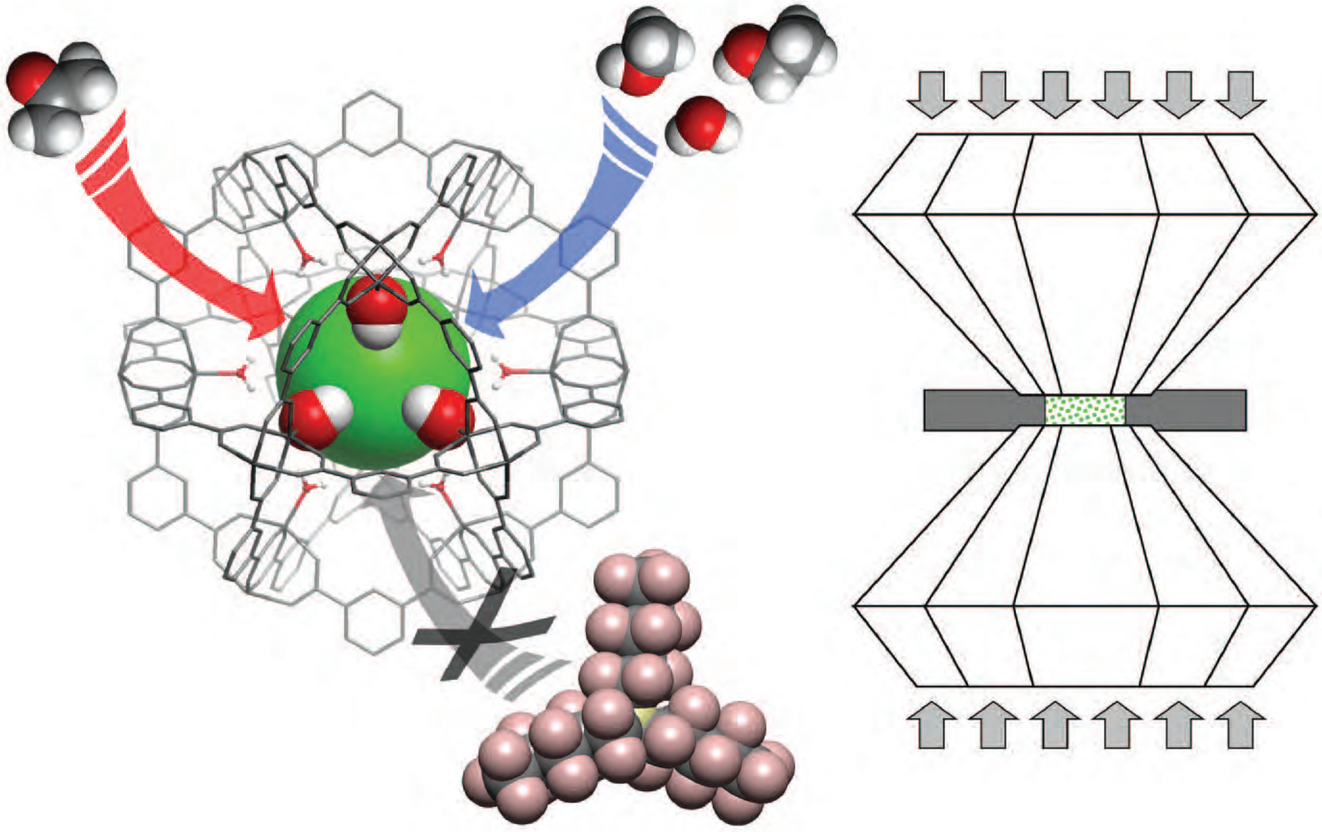


Fig. 1. The nanoporous metal-organic framework material Cu$_3$(1,3,5-benzenetricarboxylate)$_2$(H$_2$O)$_3$•{guest} exhibits anomalous compression under applied pressure that is associated with the hyper-filling of the pore network. The dramatic hard-soft transition depends on the availability and size of potential guests relative to the framework apertures.

guest molecules contained within the MOF framework help to counteract the external pressure on the MOF structure until a certain threshold pressure is reached, after which the MOF rapidly flexes and compresses. Beyond this threshold, the spaces within the MOF are compressed to the point where they are unable to allow any further guest molecules into the cavities. The pressure threshold depends on the size of the guest molecules; the larger the molecules, the lower the transition pressure. Smaller guest molecules also remain more mobile and able to seek out pores for longer times under pressure. The framework compressibility and flexing that occurs as the soft regime is entered is comparable to ionic solids such as NaCl. These responses of the Cu-btc MOF system to high pressure show some interesting differences when compared to those of other industrially important porous materials, such as nanoporous zeolites, that seem to be based on their differing structures.

The work of the Argonne group has provided not only a new way to peer into the behavior of MOF systems, but also hints at the practical possibilities such materials hold.

— *Mark Wolverton*

See: Karena W. Chapman*, Gregory J. Halder, and Peter J. Chupas, “Guest-Dependent High Pressure Phenomena in a Nanoporous Metal-Organic Framework Material,” J. Am. Chem. Soc. **130**(32), 10524 (2008). DOI: 10.1021/ja804079z

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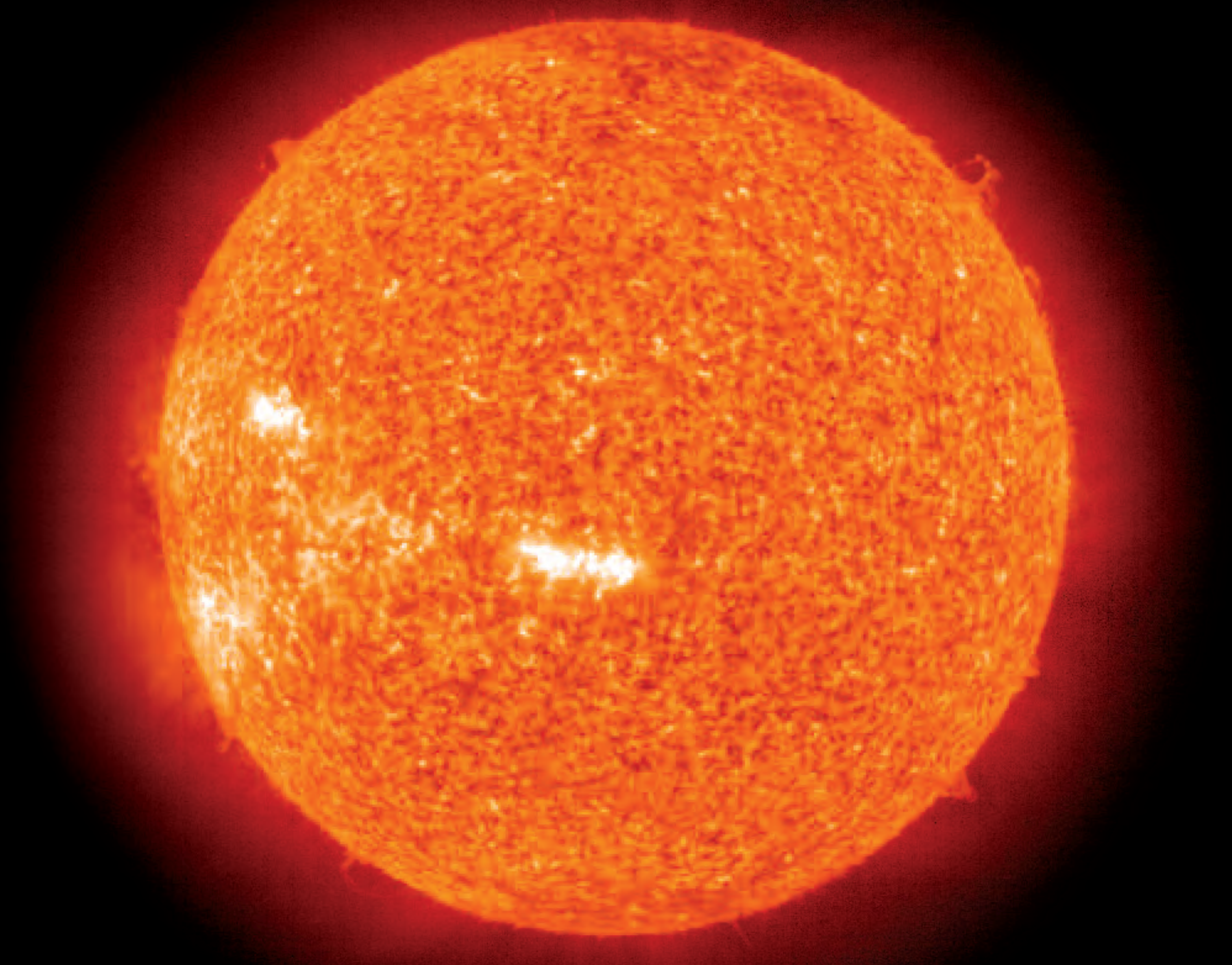
See also: Gregory J. Halder, Karena W. Chapman, Suzanne M. Neville, Boujemaa Moubaraki, Keith S. Murray, Jean-François Létard, and Cameron J. Kepert, “Elucidating the Mechanism of a Two-Step Spin Transition in a Nanoporous Metal−Organic Framework,” J. Am. Chem. Soc. **130**(51), 17552 (2008). DOI: 10.1021/ja8068038

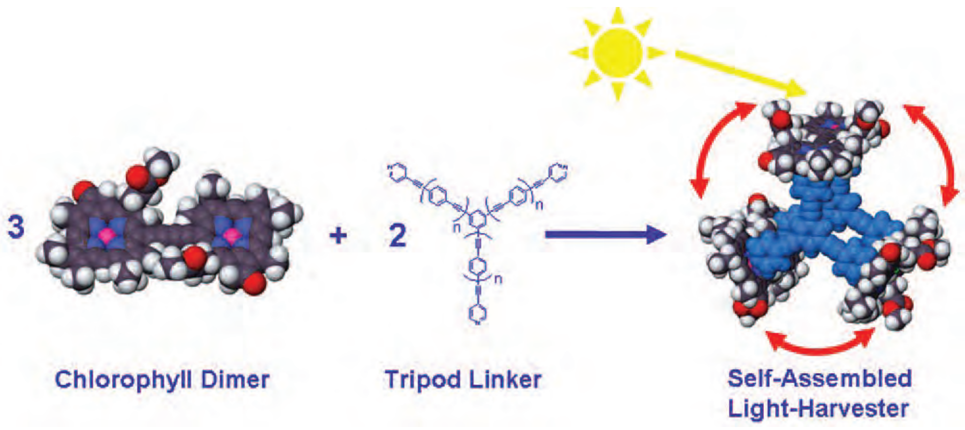
Work performed at Argonne National Laboratory and use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357. Portions of the diamond anvil cell preparation were performed at GeoSoilEnviroCARS, Sector 13 at the APS. GeoSoilEnviroCARS is supported by the National Science Foundation, Earth Sciences (EAR-0622171), and Department of Energy, Geosciences DE-FG02-94ER14466).

1-BM • XOR • Physics, materials science, chemistry • Powder diffraction • Bending magnet • Operational

SHEDDING LIGHT ON SOLAR ENERGY CONVERSION



Over millions of years, plants evolved the ultimate renewable energy resource: photosynthesis. Plants absorb light from the sun, produce a flow of electrons, and then use the electrons to power the chemical combination of carbon dioxide from the air with water to make their food. Oxygen is the main by-product of this process. Researchers using an x-ray beamline at the APS are hoping to take a leaf out of nature's book to tap into that electron flow step and convert solar energy directly into electricity. (Photo: The sun seen in extreme ultraviolet showing a coronal mass ejection. Image courtesy ESA, NASA, SOHO/EIT)



< Fig. 1. Chemical groups self-assemble to form a light-harvesting chlorophyll (prism) whose structure was determined by small- and wide-angle x-ray scattering. Upon light excitation, ultrafast energy transfer occurs between the prism faces in about ten trillionths of a second. These prisms show how ordered structures can serve as efficient light-harvesting antennae for artificial photosynthesis.

The researchers, from Northwestern University, Kyoto University, and Argonne National Laboratory, carried out x-ray scattering measurements at the XOR/BESSRC beamline 12-ID at the APS to investigate a novel chemical system that mimics photosynthesis.

One of the key requirements of a photovoltaic material based on inexpensive organic compounds rather than costly and fragile semiconductors, is that it efficiently transfer the energy trapped from sunlight across the relatively long distance to the point where electrons are generated and from which a current can be tapped off.

Chlorophylls are the light-absorbing molecule in green leaves. Other researchers have tried to build arrays of chlorophyll molecules to act as the light traps. Linking these arrays together can be done using organic groups, including constructed ethynyl and butadiynyl linkers. These linkers can boost the absorption of light energy, but allow the chlorophylls to rotate within the array, making overall efficiency lower than it might be.

To combat this problem, the researchers in this study exploited the concept of self-assembly (the organization of molecular units into ordered structures by non-covalent interactions) to build rigid, flat arrays of chlorophylls with optimal light-absorbing capacity. Using specially designed linkers, the chlorophylls lock together, lying flat with no possibility of rotation and none of the stressed bending seen with rigid, metal-based linkers that have been used by other research groups. Utilizing a butadiyne linker combined with the triethynylpyridylbenzene molecule allowed the team to construct sophisticated supramolecular assemblies. By adding a metal-containing chemical group, or coordinating ligand, the team triggered spontaneous self-assembly of chlorophyll into prismatic structures in which pairs of chlorophyll molecules form the faces of the prisms.

The resulting chlorophyll faces are entirely flat—which is essential for efficient light-absorption—while the close proximity of the faces allows energy to bounce from one unit to the next via the faces. Moreover, the three-dimensional structure of the units gave the researchers the opportunity to bias the orientation of the molecular prisms in the solid phase, again allowing them to boost light absorption and energy transfer efficiency.

To demonstrate that the relative rate of rotation of the chlorophyll groups around the butadiyne bond linking them is essentially zero, the team used high-speed femtosecond transient absorption spectroscopy. They turned to small-angle x-ray scattering experiments in solution using the synchrotron source to confirm the detailed structure of the light-absorbing materials (Fig. 1).

To test the viability of their prism arrays as mimics of plant photosynthesis, the team carried out photoexcitation experiments. They found that light shone on the prismatic assemblies was absorbed efficiently, and energy transferred well between the pairs of chlorophylls within the prisms. They were able to fine tune the response of the assemblies by using metal-binding ligands of different sizes to vary the size of the prisms and so control the separation between their faces.

The insights the team has obtained into how to control the absorption of light and energy transfer within artificial photosynthesis units will be crucial to the design of future materials for solar energy conversion that will bring us closer to emulating how plants use renewable energy sources so effectively. — *David Bradley*

See: Richard F. Kelley[1], Suk Joong Lee[1], Thea M. Wilson[1], Yasuyuki Nakamura[3], David M. Tiede[2], Atsuhiro Osuka[3], Joseph T. Hupp[1], and Michael R. Wasielewski[1,2]*, "Intramolecular Energy Transfer within Butadiyne-Linked Chlorophyll and Porphyrin Dimer-Faced, Self-Assembled Prisms," J. Am. Chem. Soc. **130**, 4277 (2008). DOI: 10.1021/ja075494f

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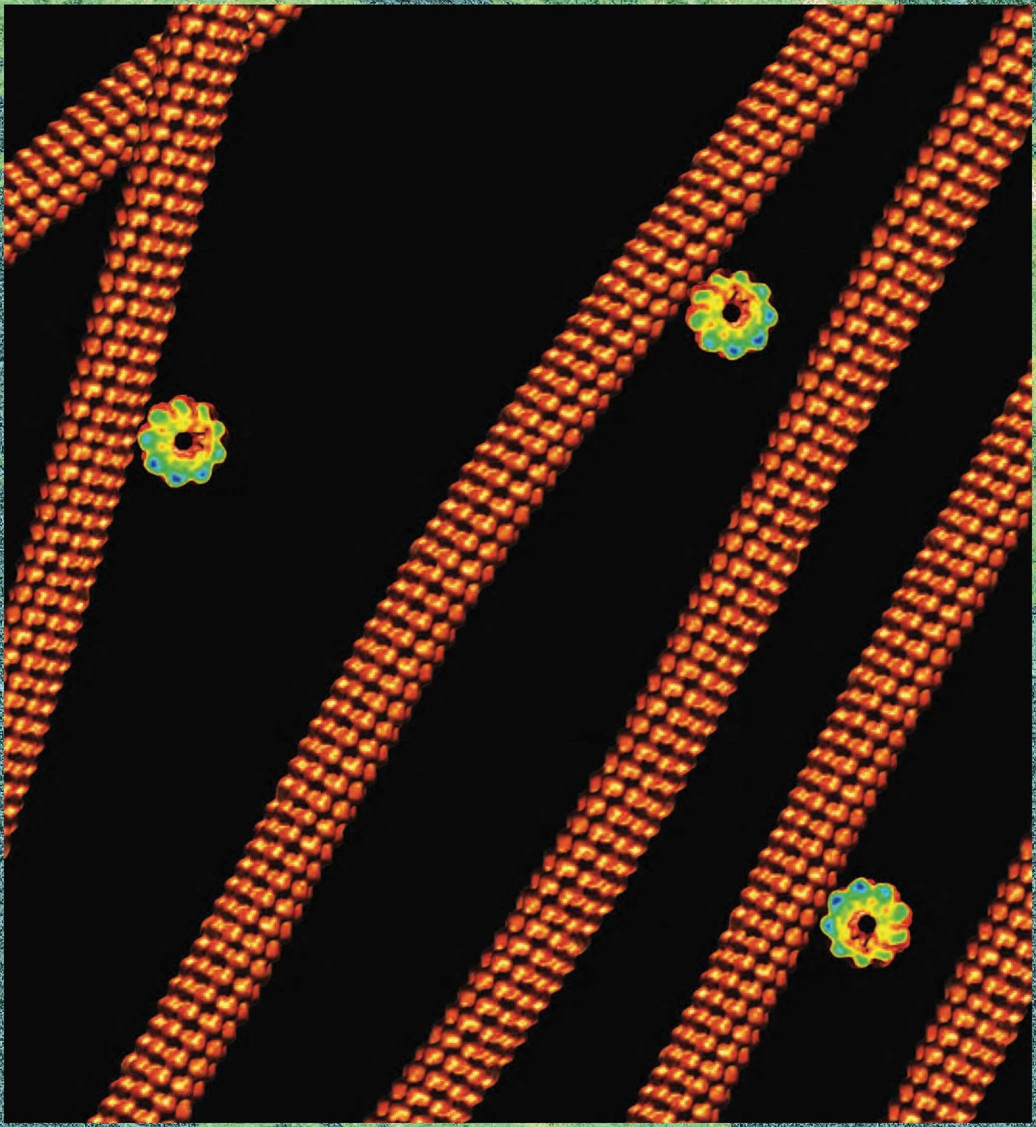
This work was supported by the Chemical Sciences, Geosciences, and Biosciences Division, Office of Basic Energy Sciences, DOE, under Grant Nos. DE-FG02-99ER14999 (M.R.W.) and DE-FG02-87ER13808 (J.T.H.) and under Contract DE-AC02-06CH11357 (D.M.T.). Y.N. thanks the Japan Society for the Promotion of Science for a Young Scientists Research Fellowship. SAXS studies at the Advanced Photon Source were supported by the Office of Science, Office of Basic Energy Sciences, DOE, under Contract No. DE-AC02-06CH11357.

12-ID • XOR/BESSRC • Chemistry, physics, materials science • Small-angle x-ray scattering, wide-angle x-ray scattering, grazing incidence small-angle scattering, surface scattering • 3.3-cm Undulator A • Accepting general users

REVEALING THE STRUCTURAL SECRETS OF PLANT VIRUSES



Viruses are extremely successful at finding ways to circumvent just about every host defense system. The secrets to this success seem to lie in their simplicity—small genomes and a metabolism that relies in part on the biochemistry of the host—and in their elegant, often breathtakingly beautiful and highly functional structures. Viral architecture, especially the coat protein structure, is intricately intertwined with successful invasion and infection of the host. Yet for many viruses, and particularly for a very large group of plant viruses, details of their structures have remained elusive. But researchers using a high-brilliance x-ray beamline at the APS have obtained important details about the structures of a soybean and a potato virus. This is good news for crop scientists concerned with finding ways to combat viral infestations.

Over the years, scientists have has invested much time and effort searching for methods to learn more about the structures of flexible filamentous viruses. By doing so, they hoped to find ways of combating the economic devastation resulting from crop loss due to viral infestations. The researchers in this study, from Vanderbilt University, the Boston University School of Medicine, the Illinois Institute of Technology, the University of Kentucky, and Brookhaven National Laboratory, used a variety of techniques, including fiber diffraction data collected on the Bio-CAT beamline 18-ID at the APS, to determine that the viruses they studied, and by extension most flexible filamentous viruses, have similar coat protein folds and helical symmetry, with a little less than nine subunits per helical turn. This new knowledge marks great progress in understanding how these plant viruses operate and will help scientists figure out how to outsmart the viruses and prevent viral infections.

The research team determined the symmetry and low-resolution structures of a potyvirus (soybean mosaic virus), and a potexvirus (potato virus X). These viruses represent the two largest families of flexible filamentous viruses, the *Potyviridae* and the *Flexiviridae*.

< Fig 1. Segments of the potyvirus soybean mosaic virus; several virions are also shown in cross-section. The symmetry and low-resolution structure of this virus are very similar to those of the potexvirus potato virus X, suggesting that flexible filamentous plant viruses share a common coat protein fold and approximate helical symmetry.

Together with some smaller families, they make up the largest group of plant viruses. These viruses are of enormous economic importance. Members of the potyvirus family account for half of the viral crop damage worldwide, but their structures had proved difficult to characterize because of such factors as flexibility, instability, and low levels of expression. The variety of methods the research team employed—fiber diffraction at the Bio-CAT beamline, cryo-electron microscopy (cryo-EM), and scanning transmission electron microscopy (STEM)—allowed them to overcome these problems and to finally produce structural data.

The researchers obtained, for the first time, well-oriented fiber diffraction data from a potyvirus. They then used these data to determine radial density and, when combined with the STEM and cryo-EM data, viral symmetry. The cryo-EM, together with the fiber diffraction data, allowed the group to determine the overall viral structure and produce a reconstructed image that showed the subunit shape and arrangement in this potyvirus (Fig. 1).

For comparison, the group then went on to study the structure of potato virus X at a comparable resolution and to confirm the previously characterized symmetry of this virus. The structures and symmetries of the two viruses were unexpectedly similar, suggesting that these two virus families, the *Potyviridae* and the *Flexiviridae*, are structurally related.

The latter result is surprising in that previous work showed little similarity in the proteins making up the coats of these viruses. Now that good structural data are available, however, the evidence points to similarity and evolutionary relationships between soybean mosaic virus and potato virus X, and by implication among all flexible filamentous plant viruses. This is good news to crop scientists concerned with finding ways to combat viral infestations. It means that when an anti-viral treatment based on viral structure works against one virus, there is a good chance it will work on others in this group. How viruses so successfully infest plants has just become a little less secretive. — *Mona Mort*

See: Amy Kendall[1], Michele McDonald1, Wen Bian[1], Timothy Bowles[1], Sarah C. Baumgarten[1], Jian Shi[1†], Phoebe L. Stewart[1], Esther Bullitt[2], David Gore[3], Thomas C. Irving[3], Wendy M. Havens[4], Said A. Ghabrial[4], Joseph S. Wall[5], and Gerald Stubbs[1*], "Structure of Flexible Filamentous Plant Viruses," J. Virol. **82**(19), 9546 (October 2008). DOI: 10.1128/JVI.00895-08

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18-ID • Bio-CAT • Life science • Microfluorescence (hard x-ray), microdiffraction, small-angle x-ray scattering, time-resolved x-ray scattering, micro-x-ray absorption fine structure, fiber diffraction • 3.3-cm Undulator A • Accepting general users

DNA STRETCHES BETTER WHEN RELAXED

When DNA takes part in crucial biomolecular processes, such as transcription or cell division, it must partly or wholly uncoil out of the compact form it assumes in cell nuclei. Because the shape of DNA can influence its biochemical interactions, scientists have long been interested in the molecule's physical characteristics, and have modeled it as an elastic rod that can stretch, bend, and twist. Experiments performed at XOR/BESSRC beamline 12-ID at the APS, and at the Stanford Synchrotron Radiation Laboratory add a new wrinkle to this model, indicating that DNA in a relaxed state is much less stiff than direct stretching measurements have indicated. The results also imply that fluctuations in the length of a DNA segment occur through cooperative variations among its constituent base pairs. The findings hint at the possibility of novel biomolecular mechanisms.

Researchers have directly imaged double-helix DNA segments some thousands of base pairs long, dissolved in a neutral medium, in order to track the random structural variations that occur in the absence of any external influences. From such measurements the stiffness of DNA's molecular structure can be inferred, but in practice it has been difficult to separate out stretching, bending, and twisting motions, each of which has a different stiffness coefficient.

To simplify the problem, a team of Stanford University researchers generated DNA segments ranging from 10 to 35 base pairs (bp) long, in 5-bp increments. These snippets, the researchers argued, should undergo negligible bending and twisting, so that length variations will come about only through stretching and compression of the molecular structure. To measure those variations, the team chemically attached gold nanoparticles to both ends of each DNA segment, then recorded the interference fringes created by small-angle x-ray scattering from solutions containing the gold-augmented DNA.

X-rays scattered by the DNA and the gold nanoparticles contribute to the interference pattern. The researchers also recorded the scattering of x-rays by DNA with no gold nanoparticles, and by DNA with nanoparticles at one end only. Comparison of the different scattering patterns yielded a prominent interference peak due to x-rays scattering from nanoparticles at either end of the same DNA segment. The position of that peak gives the average distance between the two nanoparticles—and therefore the average length of a DNA segment—while the width of the peak corresponds to the fluctuation in that length.

Two surprising results emerged. First, the length variations were considerably larger than would have been calculated from the stiffness coefficient derived from experiments in which a length of DNA is physically stretched. The Stanford scientists deduced that DNA, in a relaxed state, is at least 10 times “softer” than when under tension. As a possible explanation for this finding, they suggest that each interval between base pairs can switch easily between two conformations of slightly different length, but that when DNA is under tension, all base-pair intervals move into the longer conformation, and resistance to further lengthening becomes much greater.

Second, the statistical variance in the length of DNA segments increased quadratically with the number of base pairs, whereas for a simple elastic rod the variance should be directly proportional to the number of base pairs. Quadratic behavior naturally arises if length fluctuations of DNA occur in a cooperative manner along the length of the molecule—that is, all intervals between adjacent base pairs tend to stretch or contract in unison.

The researchers' interpretation of their findings suggests ways in which the mechanics of DNA could influence its biochemistry. For example, some proteins may bind better to DNA when it is in the longer of the two possible conformations, and the cooperative behavior of the molecule would then put neighboring segments of DNA in the longer conformation, which could in turn favor or disfavor the binding of other proteins. — *David Lindley*

See: Rebecca S. Mathew-Fenn[1], Rhiju Das[1,‡], and Pehr A.B. Harbury[1*], “Remeasuring the Double Helix,” Science **322**, 446 (2008).

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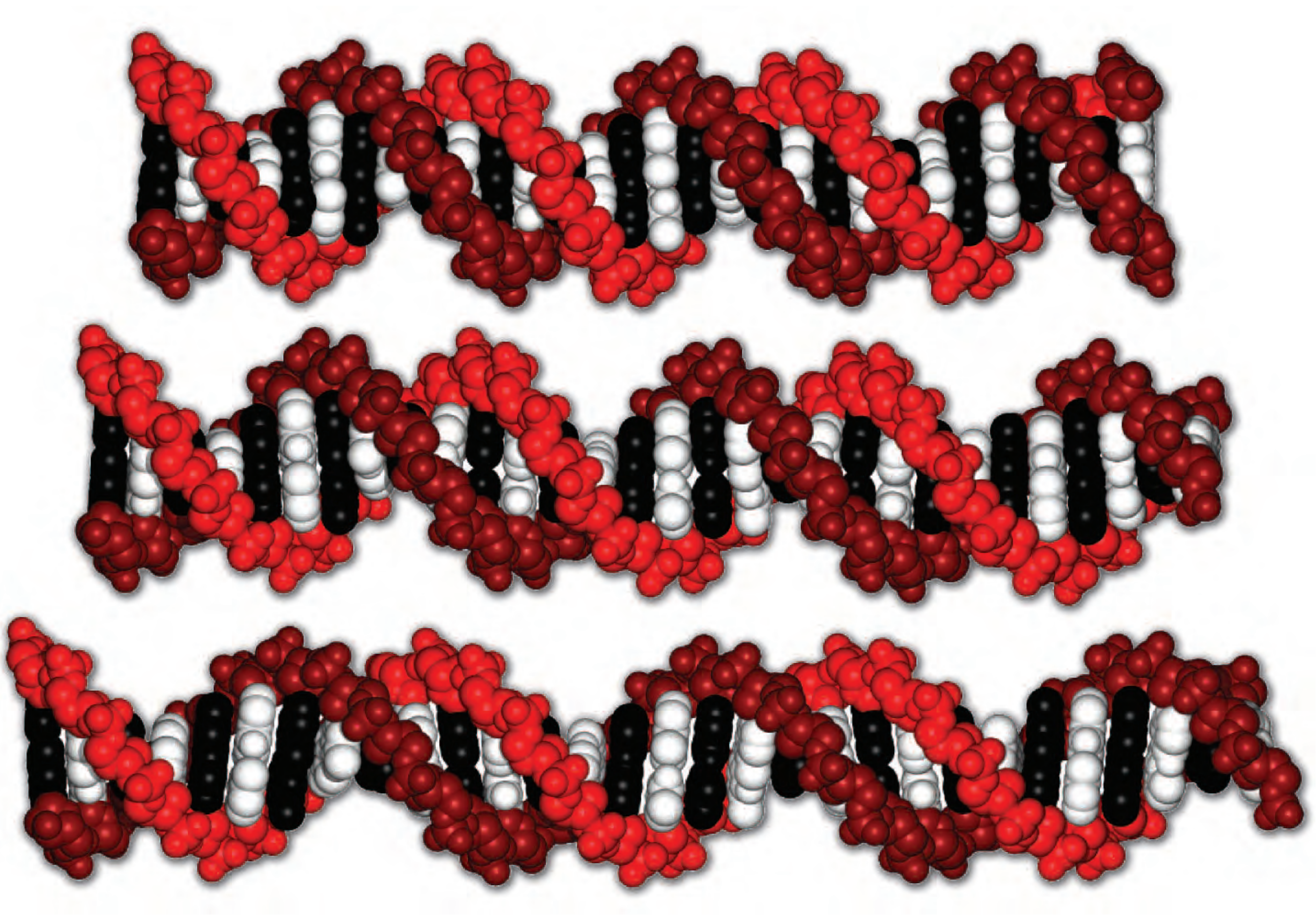
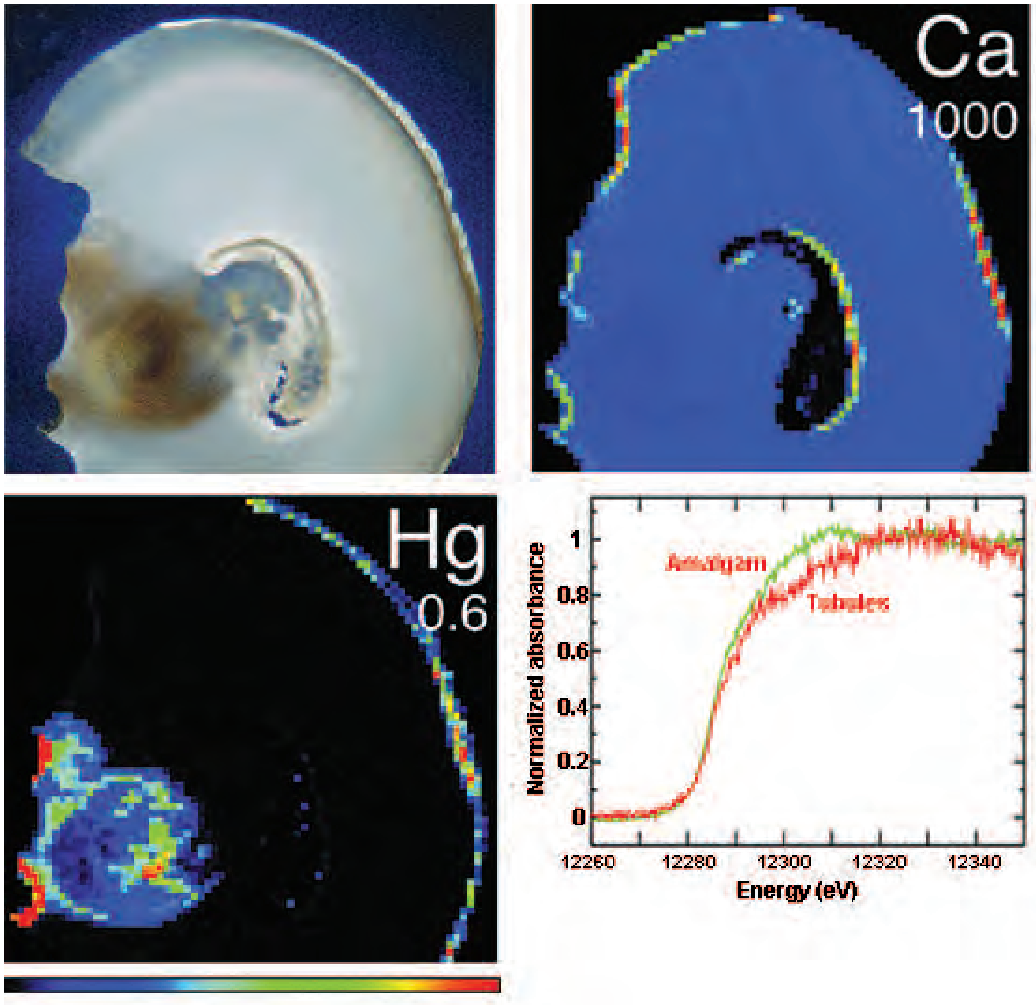
12-ID • XOR/BESSRC • Chemistry, physics, materials science • Small-angle x-ray scattering, wide-angle x-ray scattering, grazing incidence small-angle scattering, surface scattering • 3.3-cm Undulator A • Accepting general users



Calculated models of a 30-base-pair segment of DNA show how structural adjustments can cause the segment's length to decrease (top) or increase (bottom) by 10% relative to the normal length (middle). Conformational changes of this sort may explain why DNA in a relaxed state shows greater length variations than would be expected from the measured stiffness of DNA when under tension.

MERCURY TAKES A DETOUR

Mercury can be found inside thermometers and in fillings in our teeth, a purpose for which it has been used for decades. But as the pernicious effects of mercury in the human body have become better known, controversy has arisen over its use in dental fillings. While the jury is still out on whether mercury-based dental amalgam is ultimately harmful, there's no doubt that a better understanding of how mercury and other potentially harmful substances make their way from dental fillings into the body—and in what amounts—is essential. Research at an APS beamline has confirmed that measurable amounts of mercury and zinc can migrate from fillings, through the tooth, and into the dental pulp where they can be absorbed into the bloodstream.



Generally, the main avenue of dental mercury exposure has been considered to be direct inhalation or ingestion from evaporation or erosion from the surface of fillings. But another possibility is the actual migration of mercury through the tooth until it reaches the pulp and is absorbed by the bloodstream. If this is happening, it could not only skew the data of epidemiological studies dealing with the other absorption pathways, but could prove to be another significant source of mercury toxicity that needs to be considered. Can mercury find its way into the body through the teeth, and if so, in significant amounts?

A team of researchers from The University of Sydney, Stony Brook University, Eastmac Pty Ltd., and Argonne set out to probe these questions by examining human teeth using x-ray fluorescence (XRF) and x-ray absorption near-edge spectroscopy (XANES) at APS beamlines. The experimenters studied extracted teeth that had been filled with mercury-based dental amalgam for at least 20 years to see whether amalgam material had migrated from the fillings through the tooth, and whether the material had altered in chemical form, along with control samples without fillings. The experimenters used XRF and DPC (differential phase contrast) imaging at the XOR 2-ID-E beamline to determine the presence and spatial distribution of Hg, Ca, Zn, and Cu. X-ray fluorescence and XANES were employed at the XOR 2-ID-D beamline to obtain spectroscopic information on the materials distributed throughout the sample teeth.

The XRF studies showed definite migration of mercury and zinc throughout the teeth, extending from the location of the filling and filling lining to the dentine and pulp boundary. Interestingly, however, the movement of the metals through the tooth was not consistent, with some areas that would have been in direct contact with amalgam showing little or no sign of contamination. As expected, calcium showed even distribution throughout the samples. Several mercury and copper hotspots were noted to coincide with features in the DPC images, which the researchers believe are probably the result of residual amalgam diffusing through protrusions of pulp (pulp horns, small projections of vital pulp tissue directly under a cusp or developmental lobe) in the tooth.

X-ray absorption near-edge spectroscopy spectra revealed that at least some of the mercury seen in the dental tubules (minute channels in dentin, extending from the pulp cavity to the overlying cement and enamel) was partially oxidized compared to the mercury in the residual amalgam. Zinc was more evenly distributed throughout the dental material, whereas mercury seemed to concentrate in the tubules, indicating that the transport mechanisms of the two metals through the tooth are likely to be quite different.

The study confirms that both mercury and zinc can definitely migrate from fillings through the tooth into the dental pulp, and be absorbed into the bloodstream. It is clear that substantial amounts can pass into the body through this pathway. Because the samples examined were all at least 20 years old, it was not possible to determine how long the process takes on the basis of this study. But as the controversy on the hazards of dental fillings continues, these experimenters have clearly demonstrated that mercury migration through the teeth may be another significant exposure pathway that must be considered.

— Mark Wolverton

< Fig 1. X-ray fluorescence imaging of tooth sections reveals that mercury from dental amalgams migrates through human teeth to an area with an active bloodstream. Top left: Optical micrograph of a human tooth filled with amalgam for >20 years. Top right and bottom left: XRF (100-μm resolution) elemental distribution maps for 100-μm-thick horizontal section. The mercury map (bottom left) also indicates that mercury accumulates in calculus on the right-hand side of the tooth. The site of the fillings is on the left side of the tooth. It is noted that some of the enamel from the top of the tooth was lost prior to XRF imaging. Maxima for each element in mg g-1 (assuming a density of 2.1 g cm-3) are given below the element symbol. Bottom right: Hg L_{III}-edge XANES spectra from 0.25-μm × 0.25-μm spots, as indicated in the Hg map, indicates that mercury is chemically altered either during or after the transport process. (© International Union of Crystallography)

See: Hugh H. Harris,[1*‡] Stefan Vogt[2], Harold Eastgate[3], Daniel G. Legnini[2], Benjamin Hornberger[4], Zhonghou Cai[2], Barry Lai[2], and Peter A. Lay[1**], “Migration of mercury from dental amalgam through human teeth,” J. Synchrotron Radiat. **15**, 123 (2008).
DOI: 10.1107/S0909049507061468

Author affiliations: [1]The University of Sydney, [2]Argonne National Laboratory, [3]Eastmac Pty Ltd., [4]Stony Brook University ‡Present address: The University of Adelaide
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2-ID-E • XOR • Life science, environmental science, materials science • Microfluorescence (hard x-ray) • 3.3-cm Undulator A • Accepting general users

2-ID-D • XOR • Life science, materials science, environmental science • Microfluorescence (hard x-ray), micro-diffraction, micro-x-ray absorption fine structure • 3.3-cm Undulator A • Accepting general users

A BETTER UNDERSTANDING OF THE DIPHTHERIA TOXIN

Bacteria and viruses are good at guarding the secrets to their toxic effects on humans. It is just those secrets that must be revealed in order for science to develop adequate prevention and treatment for microbial diseases. One particularly well-studied toxin is produced by some strains of the bacterium *Corynebacterium diphtheriae*, which itself must be infected by an enemy known as a bacteriophage before it produces the cellular poison that causes diphtheria symptoms in humans. On a broad scale, how *C. diphtheriae* operates is well understood: it uses enzyme systems to modify existing compounds in a cell's cytoplasm. But despite considerable research, a detailed description of the entire toxin-producing process has proved elusive, and it is exactly those particulars that are necessary for progress in post-exposure treatment of the effects of diphtheria and other similar acting bacterial toxins, and in re-engineering these toxins for therapeutic purposes. Scientists using an array of research techniques at three facilities including the APS, have uncovered new details about how the diphtheria toxin invades cells.

The breakthroughs achieved by the research team came in part by combining a variety of techniques. X-ray reflectivity (XR) and grazing incidence x-ray diffraction (GIXD) carried out at the XOR/CMC 9-ID beamline at the APS are especially sensitive to the lipid membrane. The neutron reflection (NR) and adsorption studies at the National Institute of Standards and Technology Center for Neutron Research and the Los Alamos Neutron Science Center revealed changes in the shape, or conformation, of the protein. Finding that the various data sets produced consistent and complementary results, the researchers created an elegant model of how the diphtheria toxin is released from its entry compartment into the cellular fluid. The complexity of the process explains why it had been so difficult to fully understand toxin release.

Already known from previous work was that the diphtheria toxin has three separate regions: one for receptor binding, another for translocation, and a third for enzymatic, or catalytic, activity. When it binds to cells, the diphtheria toxin is encased in a small compartment within the cellular fluid, called an endosome. In its compartment, the translocation region of the toxin works to release the catalytic portion back into the cytosol, where it performs its toxic damage. That translocation process is critical; if the catalytic portion of the toxin cannot get back into the cytosol, then it can do no harm. And it is exactly that step—specifically the conformational changes that occur—that had been so difficult to visualize, in part because the protein is membrane-bound.

The team of researchers from Sandia National Laboratories, the National Institute of Standards and Technology, the Los Alamos Neutron Science Center, and Argonne National Laboratory discovered that obtaining the correct conformational changes for translocation was dependent on the binding of two or more toxin molecules to form chains. These chains, known as oligomers and detected for the first time in this study, were found to be perpendicular, instead of lateral, to the membrane. The tendency to produce the oligomers grew with increasing concentration of diphtheria toxin and decreasing pH, and led to both an open conformation and deep insertion of the toxin, both of which are necessary conditions for translocation (Figs. 1 and 2). The presence of the oligomers is a new and potentially critical insight for understanding the translocation process.

Because the diphtheria toxin is bound to the membrane in its compartment, it had been particularly difficult to study the conformational changes necessary for translocation of the molecule's catalytic portion into the cytosol. By studying the molecular complex with XR, GIXD, and NR, the research team has produced a new molecular model for the action of diphtheria toxin inside endosomes. Knowing that oligomerization may be a key step in the process by which diphtheria toxin invades cells should ultimately aid efforts to re-engineer these toxins to deliver therapeutic proteins. — *Mona Mort*

See: M.S. Kent[1*], H. Yim[1], J.K. Murton[1], S. Satija[2], J. Majewski[3], and I. Kuzmenko[4], "Oligomerization of Membrane-Bound Diphtheria Toxin (CRM197) Facilitates a Transition to the Open Form and Deep Insertion," Biophys. J. **94**, 2115 (March 2008).
DOI: 10.1529/biophysj.107.113498

Author affiliations: [1]Sandia National Laboratories, [2]National Institute of Standards and Technology, [3]Los Alamos Neutron Science Center, [4]Argonne National Laboratory
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Posters on facing page: Top: Courtesy of National Library of Medicine, U.S. Department of Health & Human Services. Center: C.N. Crittenton Co., "Save the children, Diphtheria Can Be Cured," 4-page pamphlet, Brooklyn, New York, 1881, courtesy of the National Library of Medicine, National Institutes of Health. Bottom: Works Progress Administration.

9-ID • XOR/CMC • Physics, materials science • Liquid scattering, inelastic x-ray scattering, resonant inelastic x-ray scattering • 3.3-cm Undulator A • Accepting general users

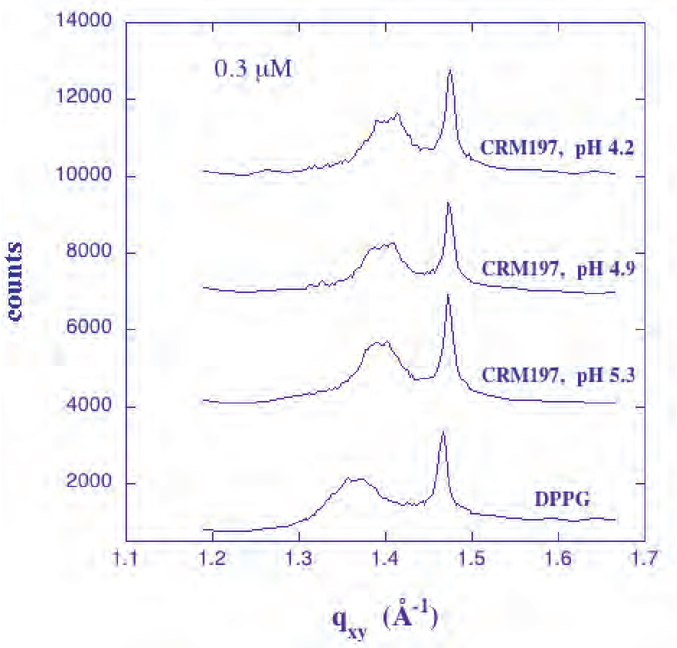


Fig. 1. Bragg peaks from GIXD for a DPPG monolayer alone at 30 mN/m and after injecting CRM197 at 0.3 mM and reducing the pH to 5.3, 4.9, and 4.2. The two peaks arise from the distorted hexagonal lattice of the DPPG tails in the gel phase. The peaks are relatively unchanged after injecting CRM197 at 0.3 mM and lowering the pH to 4.2, indicating little or no insertion of protein segments into the tails and preservation of the alkyl tail in-plane ordering.

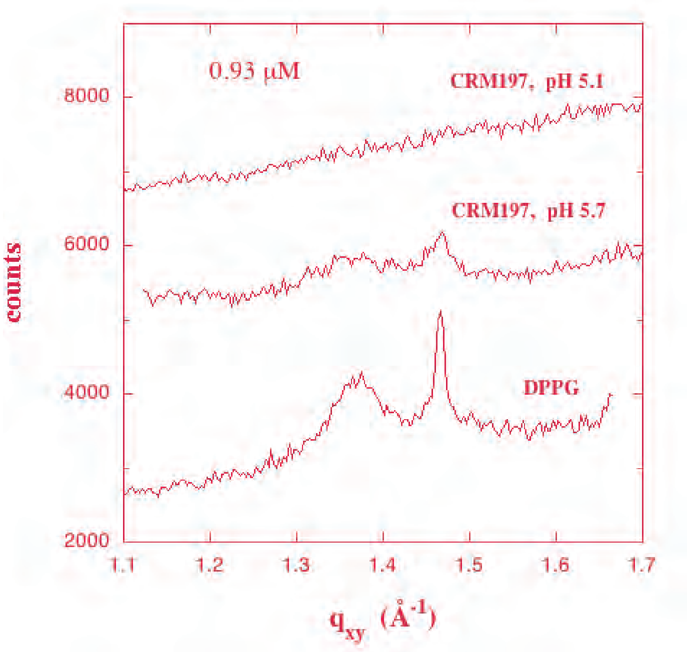
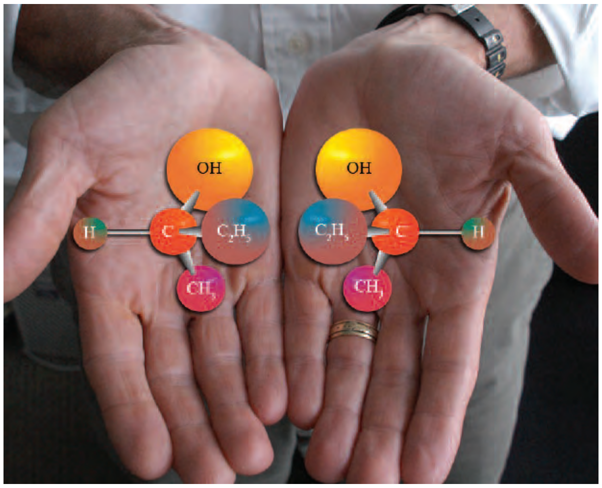


Fig. 2. Bragg peaks for a DPPG monolayer alone and after injecting CRM197 at 0.93 mM and reducing the pH to 5.7 and 5.1. The absence of the peaks after injecting CRM197 and lowering the pH to 5.1 indicates disruption of the in-plane order, suggesting strong insertion of protein segments into the DPPG monolayer.

ON THE OTHER HAND...



Research by a team using the APS explains how handedness, known to chemists as chirality, is fundamental to life on Earth. Chiral molecules can exist in a left and a right-handed form in which the chemical groups within the molecule are arranged so that the two distinct forms are non-superimposable mirror images, like a pair of hands. Irradiating a magnetic material with x-rays can produce spinning electrons that can bias the chemical reactions of another material toward one handed form and not the other. The work described here has implications for helping us gain a greater understanding of the origins of life.

The molecular building blocks of life, amino acids, sugars, DNA and RNA, and proteins are usually found in just one chiral form. Almost all natural amino acids, for instance, are left-handed, while sugars found in nature are right handed.

This handedness is important in terms of how chiral molecules interact with other chiral molecules. For instance, usually only one chiral form of a drug molecule will fit its target protein like a glove, while the opposite form will not. Indeed, one chiral form may be an effective treatment for the disease, whereas the other form may at best be inactive or less effective, and at worst can cause debilitating side effects. Similarly, chiral pesticides can be produced that are effective against pests but do not affect beneficial species.

The concept of chirality goes much deeper than chemical technology, however. Given the handed bias in nature, researchers would like to understand what first gave rise to life using just one chiral form of biomolecules. Once a particular handed form had been induced in the primordial soup, then natural selection at the molecular level would have ensured that the other handed form would simply be excluded from the processes that ultimately led to life on Earth.

Explanations based on asymmetric adsorption, asymmetric photolysis, symmetry breaking, and other notions have been put forward, but none have proved totally satisfactory. Now, the researchers from Argonne and the Ames Laboratory at the University of Iowa have taken a step toward a possible explanation.

They suggest that a previously unrecognized phenomenon might be at play in pushing a chemical reaction down one or other of the left or right pathways. Their hypothesis involves the production of low-energy, spin-polarized secondary electrons ejected by an irradiated magnetic material.

To test their hypothesis, they produced these handed electrons by irradiating a magnetized Permalloy (a nickel-iron alloy) film with APS x-ray beams. They then made detailed measurements of the reaction rate for a model organic compound, (R, for the right handed form)- or (S, for the left handed)-butan-2-ol on the surface of the Permalloy undergoing C-O bond cleavage.

Using the XOR 4-ID-C beamline at the APS in their studies, they observed a small, but significant (10%), bias towards the left- or right-handed product of this reaction. The outcome depended on whether the electrons themselves were chirally left or right handed.

The team points out that a 10% chiral selectivity is much larger than the majority of chiral effects observed previously. In earlier studies, an excess of one handed form over the other was measured at a mere fraction of one percent. It is the simplicity of the setup that suggests they may be correct in their hypothesis. Their approach requires the existence of two phenomena that are essentially ubiquitous in the universe: magnetic materials and ionizing radiation. Importantly, no predefined chiral conditions are required to produce the bias.

One can thus imagine a scenario in which prebiotic molecules adsorbed on a magnetic interstellar dust grain, comet, or meteorite and subsequently undergoing irradiation prior to being delivered to the primitive Earth may have provided the initial bias to push their behavior more down the left or right channel. — *David Bradley*

See: R.A. Rosenberg[1]*, M. Abu Haija[1], and P.J. Ryan[2], “Chiral-Selective Chemistry Induced by Spin-Polarized Secondary Electrons from a Magnetic Substrate,” Phys. Rev. Lett. **101**, 178301 (24 October 2008).
DOI: 10.1103/PhysRevLett.101.178301

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This work and use of the Advanced Photon Source were supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

4-ID-C • XOR • Physics, materials science • X-ray photoemission electron microscopy, x-ray photoemission spectroscopy, magnetic circular dichroism (soft x-ray), x-ray magnetic linear dichroism, magnetic x-ray scattering, anomalous and resonant scattering (soft x-ray) • Circularly polarized undulator • Accepting general users

THE APS RENEWAL WORKSHOP

Participants in the APS Renewal Workshop heard two days of talks on possible future research directions at a renewed APS.

Kendra Greenlee (North Dakota State University) speaks to the attendees of the “Life Sciences” breakout session.

Gene Ice (gesturing at left) of Oak Ridge National Laboratory makes a point at the breakout session on “Engineering Applications/Applied Science.”

As the APS moves through the twelfth year of user operations, with ever-increasing numbers of users, experiments, and publications, facility management has been looking to the future of photon science at this premier hard x-ray source. Several years of discussions about potential renewal and upgrade scenarios brought planners to a point where the facility sponsor—the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences (DOE-BES)— asked for a detailed, science-driven plan to cover the next five years. This renewal plan will encompass innovations in the beamlines and the x-ray source that are needed for major improvements in important areas of user science. APS management engaged users, staff, the distinguished members of the APS Scientific Advisory Committee, and other outside experts in crafting the plan. Among the spectacular impacts on science and engineering research that were offered, two overarching themes were identified that will guide technical choices for the APS Renewal: Mastering hierarchical structures through x-ray imaging, and real materials in real conditions in real time.

A planning milestone was the workshop held on October 20-21, 2008. Two days of scientific talks and breakout/discussion sessions provided a forum for topics leaders to present the outlines of forward-looking plans for experimentation in all the major scientific disciplines covered by photon science. A white paper making the broad case for renewal was written and sent to DOE-BES. The immediate next steps were finalizing reviews of proposals from users and beamline, accelerator, and other APS staff; completing the Renewal Science Case Reports written by members of the APS community; and preparing a detailed overall picture of the potential for science at a renewed APS. The white paper, presentations from and a proceedings of the workshop, and other information about renewal planning can be found at: http://www.aps.anl.gov/Renewal/

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A CLOSER LOOK AT PROTEIN BREATHING

To take a static view of proteins and regard them as simple strings of amino acids that do grunt work in cells would be a mistake. Decades of biomedical research have proven that proteins are often large, complex in structure, and, as is becoming increasingly apparent, undergo sophisticated changes in space and time in order to keep cells functioning properly. Some proteins, when in solution, exhibit dramatic fluctuations in their three-dimensional structures, movement that looks like breathing. Because this movement has usually been studied in relatively dilute solutions, and not in the crowded interior of a cell, it has been difficult to know how much of the motion would actually occur in living systems. Recognizing the need for a new approach to the problem, researchers used the APS to study the breathing motions of a diverse group of five animal proteins. Their results provide badly needed modeling of protein movement in solution and data that can be used widely in biomedical applications, such as therapeutic drug design.

The researchers from Argonne National Laboratory and the Illinois Institute of Technology used computational modeling and wide-angle x-ray scattering (WAXS) experiments performed on the Bio-CAT beamline 18-ID at the APS. They studied the breathing motions of a diverse group of five animal proteins (solutions of bovine hemoglobin, hen egg white lysozyme, hen egg white avidin, bovine serum albumen, and equine myoglobin) that represent a spectrum of size and structural differences.

By observing changes at varying protein concentrations and temperatures, the group was able to quantify spatial changes in this diverse array of molecules and, for the first time, present a set of techniques by which this quantification can be standardized.

The studies revealed motion in the three-dimensional protein structures that increased with decreasing protein concentration and increasing temperature and—perhaps most important—varied widely among the proteins. These findings point to the need for recognizing both the chemical and spatial structure of a protein (as well as its biochemical surroundings) when making estimates of protein movement, which was greatly inhibited at high protein concentration.

The proteins varied widely in their kinetic behavior, which depended on protein concentration and temperature. Because it exhibited breathing—in the form of rigid body motions—that lends itself well to observation with WAXS, hemoglobin at high concentration was chosen as the reference structure. Compared to hemoglobin, lysozyme at low concentration exhibited much less structural fluctuation. Bovine serum albumin exhibited about the same amplitude of breathing as lysozyme at very low concentration, while myoglobin and avidin exhibited movement comparable to hemoglobin (Fig. 1).

As temperature increased, the breathing in hemoglobin increased slightly; this increase was suppressed as the protein concentration, and accompanying molecular crowding, increased. Thus, the effect of temperature appears to be amplified at lower concentrations. And it seems that when proteins have more room to move (when protein concentration is low and there is more empty space nearby), more breathing occurs.

The chemical composition of a protein, called its primary structure, was also found to be important. Unlike the other proteins studied, the lysozyme and bovine serum albumin, which are stiffened by multiple disulfide bonds, showed relatively little increase in breathing in dilute solutions.

The research team used techniques that allowed an estimate of the size of rigid bodies that move during protein breathing. Concluding that secondary structures, such as alpha-helices, move like rigid bodies during breathing, the authors hypothesized that breathing involves slow collective movements. Another striking result of the study is that a protein's attributes such as size, structure class, subcellular location, or presence of multiple subunits do not seem to correlate with the measured amount of breathing. Thus, based on the usual suspects, there is no way to generalize about the expected amount of structural fluctuation. Each protein must be studied individually to learn its breathing habits under various cellular conditions, underscoring the danger of generalizing protein behavior from a limited sample.

This study provides badly needed modeling of protein movement in solution and data that can be used widely in biomedical applications, such as therapeutic drug design. — *Mona Mort*

See: Lee Makowski[1]*, Diane J. Rodi[1], Suneeta Mandava[1], David D.L. Minh[1] David B. Gore[2], and Robert F. Fischetti[1], "Molecular Crowding Inhibits Intramolecular Breathing Motions in Proteins," J. Mol. Biol. **375**, 529 (2008). DOI: 10.1016/j.jmb.2007.07.075

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18-ID • Bio-CAT • Life science • Microfluorescence (hard x-ray), microdiffraction, small-angle x-ray scattering, time-resolved x-ray scattering, micro-x-ray absorption fine structure, fiber diffraction • 3.3-cm Undulator A • Accepting general users

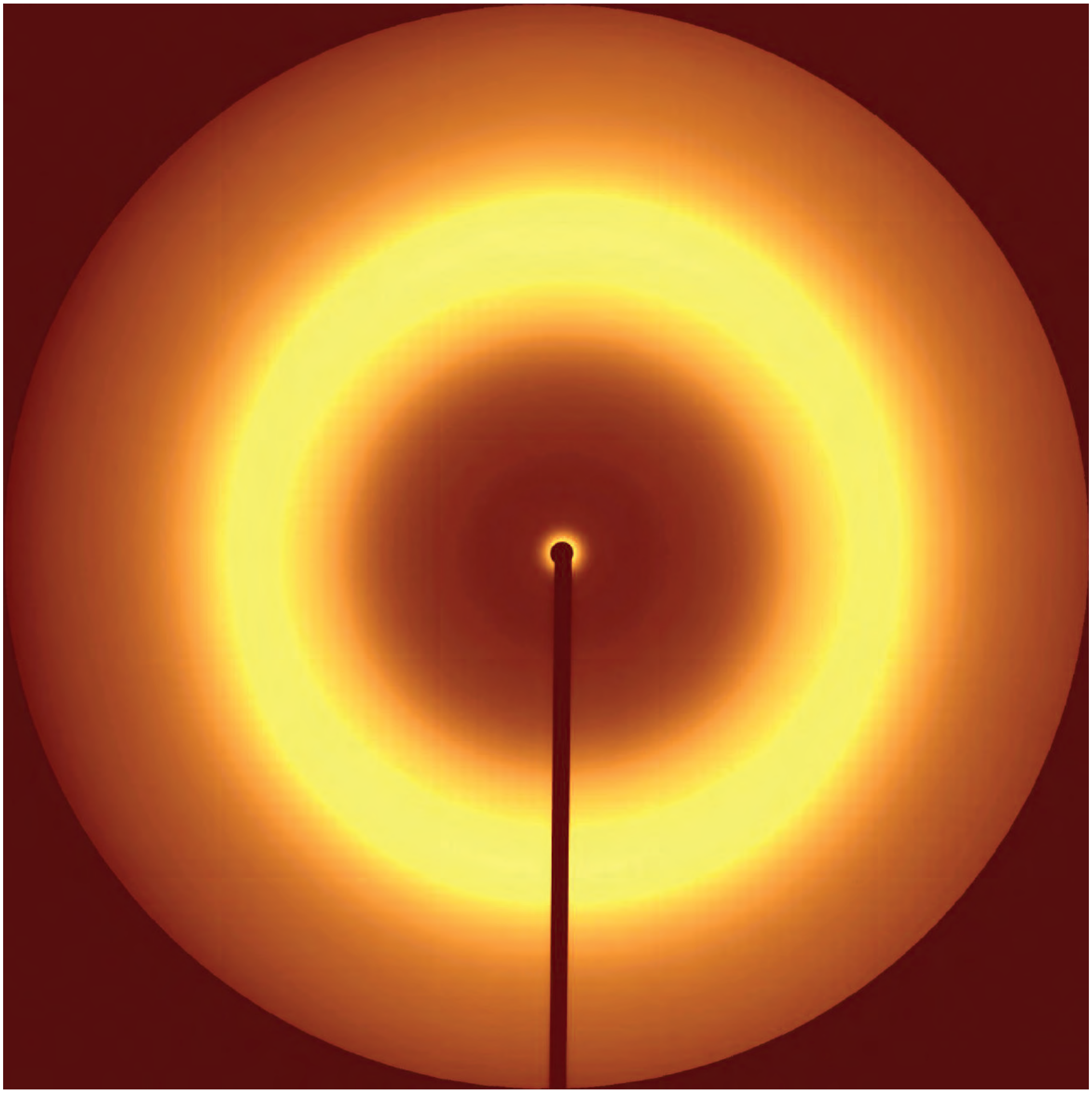
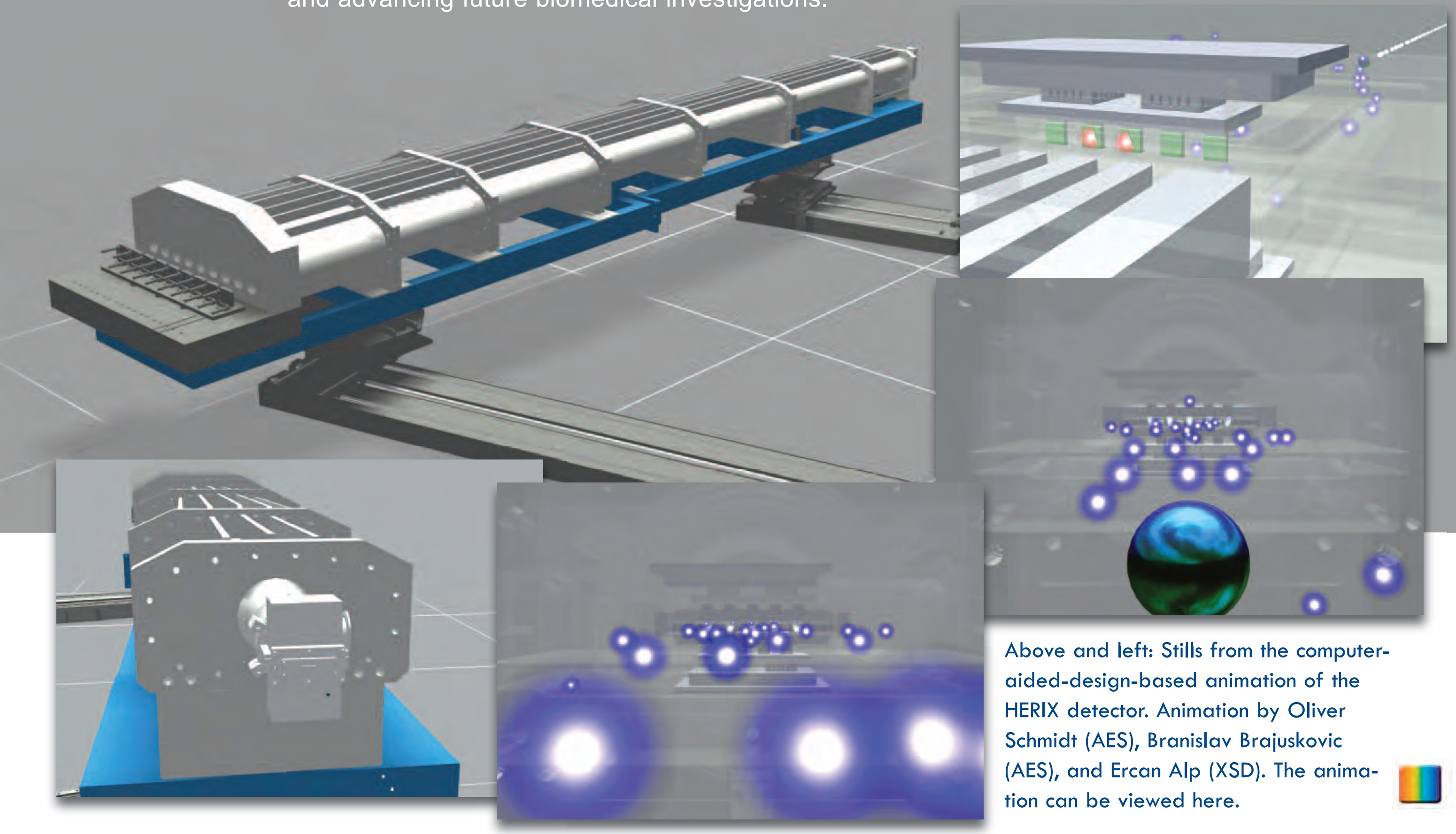


Fig. 1. A false-color scattering pattern from the protein myoglobin.

THE ATOMIC DANCE OF PROTEINS

Researchers have known for some time that proteins, the building blocks of life, undergo a temperature-dependent dynamic transition (T_D) at 220K, shifting from a liquid-like, flexible state above T_D to a glassy, less flexible state below the transition temperature. It also appears that biological functions of proteins come nearly to a standstill below T_D . But previous studies using incoherent neutron scattering and molecular dynamics simulations showed only the motion of individual hydrogen atoms in proteins and did not reveal the collective motions of molecules constituting the protein. Research at two APS beamlines has revealed the dynamic structure of two important proteins, enhancing our knowledge about the biological functions of proteins and advancing future biomedical investigations.



Above and left: Stills from the computer-aided-design-based animation of the HERIX detector. Animation by Oliver Schmidt (AES), Branislav Brajuskovic (AES), and Ercan Alp (XSD). The animation can be viewed here.

Researchers from the Massachusetts Institute of Technology, the University of Florence, and Argonne, using two APS beamlines, revealed the collective molecular motion of a specific range of wavelengths and their wave amplitudes in two hydrated globular proteins. The team used the XOR 3-ID beamline and the high-energy resolution inelastic x-ray scattering (HERIX) beamline, 30-ID, to characterize the dynamic structure of lysozyme and bovine serum albumen at low temperatures above, at, and below T_D (Fig.1).

Lysozyme and bovine serum albumen are globular proteins with very different structures. The egg white lysozyme used in this study is an enzyme with a folded ellipsoid structure measuring $2.25 \times 1.5 \times 1.5$ nm^3 and consisting of five α-helical coils and five β–sheets. Bovine serum albumen is a protein that transports lipids in blood plasma and has a larger, more elongated ellipsoid shape ($7 \times 2 \times 2$ nm^3), with helical coils and a greater molecular weight. Commercially purchased protein powder was dehydrated and then exposed to water vapor to coat the protein surface with a thin layer of water.

The proteins were probed at three different temperatures, below T_D at 170K, near T_D at 220 K, and above T_D at 250K. The dynamic structure factor measured by inelastic x-ray scattering (IXS) was analyzed with a damped harmonic-oscillator (DHO) model. The DHO analysis of the measured spectra allowed the team to extract the intra-

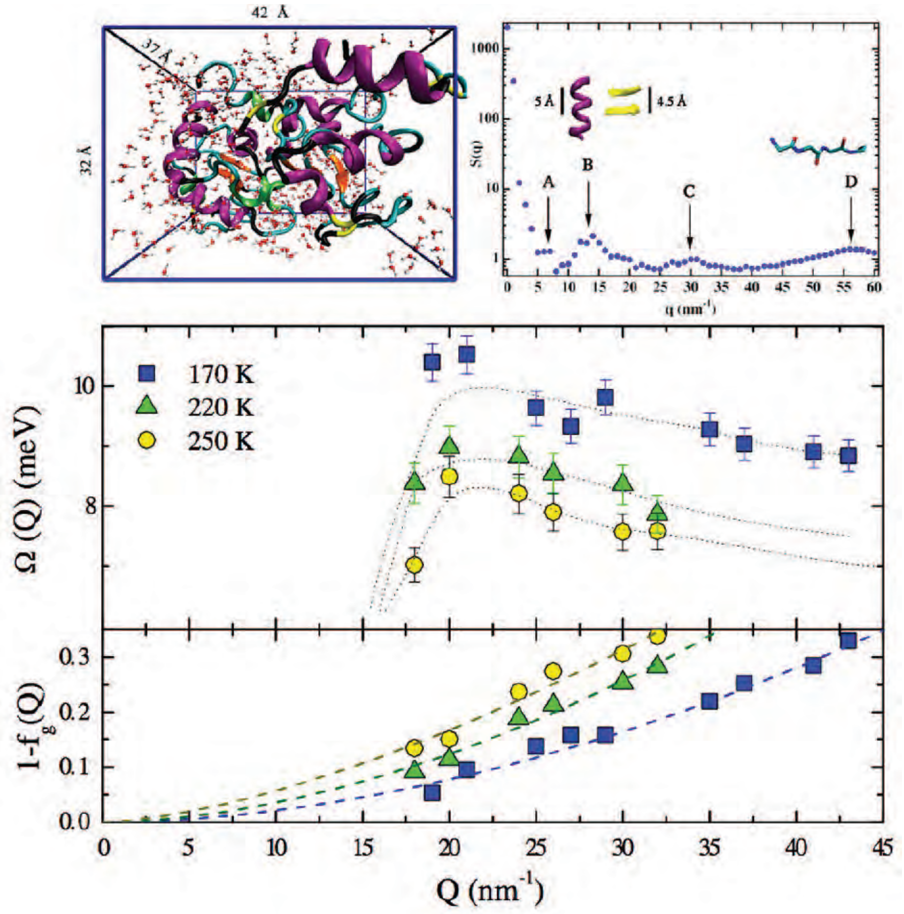


Fig. 1. Top left panel: The elements of lysozyme secondary structure are displayed with different colors: α-helices in purple, 3-10 helices in lime, β-sheets in orange, β-bridges in yellow, turns in cyan and coils in black. Top right panel: Calculated lysozyme structure factor *S*(*q*). The phonons were observed for magnitude of wave vector transfer Q around Peak B (that corresponds to some typical distances of the protein secondary structure, ~ 4.5 Å to 5 Å). This suggests the presence of wave motions that propagate along the α-helices and the β-sheets. Middle panel: Dispersion of the intra-protein phononlike collective excitations of lysozyme as a function of Q, below and above the second major peak in the structure factor. The square (blue), triangle (green), and circle (yellow) symbols indicate the phonon energies at temperatures 170K, 220K, and 250K. Bottom panel: Fractional area of the Brillouin peak vs Q. This factor is found to increase as a function of Q^2. Note that a marked softening of phonon energy is visible when the temperature is raised above the glass transition temperature of the protein at 220K when it becomes biologically active. And concomitantly, the population of the phonons at that temperature increases, as indicated in the bottom panel.

protein phonon dispersion relations. The phonon dispersion relation gives an energy of phonon propagating with the wavelength $\lambda = 2\pi/Q$, where Q is the magnitude of the momentum transferred to the protein molecules during the scattering process.

When the temperature exceeds T_D, the energies of phonon excitations with a certain Q range decrease. In other words, the molecular motions with this range of wavelengths within the protein are anharmonic and have higher amplitude at higher temperatures. It is therefore proposed from this study that this loosening, or conformational flexibility, at the higher temperature allows biological functions such as enzymatic activity to occur. It can be said that the high-energy resolution and length-scale sensitivity of IXS finally gives a plausible reason for the slowing down of biological function as temperature decreases. Below 220K, the molecules in the secondary structure of the protein continue to vibrate harmonically with low amplitude. The phonons that show softening when the temperature goes above T_D are in the Q-range corresponding to the length scale of the secondary structures of the protein, which are the α-helices and the β-sheets.

Previous studies of biomolecular assemblies using the IXS technique explored phonon dispersion relations in thin films of lipid bilayers and aligned liquid-crystalline DNA. Interprotein phonons have also been shown to exist by molecular dynamics simulation. The current study of the intra-protein phonons in the two proteins expands our knowledge about the role played by the collective motion of certain molecular groups for the biological functions of proteins and will have an impact on biomedical research in the future.

— *Elise LeQuire*

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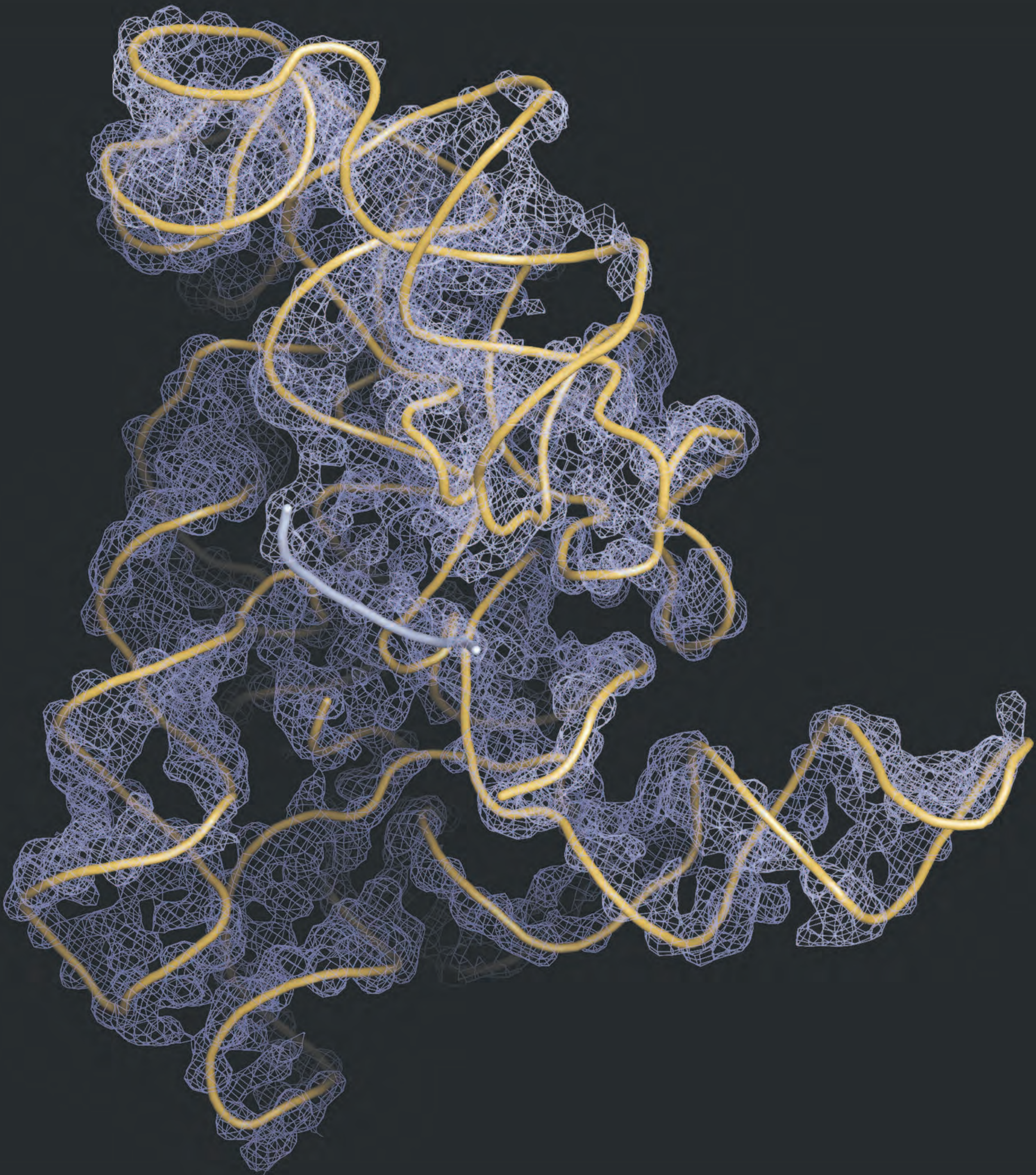
3-ID • XOR • Physics, geoscience, life science, chemistry, materials science • Nuclear resonant scattering, high-pressure diamond anvil cell, inelastic x-ray scattering • 2.7-cm undulator • Accepting general users

30-ID • XOR/IXS • Physics, materials science, geoscience, life sciences • Inelastic x-ray scattering • 3.0-cm undulator • Accepting general users

A RIBBON THAT CUTS ITSELF: THE STRUCTURE OF A GROUP II INTRON



Research carried out at two APS beamlines, and two beamlines at the National Synchrotron Light Source at Brookhaven National Laboratory, offers a glimpse into the evolution of introns—segments of a gene that have to be removed before the gene can do its work, much like movie outtakes spliced from the director's final cut. The data obtained by researchers from Yale University and the Howard Hughes Medical Institute (HHMI) have allowed them to determine the first three-dimensional (3-D) structure of a bacterial intron after it has spliced itself from its host gene. The researchers believe that such objects, called a "group II intron," were the precursors of specialized splicing machinery thought to give plant and animal cells much of their genetic complexity.

When a gene is activated, cellular proteins "transcribe" a single strand of RNA from double-stranded DNA. Called messenger RNA, the molecule then encodes instructions for building a protein. In nearly all genes, the RNA code is interrupted by short stretches—the introns—that the cell has to remove first. (The remaining pieces of the gene are called exons.) Plant and animal cells have evolved an RNA-protein machine called the spliceosome to snip out introns and stitch the exons back together. By splicing the same gene in multiple ways, organisms can pack more functions into a seemingly small number of genes, which may be how such species as humans have evolved with greater complexity than other species with a similar number of genes.

Splicing didn't evolve overnight. Group II introns, found in bacteria and in compartments of plant and animal cells that are thought to have come from bacteria, are able to splice themselves out of messenger RNA directly, without help from a spliceosome. Biochemical evidence suggests the spliceosome is actually descended from group II introns. To study these self-splicers, the researchers isolated group II introns from *Oceanobacillus iheyensis*, a deep-sea microbe, and allowed it to splice itself. They crystallized the resulting molecule and determined its structure from x-ray data collected on NE-CAT beamline 24-ID-C and SBC-CAT beamline 19-ID.

< Fig. 1. Electron density view of a self-splicing group II intron (nucleic acid backbone in beige) co-crystallized with spliced exons (gray). The intron's catalytic site—used to splice itself out from between two exons—sits in a cleft (lower right) between two structural elements that are highly conserved among introns from different species

The Yale-HHMI team reported that the structure of the intron appears to be finely tuned for splicing. The 3-D shape of the molecule depends on its sequence of nucleotides, the chemical subunits that make up the RNA strand. Researchers believe the intron adopts a complicated shape that is capable of accelerating the chemical reaction of breaking and re-fusing an RNA molecule at specific points. Such molecules are called RNA enzymes, or ribozymes.

If flattened out, the RNA molecule would resemble a six-armed starfish, with a series of hairpin shapes projecting from the center. But the hairpins clump together, giving the spliced intron a compact shape (Fig. 1). The researchers believe the area that catalyzes the splicing reaction lies within the very center of the folded molecule, containing a negatively charged pocket that holds two metal ions in place. The active site is composed of atoms within an "arm" of the molecule, including a small bulge that sits next to a region where the RNA folds together in a three-stranded twist or triple helix, which seems to anchor the bulge in place. The researchers note that the nucleotide sequences corresponding to the bulge and triple helix are separated by only a short distance and are nearly identical among different forms of life, indicating that even a slight change would likely disrupt the intron's shape enough to render it inactive.

Once a group II intron has spliced itself, it can recruit other enzymes to insert itself into the genome and convert itself into DNA, a strategy that the Human Immunodeficiency Virus and other retroviruses have also adopted. If plant and animal cells evolved by engulfing primitive bacteria, group II introns would have found a new genome to invade, being shaped by evolution until they transformed into the spliceosome. The Yale-HHMI team says its findings support the notion that group II introns evolved to colonize and shape the genomes of modern organisms. — *JR Minkel*

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19-ID • SBC-CAT • Life science • Anomalous diffraction (MAD/SAD), subatomic (<0.85 Å) resolution, ultra-low-temperature (15K) • 3.3-cm Undulator A • Accepting general users

24-ID-C • NE-CAT • Life science • Microfluorescence (hard x-ray), tomography, microdiffraction • 3.3-cm Undulator A • Accepting general users

HOW THE BRAIN MAKES CONNECTIONS

Autism, the developmental disability that typically appears during the first three years of life and affects a person's ability to communicate and interact with others, responds well to early diagnosis and intervention so that affected individuals can live productive lives. Nevertheless, autism can and does impose hardships on those with the disability, and on their families. Furthermore, the Autism Society of America estimates a lifetime-care cost range of $3.5 million to $5 million per person. In the U.S. alone, the aggregate dollar amount for autism research, treatment, educational and housing costs, etc., is nearly $90 billion a year [1]. Researchers using two x-ray beamlines at the APS have mapped the locations of two neurological mutations that earlier studies have connected to autism.

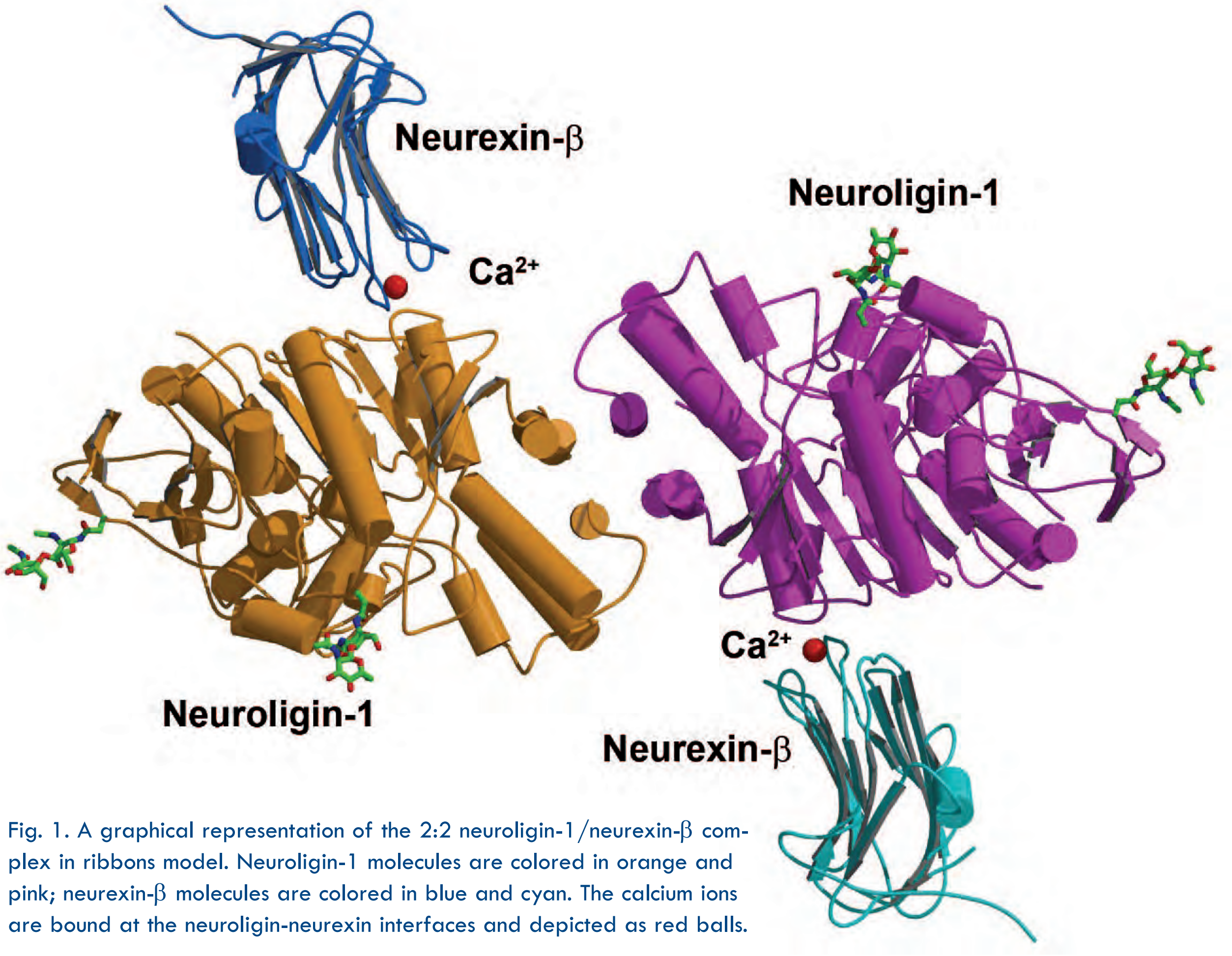

Fig. 1. A graphical representation of the 2:2 neuroligin-1/neurexin-β complex in ribbons model. Neuroligin-1 molecules are colored in orange and pink; neurexin-β molecules are colored in blue and cyan. The calcium ions are bound at the neuroligin-neurexin interfaces and depicted as red balls.

A three-dimensional structure from this research can be viewed here

Researchers using the APS have mapped the locations of two neurological mutations that earlier studies have connected to autism

Each of the ten billion neurons of the human brain is capable of forming thousands of signalling connections with other neurons. Forming this staggeringly large synaptic network requires a vast array of signalling and structural proteins. In synapse development, adhesion molecules on cell surfaces at the presynaptic and postsynaptic sites are involved in target recognition, enabling proper matching of neurotransmitter release from axon terminals with their postsynaptic receptors. Postsynaptic neuroligin on the axon and presynaptic neurexin on the target nerve cell are binding partners with crucial roles in inducing the formation of and specifying the synaptic junction.

Using the SER-CAT 22-BM-D and LS-CAT 21-ID-D beamlines at the APS, researchers from the Northwestern University Feinberg School of Medicine have succeeded in visualizing the extracellular portions of a murine neuroligin-neurexin complex to a resolution of 2.4 Å (Fig. 1). Neuroligins are important to synapse development, specificity, and stability. Point mutations in two of the four known neuroligin genes have been linked to autism. The neurexins are expressed as thousands of different isoforms generated by alternative splicing of mRNA transcripts from three genes, each with promoters for expression of a long α-neurexin and a shorter β-neurexin protein. Recognition involves the CLD of neuroligin and the LNS domains of neurexin. Target selectivity is obtained by alternative splicing to generate distinct neuroligin-neurexin pairs. CLD contains splice site A, and in neuroligin-1 (NL1) an additional splice site B; α-neurexin has five splice sites within the LNS domains, with the fourth site (SS 4) also found in the LNS of β-neurexin.

The Northwestern University researchers studied the crystallized complex formed by the CLD of mouse neuroligin-1 (NL1) and the LNS domain of mouse neurexin1-β (NX1β) in the presence of calcium ion (Ca^{2+}). The CLD of the NL1 monomer had a globular form with a central β-sheet flanked by α-helices. The NL1/NX1β complex was found to consist of a central NL1 dimer and two NX1β monomers, one on each side (Fig. 1). The dimer interface of NL1, formed by the four α-helices, two from each monomer, was large, burying a surface area of 1,590 Å2. The LNS domain of NX1β had a β-sheet sandwich form, with several loops on the side that made contact with a protruding patch on the exposed side of the central β-sheet of NL1. The residues involved in this interface were primarily hydrophilic, with water molecules filling unoccupied space; two salt bridges (weak ionic bonds) occurred near the edge of the interface.

Neuroligin-neurexin binding was known to be Ca^{2+}-dependent, but the position of the Ca^{2+} binding site had not previously been ascertained. The Northwestern University researchers found it to be located in NX1β at the looping edge of the β-sandwich. The bound Ca^{2+} has no direct contact with NL1; however, its binding appears to require the presence of NL1. Alternate splicing at site B in NL1 affects one of the salt bridges within the interface, and the structure of the SS 4 site suggests it may act on the other salt bridge by a similar mechanism. Thus, the neuroligin-neurexin interface is readily affected by a number of variables, such as ion concentration and minor sequence variations in the neurexins, thereby modulating binding affinities and enabling selectivity.

The researchers mapped the locations of neuroligin-3 and -4 point mutations that have been implicated in autism, and found that the affected amino acids were located well away from the interfaces. Since these residues are not involved in neurexin binding, the researchers proposed that these mutations act to compromise protein structure, either by insufficient folding, inadequate secretion, or reduced viability of the neuroligin, thereby altering or impairing its functions at the synapse. — *Carol Hart*

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22-BM-D • SER-CAT • Macromolecular crystallography • Bending magnet • Accepting general users

INSIGHTS INTO VIRAL MATURATION

The *Flaviviridae* family is an important group of the human pathogens that cause mosquito-transmitted disease, such as Dengue fever, West Nile virus, yellow fever, and Japanese encephalitis. The way in which these viruses mature and replicate is not completely understood, and currently, there are no effective vaccines or antiviral therapies for many of the resulting diseases. Experiments at GM/CA-CAT beamline 23-ID-D at the APS helped researchers from Purdue University find out more about a maturation step that the Dengue virus undergoes during the final stages of assembly before its release from the host cell. This and other information gleaned by the team will aid in the development of pharmaceuticals and therapies to prevent and treat a range of mosquito-transmitted diseases.

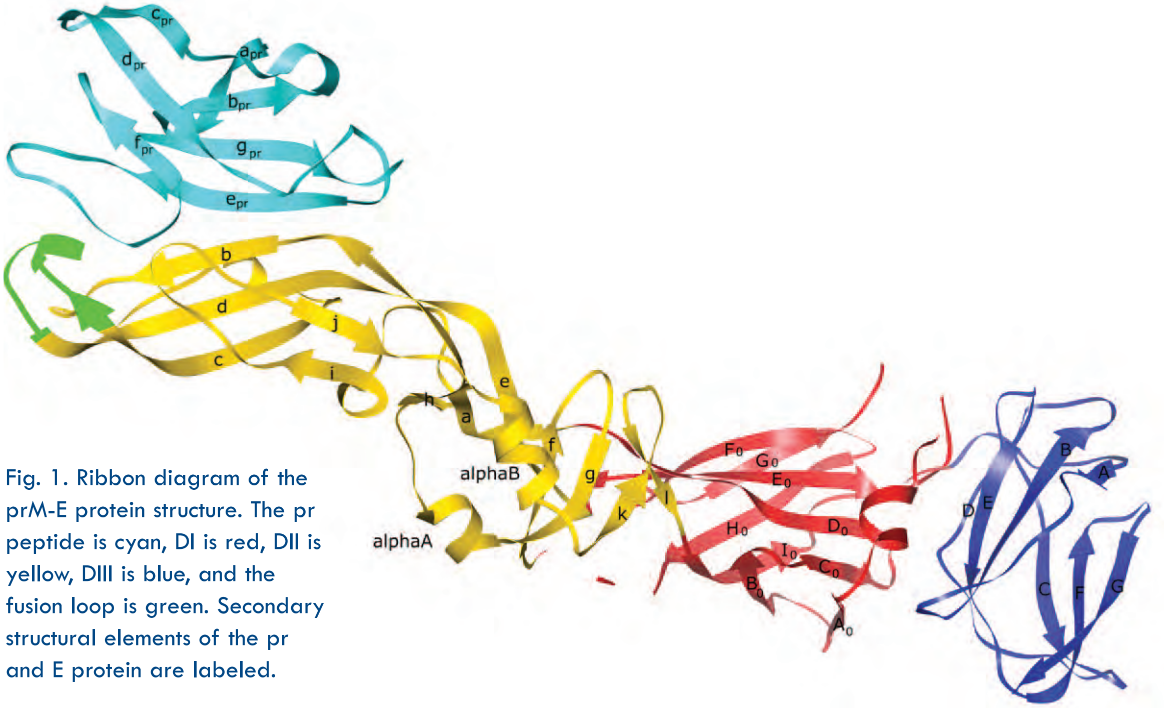

Fig. 1. Ribbon diagram of the prM-E protein structure. The pr peptide is cyan, DI is red, DII is yellow, DIII is blue, and the fusion loop is green. Secondary structural elements of the pr and E protein are labeled.

By understanding these mechanisms more can be learned about how to develop novel vaccines and treatments that will hopefully prevent and treat diseases such as Dengue fever

The team solved the crystal structure of part of the precursor membrane protein of the virus which, when cleaved, turns inert particles into infectious ones (Fig. 1). They suggest that the maturation process described is highly conserved and may have applications for other related viruses [1].

A virion, i.e., a complete virus particle, consists of nucleic acid surrounded by a protective coat of protein called a capsid. The Dengue virus polyprotein, a precursor that ultimately develops into a mature virion, contains all the components of the virion strung together linearly. The three main components of the polyprotein are the capsid protein, the precursor membrane glycoprotein, and the envelope glycoprotein.

Within an infected cell, Dengue polyproteins are threaded like stitching through the endoplasmic reticulum, a maze-like system of interconnected tubules that runs through the cell's cytoplasm. Prior to maturation, specific enzymes (proteases) cleave the components of the Dengue polyprotein into its subcomponents, and immature particles are released. These are transported through the cell, and after removal of the precursor membrane protein, they eventually develop into mature virions.

To find out more about the maturation process of the Dengue virus, a recombinant protein containing two components of the polyprotein structure joined together by an 8-amino acid linker was constructed. One component was the precursor membrane protein, which protects immature virions against premature fusion with the host membrane, and the other was the envelope protein, which participates in the fusion of the virion with the endosomal membrane at low pH.

The fusion of the Dengue virus with the host cell takes place under a low pH, but the team determined the crystal structure of their recombinant protein at pH 5.5 (low pH), as well as pH 7.0 (neutral pH). They found no structural differences at either low or neutral pH. However, they were able to resolve the low-pH structure at a higher resolution, so they used this structure for their subsequent studies.

Upon fitting the crystal structure of prM-E into the cryo-EM reconstructions of the immature virus, they found that the precursor membrane protein was positioned in a way that would prevent its fusion with the host membrane, and found several structural differences between the immature and mature proteins. They also found that furin, a protease enzyme important in the maturation process, would be unable to bind to the precursor membrane protein at neutral pH. By contrast, the low-pH conformation was found to be accessible to furin cleavage and therefore could mature [2].

The researchers also found that the structural changes that occurred in the immature virus in neutral-pH vs low-pH conditions were reversible when the precursor membrane protein was still intact. However, when the precursor membrane had been cleaved with furin, the pH changes had no effect and the cleaved precursor peptide was released [2]. They likened this mechanism of pH sensitivity to the effect of a drawstring that opens and closes a curtain. Once the string is cut (i.e., with furin), no further movement could occur, regardless of pH.

By understanding these mechanisms, which appear to be conserved among related viruses, more can be learned about how to develop novel vaccines and treatments that will stop viral maturation and release and hopefully prevent and treat diseases such as Dengue fever. — *Emma Hitt*

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23-ID-D • GM/CA-CAT • Life science • Macromolecular crystallography, microdiffraction, anomalous diffraction (MAD/SAD), subatomic (<0.85 Å) resolution • 3.0-cm undulator • Accepting general users

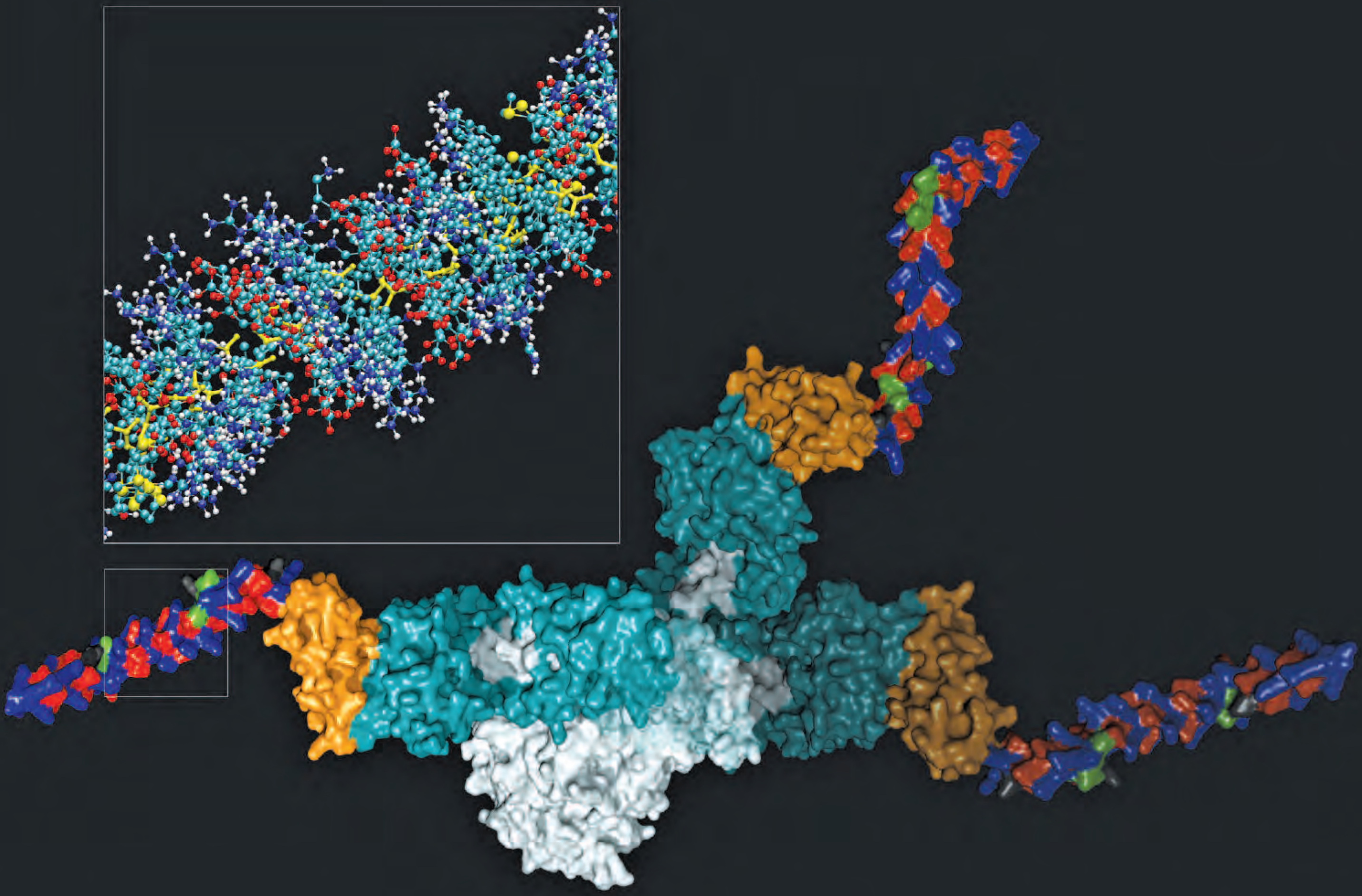

Fig. 1. Computer-generated representation of myosin VI binding to an actin filament. Actin filament (white) is shown with a myosin VI molecule attached through its globular head domain (teal) with the lever arm (yellow) and tail domains (blue, red, green) shown in three positions as they undergo a 180° swing. Inset shows representation of putative single helix predicted for the structure of MT domain of the tail. Cargo binding domain is not shown.

TAKING BIG STEPS WITH MYOSIN VI

The interaction of muscle myosin (the large family of motor proteins found in eukaryotic tissues) with actin filaments generates the force that powers muscles. In an elegant example of nature's endless ability to adapt old tools to new projects, recent research years has revealed a family of myosin proteins that move along actin filaments in unexpected ways to carry loads within cells. One of these proteins, myosin VI, is of particular interest because its predicted dimensions cannot account for its large (~36-nm) steps. In order to determine whether more information about the structure of myosin VI might uncover the secret of these large steps, researchers at Stanford University used the 12-ID beamline at the APS to study the structure of the tail portion of myosin VI that is predicted to be responsible for step size. Because there are few other natural examples in known protein structures, understanding the role this single helical domain plays in myosin VI force generation may provide a model for the design of synthetic proteins in which a single secondary structure that spans a long distance may be of value, such as in the design of novel drug delivery systems.

Muscle myosin contains a globular head that hydrolyzes adenosine triphosphate (ATP, a high-energy phosphate compound found in the body) to provide the force to ratchet the molecule along actin filaments in a stepwise manner. Association of the elongated myosin tail with oppositely aligned myosins on other actin filaments creates a sliding motion that is typical of skeletal muscle movement.

Using small-angle x-ray scattering (SAXS) data collected at the XOR/BESSRC beamline 12-ID in combination with other techniques, the Stanford researchers obtained evidence that myosin VI takes its big steps by virtue of a rare, single-helical domain. Analysis of the amino acid sequence of myosin VI revealed the predicted globular head region followed by a lever arm, tail region, and cargo binding domain. The tail region is predicted to contain three domains that may be involved in step size; these are called the proximal, medial, and distal tail regions on the basis of their location relative to the myosin head domain.

Working with expression constructs of the tail region, investigators studied the role of these domains. The proximal tail (PT) region, closest to the lever arm and head, has been proposed to form a random coil that may allow for the flexibility required for the elongated step. Hypothesizing that substitution of amino acids would not disrupt the function of this region if it was a random coil but would if the coil was structured, the team made a series of mutations in the PT and found that these changes significantly affected the step size of the myosin. Their data do not support a model in which step size is facilitated by the elongated random coil structure of the PT, but do show that the PT is likely to have the three-dimensional structure required for myosin VI activity.

The researchers next investigated the role of the medial tail and distal tail (MT-DT) regions in step-size generation. Two possible structures for this region have been proposed. The first is that the region forms a dimer with its counterpart on another myosin molecule. The second is that this region is maintained as a single α-helix. In order to test these possibilities, investigators used SAXS to assess the structure of the MT-DT region and found the MT to be a single extended α-helix with sufficient length to account for the large myosin step (Fig. 1). Further experiments with the purified MT-DT in solution showed that it was unlikely to form a dimer under a variety of conditions. Instead, the authors propose that the cargo binding domain is responsible for bringing two myosin VI molecules together as they work in pairs to carry their cargo. — *Sandy Field*

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12-ID • XOR/BESSRC • Chemistry, physics, materials science • Small-angle x-ray scattering, wide-angle x-ray scattering, grazing incidence small-angle scattering, surface scattering • 3.3-cm Undulator A • Accepting general users

HELPING TO CONQUER THE WIDE-RANGING EFFECTS OF OBESITY

The worldwide prevalence of obesity underscores the need for improved treatment for heart disease, diabetes, and other health issues related to excess weight. One consequence of obesity is an increased risk of the metabolic syndrome, which is defined as a group of risk factors for heart disease that occurs simultaneously and includes conditions such as visceral obesity, hyperglycemia, elevated blood cholesterol levels, and high blood pressure. In a study carried out with the help of an x-ray beamline at IMCA-CAT at the APS, researchers from Merck Research Laboratories sought to find out more about the farnesoid X receptor (FXR) and how it might bind to an activating ligand. A therapy that targets this receptor may play an important role in helping to counteract some of the effects of obesity.

The farnesoid X receptor represents a novel therapeutic target that may help prevent components of the metabolic syndrome, specifically hyperglycemia and high blood cholesterol levels. The FXR is a receptor that normally binds bile acids, and when activated in this way, shuts down the synthesis of bile from cholesterol and accelerates the elimination of bile from the body. This conversion process is one of the major clearance mechanisms for excess cholesterol in the body. Recent work has shown that activation of FXR also decreases circulating glucose levels and increases insulin sensitivity. The possible end result of FXR activation by bile acids, or specially designed agonists such as the potent synthetic FXR agonist called MFA-1, is a return to more healthy blood cholesterol and glucose levels.

The family of receptors to which FXR belongs consists of a domain that binds to specific sequences within DNA coupled to another smaller domain that binds an activator molecule or ligand, which, with the help of other proteins, activates the receptor and causes DNA transcription.

The researchers identified MFA-1, a molecule that activates FXR, from about one million other compounds on the basis of its ability to induce binding of FXR to a helper protein called a coactivator, indicating an agonist effect. MFA-1 was found to be nearly 500 times more potent than the highest-affinity naturally occurring bile acid that normally binds to FXR. MFA-1 was also found to be as potent as

"Obesity" *continued on page 80*

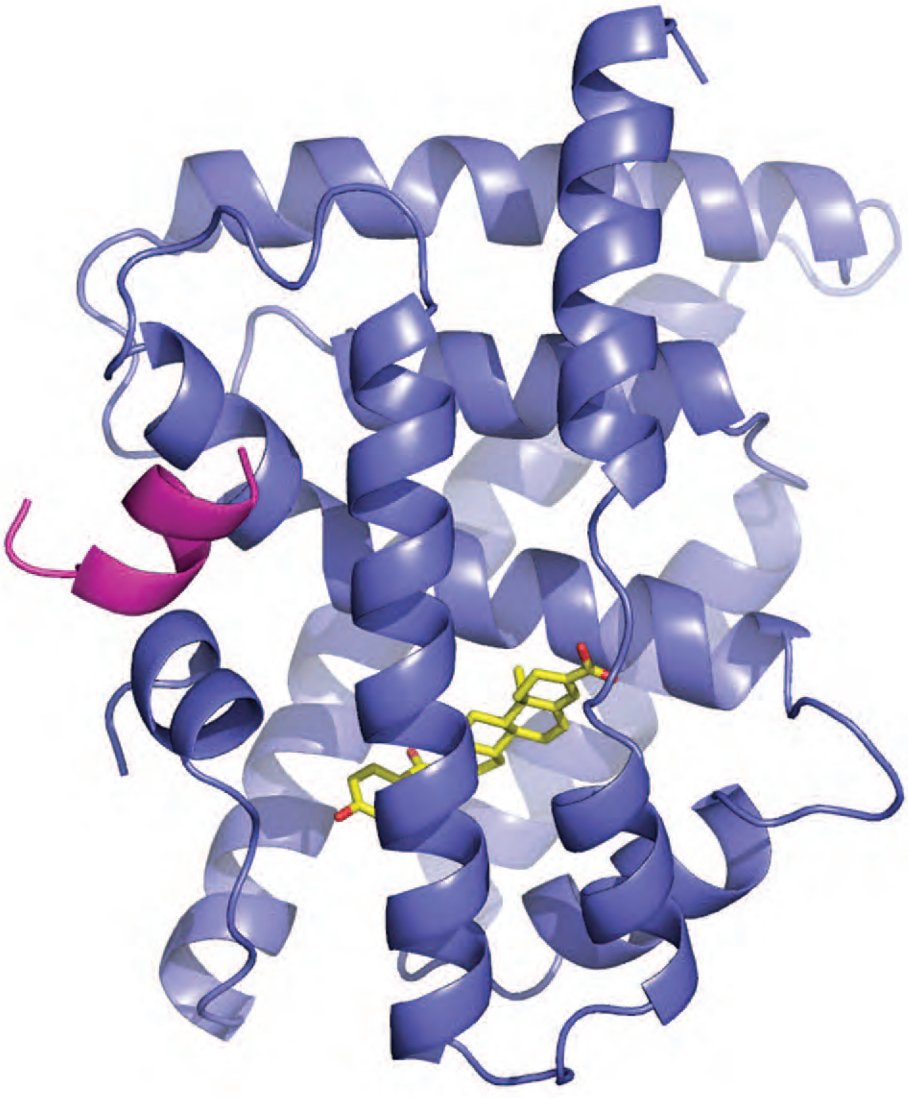

Fig. 1. Ribbon representation of the structure of human FXR (blue) with bound activating ligand MFA-1 (yellow) and a 25-residue peptide derived from co-activating protein SRC-1. (© 2008 by the National Academy of Sciences)

A NUCLEAR RECEPTOR COMPLEX REVEALED

Regulation of many aspects of metabolism is managed by small molecules that circulate in the blood, pass through the plasma membrane, and bind to nuclear receptors that can affect DNA transcription. These nuclear receptors are responsible for appropriate uptake, storage, and breakdown of lipids and carbohydrates in our cells. For patients with severe metabolic disorders such as diabetes mellitus, regulation of metabolism is crucial. One group of nuclear receptors, the peroxisome proliferator-activated receptors (PPARs), has been identified as important for lipid metabolism; their activation by a class of drugs known as thiazolidinediones can improve glucose uptake to relieve symptoms of diabetes in patients. Peroxisome proliferator-activated receptors work as part of a complex with retinoid X receptors (RXR) to bind specific DNA sequences and activate transcription of metabolic genes. Recent work completed by researchers using the SER-CAT 22-ID beamline at the APS determined the structure of one of these transcription complexes for a nuclear receptor called PPAR-γ. This structure increases our understanding of how nuclear receptors regulate genes involved in human disease and could lead to drugs that are more effective with fewer side effects.

Drugs that activate PPAR-γ, such as rosiglitazone, have shown promise as treatment for metabolic disorders such as type 2 diabetes, hyperinsulinemia, and hyperglycemia. In addition, due to other beneficial effects, rosiglitazone is being considered for treatment of inflammatory diseases, atherosclerosis, hypertension, and Alzheimer's disease. However, these drugs have been reported to have side effects including increased risk of heart attack. Drug design efforts and previous structural studies have focused on the structure of the PPAR-γ ligand binding domain (LDB) responsible for interaction with the thiazolidinediones. Elucidation of the structure of the entire DNA binding complex of PPAR-γ provides additional information that may allow science to design drugs with increased efficacy and fewer side effects.

First, the researchers, from the University of Virginia Health System, the ExSAR Corporation, and the Louisiana State University Health System, crystallized the complex, which included PPAR-γ; RXR-α, the ligand for RXR-α called 9-*cis*-retanoic acid; rosiglitazone, the DNA sequence that is recognized by the two protein receptors; and two co-activator peptides. In order to determine whether different ligands would change the configuration of the complex, two other complexes were crystallized that contained a partial activator or a suicide inhibitor for PPAR-γ instead of rosiglitazone. The

"Nuclear" *continued on page 80*

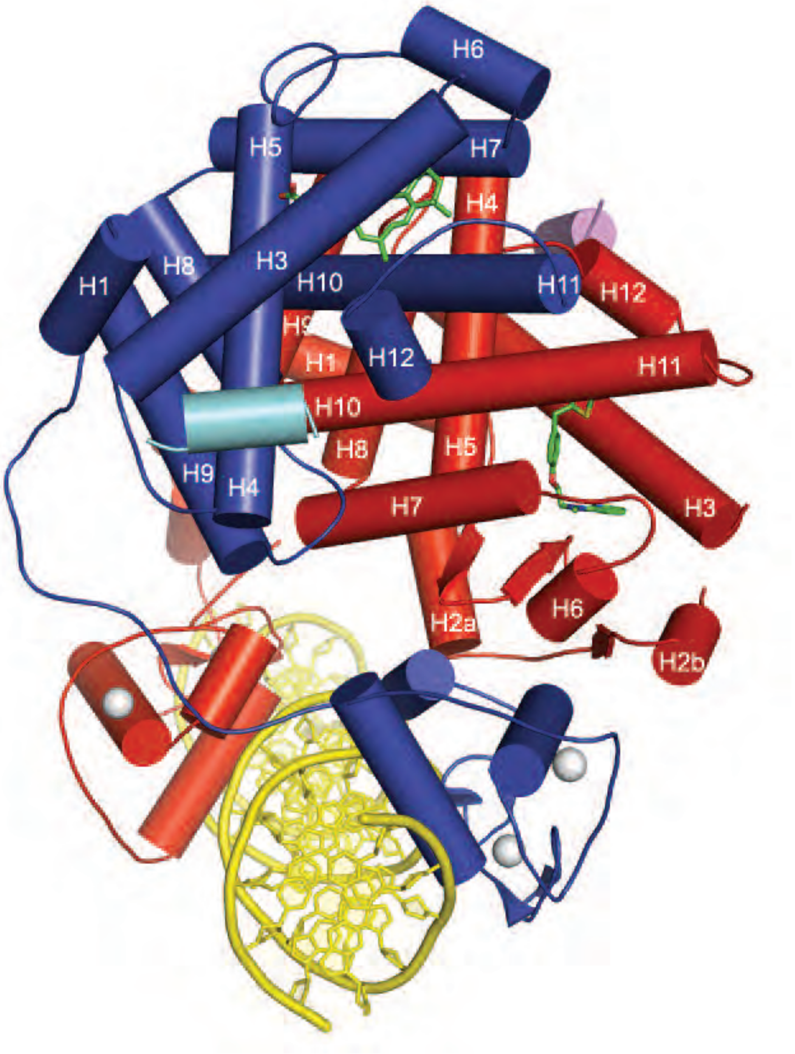

Fig. 1. Structure of the PPAR-γ nuclear complex. PPAR-γ is shown in red, RXR-α is shown in blue, DNA response element is yellow, receptor ligands rosiglitazone and 9-*cis*-retanoic acid are shown in green, Zn(II) ions are white and coactivator peptides are in light blue and purple.

"Nuclear" from page 79

structures were solved at 3.1-Å to 3.2-Å resolution by single anomalous dispersion phasing for the rosiglitazone structure and molecular replacement for the other ligands. All structures were similar in the relative arrangement of the receptors and their domain interactions with each other, and with the DNA sequence. The center of the complex is the PPAR-γ LBD, which has contacts with many other domains in the structure (Fig. 1). In contrast, the LBD of the RXR-α has no additional contacts with other parts of the complex except for the PPAR-γ LBD.

Both RXR-α and PPAR-γ interact with DNA through C-terminal DNA binding domains (DBD) that have α-helical structures aligned with the DNA major groove at the conserved sequences for binding. The C-terminal extension of RXR-α forms a DNA-dependent contact with the PPAR-γ DBD, but has no other secondary structure. This may be due to the fact that RXR-α is known to interact with other nuclear receptors and requires flexibility in this region to accommodate these alternate interactions.

In addition to the interaction between the DBDs of the two proteins, the structure of the PPAR-γ complex revealed two other DNA-dependent interactions between RXR-α and PPAR-γ. First, the two proteins interact at an interface between the two LBDs, and second, the PPAR-γ LBD interacts with the C-terminal DNA-binding domain of RXR-α. This previously unknown DNA-dependent interaction helps to explain why intact receptors have a higher affinity for DNA than the isolated DNA binding domain alone. In fact, the researchers show here that mutations that disrupt this binding interaction reduce the affinity of the receptor for DNA and also disrupt transcriptional activation by the complex.

The insights provided by this increased understanding of the PPAR-γ nuclear receptor complex will be useful to researchers and clinicians hoping to expand the therapeutic value of nuclear receptor activation in human disease.

— *Sandy Field*

See: Vikas Chandra[1], Pengxiang Huang[1], Yoshitomo Hamuro[2], Srilatha Raghuram[1], Yongjun Wang[3], Thomas P. Burris[3], and Fraydoon Rastinejad[1]*, "Structure of the intact PPAR-γ–RXR-α nuclear receptor complex on DNA," Nature **456**, 350 (20 November 2008). DOI:10.1038/nature07413

Author affiliations: [1]University of Virginia Health System, [2]ExSAR Corporation, [3]Louisiana State University System

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SER-CAT, an organization consisting of 25 member institutions, is operated by the University of Georgia. Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

22-ID • SER-CAT • Life science • Macromolecular crystallography, multi-wavelength anomalous dispersion • 3.3-cm Undulator A • Accepting general users

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"Obesity" from page 78

two other known synthetic agonists, GW4064 and fexaramine.

Once the researchers had identified MFA-1 as being a potent agonist of FXR, they next sought to glean some insights into how MFA-1 interacts with FXR by determining the crystal structure of the FXR in complex with MFA-1. Notably, the structure of human FXR in complex with MFA-1 was similar to previously reported structures of rat FXR in complex with bile. FXR was also similar in structure to other members of the same receptor family, which includes the estrogen and progesterone receptors.

X-ray crystallography carried out at the IMCA-CAT beamline 17-ID showed that the FXR consisted of 12 coils or helices and that MFA-1, when bound, was buried deep within the FXR structure. The researchers also found that the steroid ring system of MFA-1 was bound in an orientation that was flipped by 180 degrees compared with the natural bile acid ligands. They suggest that the presence of a negative charge on MFA-1 may play a role in dictating the orientation of the ligand in the binding pocket. These findings help to dispel previous suggestions that FXR uses shape discrimination to preferentially bind bile acids over conventional steroids. In fact, FXR may use elements other than the binding orientation and steroid rings to select ligands. The researchers also speculated that MFA-1, like other FXR agonists, might activate the FXR by helping to stabilize the structure of the receptor.

Future efforts are likely to focus on developing additional molecules that can bind to the FXR and that may be useful in preventing or treating the metabolic syndrome. — *Emma Hitt*

See: Stephen M. Soisson*, Gopalakrishnan Parthasarathy, Alan D. Adams, Soumya Sahoo, Ayesha Sitlani, Carl Sparrow, Jisong Cui, and Joseph W. Becker, "Identification of a potent synthetic FXR agonist with an unexpected mode of binding and activation," Proc. Nat. Acad. Sci. USA **105**(14), 5337 (April 8, 2008). DOI: 10.1073pnas.0710981105

Author affiliation: Merck Research Laboratories

Correspondence: *stephensoisson@merck.com

Use of the IMCA-CAT beamline 17-ID at the APS was supported by the companies of the Industrial Macromolecular Crystallography Association through a contract with the Center for Advanced Radiation Sources at The University of Chicago. Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

17-ID • IMCA-CAT • Life science • Macromolecular crystallography, anomalous diffraction (MAD/SAD) • 3.3-cm Undulator A • Accepting general users

A New Life Sciences Facility at the APS

LS-CAT Operations Manager Keith Brister (Northwestern University) at the MD2 diffractometer in the 21-ID-D enclosure.

The Life Sciences Collaborative Access Team (LS-CAT) on APS Sector 21 is the latest macromolecular crystallography sector providing state-of-the-art x-ray diffraction facilities at the APS. LS-CAT is open to general-user (GU) proposals through the APS GU proposal system, and to researchers from member institutions. Facilities at LS-CAT include four experiment stations (21-ID-C, -D, -E, and -G) taking beam from two insertion devices (IDs). The main beamline (21-ID-D) uses a shortened APS Undulator A and a double-crystal monochromator in a layout very similar to the XOR 4-ID beamline, and the NE-CAT ID beamline on Sector 24. The other three LS-CAT experiment stations share a 3.0-cm undulator.

The 21-ID-F and 21-ID-G stations use diamond Laue monochromators—along with beryllium lenses—to deliver focused beam to the stations. This arrangement, much like the ID14 beamline at the European Synchrotron Radiation Facility, allows macromolecular crystallography experiments to be done at the selenium edge (12.668 keV). The fourth station, 21-ID-E, is scheduled to come on line in 2009 using a large offset monochromator.

Each of the four stations is equipped with a MAATEL MD2 microdiffractometer for high-throughput crystallography. The MD2 provides a beam-axis video view of the sample without parallax error.

LS-CAT manages user data using the Lustre file system, originally developed for supercomputer centers. This system allows very fast access for data analysis. The APS Experiment Safety Review System (ESAF, see page 140) has been integrated into the data collection process. ESAF approval generates the user accounts required to use the LS-CAT systems, elevating the ESAF to an engineered control that enhances user safety.

To automate sample manipulation, four Cryogenic Automated Transfer Systems (CATS), one for each experimental enclosure, are being installed. Each of the robots is equipped for both SPINE and Cryotong grippers to provide the greatest flexibility for users.

LS-CAT was formalized in 2003 with seed money from the State of Michigan through the Michigan Core Technology Alliance. Northwestern University was selected as the managing partner for the collaboration. Current LS-CAT members are Michigan State University, the University of Michigan, Wayne State University, the Van Andel Research Institute, Northwestern University, the University of Wisconsin-Madison, Vanderbilt University, and the University of Illinois at Urbana-Champaign.

Contact Keith Brister
(k-brister@northwestern.edu)

UNRAVELING THE PRODUCTION OF BACTERIAL ANTIGENS

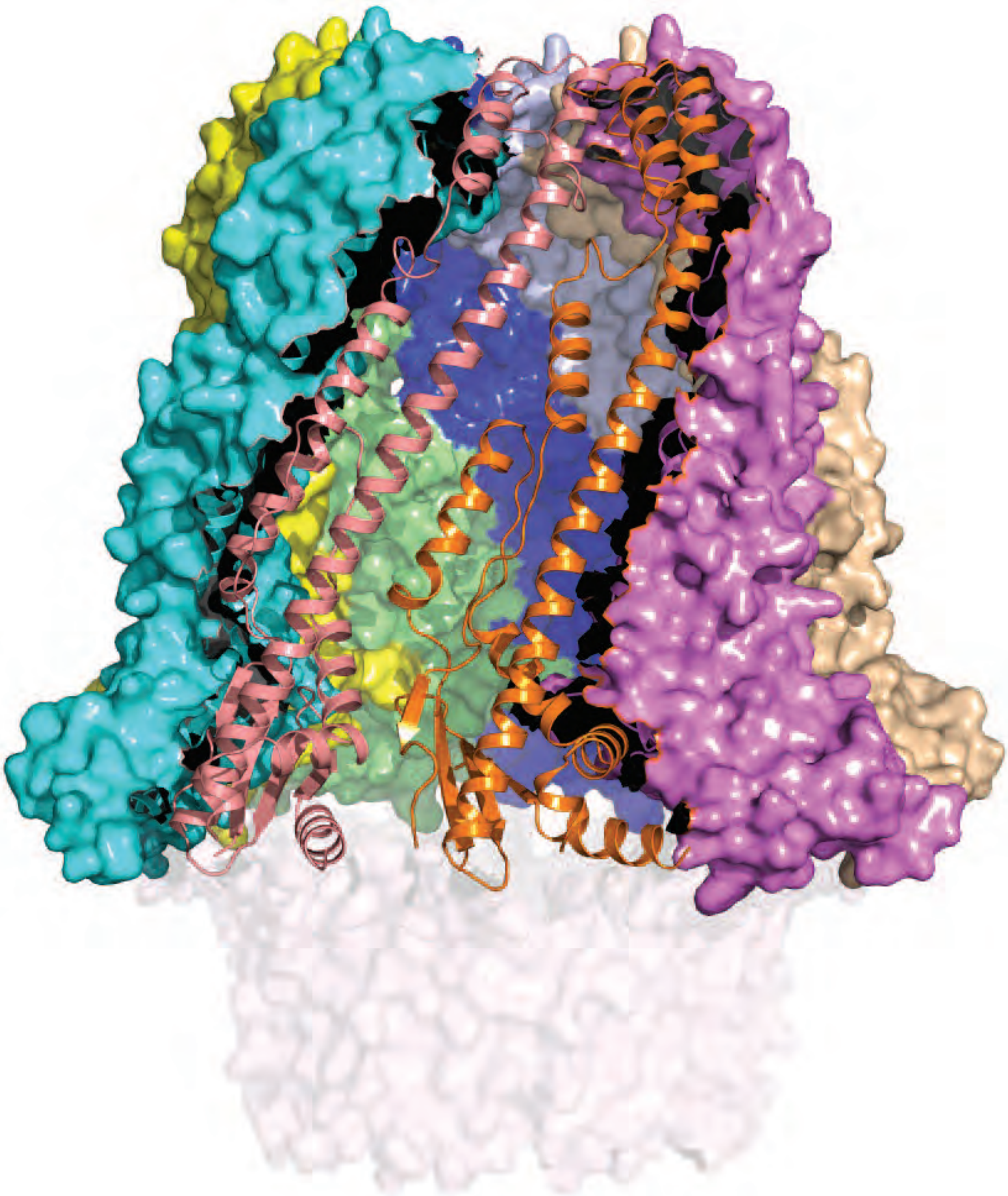

Fig. 1. The representation of a FepE nonamer. Each protomer is painted in a different color. This assembly creates a large internal cavity. The pale surface at the bottom of the bell represents a model of the possible arrangement of the transmembrane helices (18 in total). The transmembrane regions were not part of the crystal structure.

Three-dimensional structures from this research can be viewed here.

Bacterial pathogens protect themselves from their hosts with the aid of a great variety of complex polysaccharides present on their cell surfaces. The variability in these polysaccharides from one strain to another helps pathogens circumvent both host defenses and pharmacological intervention. The chain length of some of these surface polysaccharides, such as O-antigen in gram-negative bacteria, is a key determinant of their virulence. Chain length is known to be regulated by polysaccharide co-polymerases (PCPs) located on the inner membrane and extending into the periplasmic space. Bacterial PCPs are themselves highly variable: over 1,150 have been identified and grouped into three classes. Researchers using the APS have succeeded in describing the three-dimensional (3-D) structures of PCPs derived from two of the pathogens most frequently implicated in bacterial gastroenteritis: *Salmonella enterica* and *Escherichia coli* O157:H7, providing new tools for studies of the processes involved in bacterial polysaccharide biosynthesis.

The researchers, from McGill University, the University of Adelaide, the National Research Council of Canada, the Hospital for Sick Children, and the University of Montreal determined the 3-D structures of the periplasmic domains of four PCPs that confer different polysaccharide chain lengths, one (WzzB) from *S. enterica* serotype Typhimurium and three from *E. coli* O157:H7 (FepE, WzzE, and WzzB). X-ray diffraction data were collected at the SGX-CAT 31-ID beamline at APS and beamlines X8C, X12B, and X29 at the National Synchrotron Light Source at Brookhaven National Laboratory. The structures were resolved to 2.7 Å (FepE), 3.1 Å (*S. enterica* WzzB), 2.4 Å (WzzE), and 3.6 Å (O:157:H7 WzzB). All four proteins belong to the PCP1 group and participate in the Wzy pathway for complex polysaccharide synthesis.

As is generally true for PCPs, sequence identity between the four proteins was low, in the range of 16–22% for their periplasmic segments. However, they showed striking structural similarities at the subunit (protomer) level. The protomers making up the four proteins had two structural components: an α/β base domain placed close to the inner membrane and an α-helix hairpin extending out into the periplasmic space. Visualized from below, the α/β base forms a trapezoid in cross-section. The α-helix hairpin consists of an elongated (100-Å-long) helix, followed by a pair of helices that fold back toward the inner membrane for a coiled-coil interaction with the 100-Å helix. The close correspondence in the structures of the four PCP1 group proteins suggests that all the class 1 PCPs might have similarly structured protomers despite their low sequence identity.

In the crystals, the protomers self-assembled into intriguing thimble- or bell-shaped oligomers around an internal cavity, with the curvature resulting from the trapezoid bases of the protomers. The FepE oligomer typically crystallized with 9 protomers (Fig. 1), the WzzE with 8, and the *S. enterica* WzzB with 5. The *E. coli* WzzB adopts an open trimeric arrangement in the crystal corresponding to half a bell structure; when two such trimers are assembled together, they form a closed hexameric bell. The number of protomers in the bell-shaped oligomer correlates to some extent with the length of the synthesized polysaccharide in that FepE, the largest of the three oligomers, producing extremely long O-antigen chains (~80 repeat units).

The PCP crystals represented only the periplasmic domains of the proteins. The researchers next sought to determine how the crystallized periplasmic segment corresponds to the structure of a full-length PCP1 by using electron microscopy studies of purified WzzE. They identified complexes with consistent shapes and dimensions that corresponded very well to the octamers in the crystal.

Based on the structure of the crystallized PCPs and their investigations of the effects of specific mutations on PCP function, the researchers proposed that it is the external thimble shape of the PCP oligomers, rather than any protein-protein interaction that regulates the length of the synthesized polysaccharide chain. In this model, the transmembrane base of the PCP oligomer serves as an organizing scaffold for polysaccharide assembly by multiple Wzy polymerases, while the top of the oligomer measures the polymer length. — *Carol Hart*

See: Ante Tocilj[1], Christine Munger[1], Ariane Proteau[1], Renato Morona[2], Leanne Purins[2], Eunice Ajamian[1], John Wagner[3], Magdalene Papadopoulos[2], Luisa Van Den Bosch[2], John L. Rubinstein[4], James Féthière[5], Allan Matte[3], and Miroslaw Cygler[1,3]*, "Bacterial Polysaccharide Co-polymerases Share a Common Framework for Control of Polymer Length," Nat. Struct. Mol. Biol. **15**, 130 (February 2008). DOI: 10.1038/nsmb.1374

Author affiliations: [1]McGill University; [2]University of Adelaide; [3]National Research Council, Canada; [4]Hospital for Sick Children; [5]Université de Montréal

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31-ID • SGX-CAT • Life science • Macromolecular crystallography, single-crystal diffraction, fiber diffraction, single-wavelength anomalous dispersion • 3.3-cm Undulator A • Accepting general users

USING VIRUSES TO TARGET CANCER

Viruses are small particles composed of protein and nucleic acid that are known for their ability to cause infectious diseases, such as the flu, and some cancers. What they are less known for is their ability to treat cancer. However, this possibility has been studied since the 1950s, when the first clinical trials investigating the use of viruses to treat cervical cancer were initiated. Research has progressed in this area and new viruses have been identified that can selectively kill tumor cells. One of these is the new picorna family virus, Seneca Valley Virus-001 (SVV-001), which is unique enough to be given its own genus. In recent work performed at the BioCARS 14-BM beamline at the APS under biohazard safety level 2 (BSL2) conditions, researchers elucidated the three-dimensional structure of this remarkable RNA virus. This work produced important information about a new viral genus and may provide answers to the question of how some viruses specifically recognize and kill cancer cells while other related viruses do not.

Picornaviruses are single-stranded, positive-sense RNA viruses. This family includes more than 150 members that cause human disease, including polioviruses, human rhinoviruses (HRV) that cause the common cold, and the cardioviruses such as Mengo encephalomyocarditis virus (MEV), that could cause acute fever. Their RNA genome codes for four structural proteins that make up the repeating structure of the outer coat of the virus and seven other non-structural proteins. The structure of SVV-001, determined at a resolution of 2.3 Å, was solved for the outer coat proteins known as VP1, VP2, VP3, and VP4. In this study, the structure of SVV-001 was solved by molecular replacement against the known structure of the cardiovirus MEV, with which it shares 42% sequence similarity. The majority of the core structural features of SVV-001 are similar to other picornaviruses; however, there exist important differences in the surface exposed "loops" of the VP1 and VP2 subunits that may be responsible for the differences in binding to different cell types, otherwise known as cell tropism.

The serendipitous discovery of the SVV-001 as a cell culture contaminant in the 1990s has led researchers to identify it as a possible therapeutic tool because, although it does not infect human cells, it can infect tumor cells of neuroendocrine origin. In fact, this study undertook to use their structure to investigate possible surface motifs on the virus that might be important for binding to tumor cells with neuroendocrine features. Comparison of exposed sequence motifs to known motifs that bind surface receptors such as integrins and the low-density lipoprotein receptor (LDLR) revealed possible amino acid sequences that could be responsible for cellular attachment. For example, comparison of SVV-001 loop regions to those of the closely related MEV, which does not bind to cancer cells, showed that SVV-001 contains possible LDLR binding regions that are not observed in MEV. In contrast, HRV2, which is known to bind to the LDLR, has a very similar fold to SVV-001 in this area. Seneca Valley Virus-001 also contains two amino acid motifs in exposed loop regions that have the hallmarks of proteins that bind to cell surface integrins.

The team was also able to learn more about the interactions between the structural proteins making up the viral outer shell, known as the capsid, and the RNA genome housed within. This analysis was achieved at a resolution of 20 Å and is the first time that this type of x-ray crystallographic data has been available for a picornavirus. Crystallographic data revealed that the RNA genome is in almost constant contact with the capsid, with particularly prominent contacts with VP2 and to a lesser extent with VP4.

Elucidation of the structure of the SVV-001 represents a significant step forward in understanding picorna family viruses and in advancing our understanding of how viruses that recognize cancer cells do so with such specificity. This knowledge is essential to the development of these viruses as potential cancer therapeutics.

— *Sandy Field*

See: Sangita Venkataraman[1], Seshidhar P. Reddy[2], Jackie Loo[1], Neeraja Idamakanti[2], Paul L. Hallenbeck[2], and Vijay S. Reddy[1]*, "Structure of Seneca Valley Virus-001: An Oncolytic Picornavirus Representing a New Genus," Structure **16**, 1555 (October 8, 2008).
DOI: 10.1016/j.str.2008.07.013

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This work was partially supported by the National Institutes of Health (NIH) Grant R56 AI070771 to V.S.R. Partial salary support to V.S.R. by NIH Research Resource Multiscale Modeling Tools for Structural Biology (MMTSB; RR12255) is acknowledged. BioCARS is supported by the National Center for Research Resources of the NIH. Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

14-BM • BioCARS • Life science • Macromolecular crystallography, fiber diffraction, biohazards at the BSL2/3 level, subatomic (<0.85 Å) resolution • Bending magnet • Accepting general users

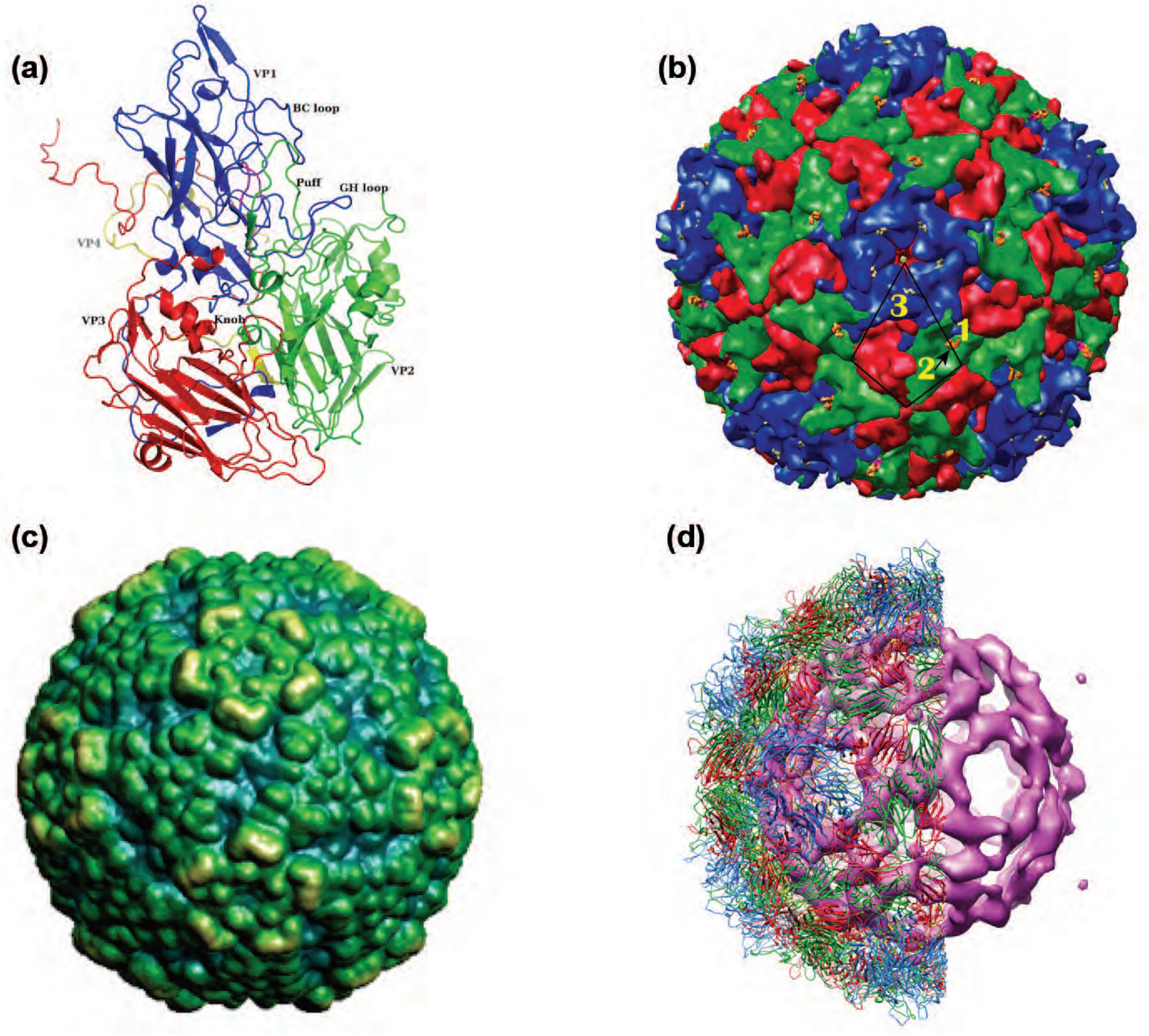

Fig. 1. Salient features of the structure of SVV-001. (a) Subunit organization highlighting the important loop regions in VP1 (blue), VP2 (green), VP3 (red) and VP4 (yellow). (b) Organization of the above subunits in the assembled capsid. (c) Surface-rendered image of SVV-001 showing the most exposed residues in shades of yellow and the least in shades of blue. (d) Cutaway view showing the organization of RNA (magenta) in the SVV particle. Half of the protein subunits surrounding the RNA are shown as ribbons.

THE CHOREOGRAPHY OF MEMBRANE TRAFFIC

How does a cell transport the biochemicals that need to be in a certain place at a certain time in order for the show to go on? The answer is choreography, choreography, choreography. Membrane-bound packets, known as "vesicles," serve as the dancers that enclose and carry molecules from one membrane-bound compartment to another, where fusion creates a channel through which the molecules arrive at their new location. Multitudes appear to be the key here, in the form of hundreds of proteins and nucleotides that associate in complexes on both the carrier membrane and the target membrane. Only when all are present and active does metabolism proceed correctly. So it is not surprising that biochemists have labored long and hard to identify and visualize the components of membrane transport systems. Researchers using high-brightness x-ray beams from the APS have gathered data that show which molecules need to be where and how their actions result in the required steps for fusion, providing much-needed insight for investigating metabolic disorders.

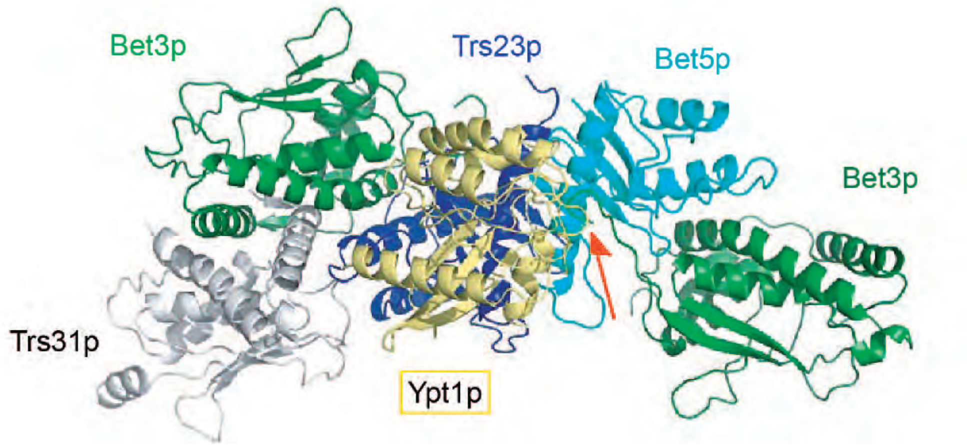

Fig 1. Structure of a TRAPP subcomplex as it activates the Rab GTPase Ypt1p; TRAPP subunits are Bet3p, Bet5p, Trs23p, and Trs31p. The C-terminus of one copy of Bet3p (red arrow) invades the nucleotide-binding site of Ypt1p as part of the mechanism for activation.

The proteins required for membrane transport include the membrane fusion machinery as well as coat proteins that are needed for cargo selection and vesicle budding, small regulatory GTPases, and large tethering complexes that mediate the recognition between a vesicle and its target compartment. One such tethering complex, TRAPPI, is present in all nucleus-containing cells, including human cells, and therefore is critical to understanding metabolic disease. With the help of NE-CAT beamline 24-ID-C at the APS, the researchers from Yale University, the University of Kentucky, and the Yale University School of Medicine determined the crystal structure of a TRAPPI complex needed for an event directly preceding membrane fusion, resulting in a model that is consistent with new and existing data.

The researchers set out to understand how TRAPPI subunits cooperate in activating an enzyme known as Rab GTPase Ypt1p. Activation of Ypt1p, or conversion from its GDP- to GTP-bound state, is necessary for subsequent membrane fusion and requires a complex of four different TRAPPI subunits. The team studied a TRAPPI subassembly containing the TRAPPI subunits critical to the activation process (two copies of Bet3p and one each of Bet5p, Trs23p, and Trs31p) in complex with Ypt1p (Fig. 1).

In an elegant progression of steps, TRAPPI stabilizes the nucleotide-bind-

"Traffic" continued on page 88

OPTIMIZING THE USE OF BACTERIAL INVADERS

Phages do to bacteria what some bacteria do to humans—threaten their health by infecting them. Phages are simple packages of genetic material, either DNA or RNA, surrounded by a protein coat, and they are so adept at infecting and killing bacteria, that they have even been investigated as a form of antibacterial therapy. In the U.S., phages are used to eliminate potentially toxic Listeria bacteria from some types of cheeses. Phages can also be used to attach fluorescent molecules to RNA so that researchers can view them using the live-cell imaging technique. Researchers from the Albert Einstein College of Medicine sought to find out more about another use for phages, called "RNA affinity purification," a technique used to purify pieces of RNA from a mixture of molecules. Their research yielded a greater understanding of how a particular bacteriophage—PP7—binds to RNA; this information could expand the uses of fluorescent labeling of RNA for cell imaging.

In their study, the group focused on the PP7 bacteriophage and the way it recognizes the RNA to which it attaches with the help of the SGX-CAT Express Crystallography service and 31-ID beamline at the APS.

During the life cycle of the phage, which involves attachment and penetration of the bacterial host and then its own replication, the protein coat of the PP7 phage serves not only a structural function, but also a regulatory function by attaching to its inner genetic material, in this case RNA. Specifically, the protein is able to recognize a kink in the RNA, called a "hairpin," which contains a unique sequence of RNA. It is the ability to recognize and attach to this piece of RNA that makes the phage useful in other applications, such as purifying RNA and labeling RNA with fluorescent tags.

The researchers found that the structure of the PP7 phage coat protein attached in a manner that was distinct from that of the coat protein of another type of phage, called MS2, which has been very well characterized in previous studies. Both the PP7 coat protein and the MS2 coat protein are able to bind their own RNA targets with high affinity. The distinct specificities allow PP7 and MS2 to be used together with distinct fluorescent proteins to detect multiple RNA species in living cells.

"Invaders" continued on page 88

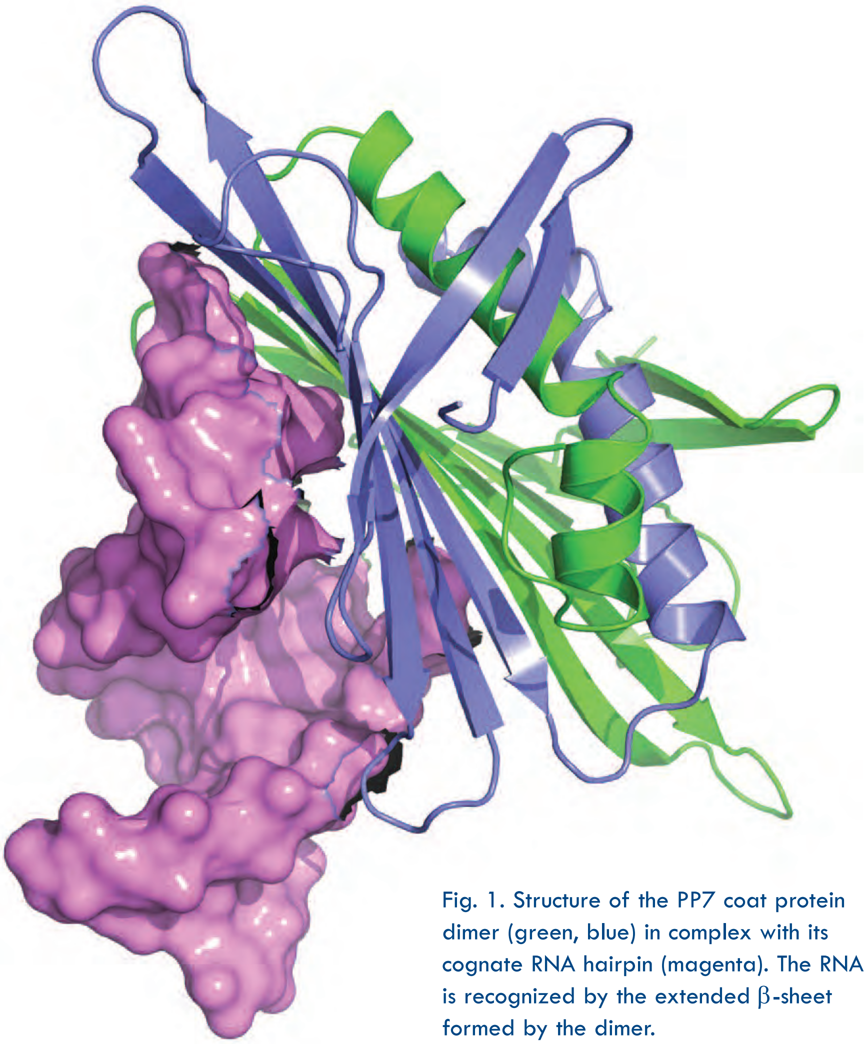

Fig. 1. Structure of the PP7 coat protein dimer (green, blue) in complex with its cognate RNA hairpin (magenta). The RNA is recognized by the extended β-sheet formed by the dimer.

Three-dimensional structures from this research can be viewed here

"Invaders" frompage 87

The researchers sought to solve the protein structure of the PP7 protein coat in complex with its RNA hairpin recognition site. Specifically, they used a shortened version of the protein and solved the structure in its unbound form and also in complex with a 25-nucleotide piece of RNA containing the recognition site. Interestingly, they found that the PP7 protein coat had "co-evolved" with its RNA recognition site and was able to bind two RNA adenosine bases at a time through symmetrically positioned protein pockets in the PP7 protein coat.

Now that the way in which PP7 can bind to RNA is more precisely understood, future research may enable the design of additional proteins that can be used to purify various types of RNA and expand applications in fluorescent labeling of RNA for cell imaging. — *Emma Hitt*

See: Jeffrey A. Chao, Yury Patskovsky, Steven C. Almo, and Robert H. Singer*, "Structural basis for the coevolution of a viral RNA–protein complex," Nat. Struct. Mol. Biol. **15**(1), 103 (January 2008). DOI: 10.1038/nsmb1327
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31-ID • SGX-CAT • Life science • Macromolecular crystallography, single-crystal diffraction, fiber diffraction, single-wavelength anomalous dispersion • 3.3-cm Undulator A • Accepting general users

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"Traffic" from page 86

ing pocket of Ypt1p in an open conformation to facilitate nucleotide exchange. Three of the TRAPPI subunits—Bet3p, Bet5p, and Trs23p—are involved in stabilizing the form while one end of the Bet3p helps to remodel the complex by invading the pocket. The Trs31p unit works to change the shape and position of a region of Trs23p that helps to bind Ypt1p.

The research team was able to extend their conclusions from studying the TRAPPI complex to the related TRAPPII membrane-tethering complex, which has the same four subunits necessary for nucleotide exchange and also activates Ypt1p. It is likely that TRAPPII activates the Ypt1p complex by a mechanism identical to that discovered for TRAPPI. Both TRAPPI and TRAPPII are involved in necessary cellular processes, namely proper functioning of cellular transport mechanisms to the Golgi apparatus. Thus, the data provide a general framework for understanding how a membrane-tethering complex that includes several subunits activates the steps necessary to membrane fusion. Without these important membrane-tethering molecules, and the rest of the molecules in the picture, the initial interactions required for fusion of the carrier and target membranes cannot occur.

The data show which molecules need to be where and how their actions result in the required steps for fusion, providing much-needed insights for investigating metabolic disorders

Interestingly, when taken separately, the TRAPPI subunits by themselves do not seem to be responsible for any single part of the activation process. It is the interaction among the subunits that results in the correct turn of events, just as it is the interaction among the hundreds of molecules involved in the dance of cellular transport that turns it into a fully formed production. — *Mona Mort*

See: Yiying Cai[1], Harvey F. Chin[2], Darina Lazarova[1], Shekar Menon[1], Chunmei Fu[1], Huaqing Cai[1], Anthony Sclafani[1], David W. Rodgers[3], Enrique M. De La Cruz[2], Susan Ferro-Novick[1]*, and Karin M. Reinisch[1]**, "The Structural Basis for Activation of the Rab Ypt1p by the TRAPP Membrane-Tethering Complexes," Cell **133**, 1202 (June 27, 2008).
DOI: 10.1016/j.cell.2008.04.049
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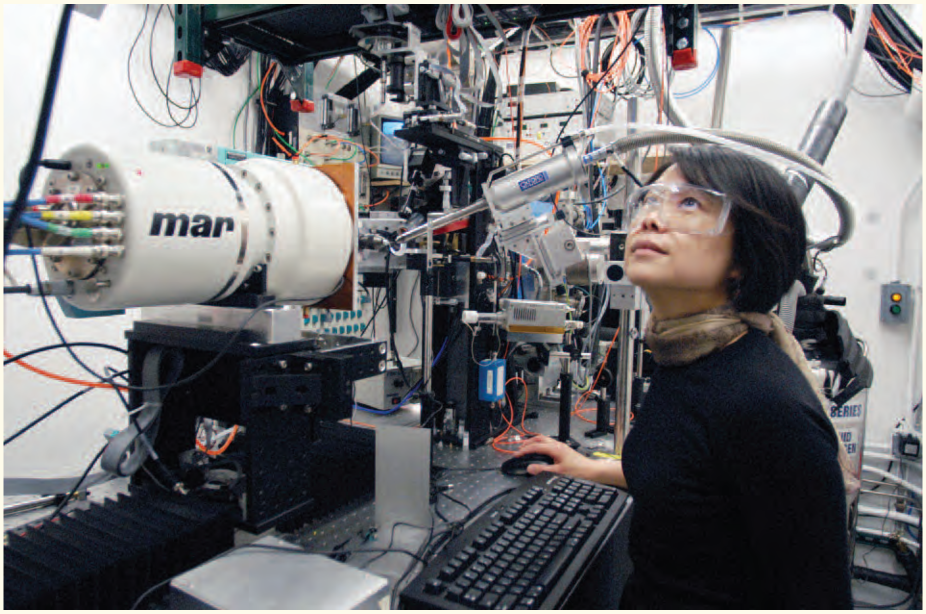
24-ID-C • NE-CAT • Life science • Microfluorescence (hard x-ray), tomography, microdiffraction • 3.3-cm Undulator A • Accepting general users

100-ps Time-Resolved Crystallography at BioCARS



Xiaojing Yang, a scientist with Keith Moffat's group at The University of Chicago, working on her time-resolved crystallography project involving bacteriophytochrome crystals in the 14-ID-B experiment station.

BioCARS beamline 14-ID-B at the APS has been upgraded to a new role as a leading facility worldwide for 100-ps time-resolved x-ray crystallography. The upgrade is the result of a collaboration between BioCARS, one of four beamlines at the APS operated by the Center for Advanced Radiation Sources (CARS) at The University of Chicago; the National Institutes of Health, National Institute of Diabetes and Digestive and Kidney Diseases (NIH/NIDDK); and the APS.

The upgrade, which encompasses new beamline optics and improved time resolution, features installation of several new pieces of equipment: two undulators that operate collinearly, a new Kirkpatrick-Baez mirror system providing 90-μm (horizontal) by 35-μm (vertical) x-ray beam size at the sample, a new monochromator, an upgraded BioCARS ultrafast x-ray chopper capable of isolating single x-ray pulses in the 24-bunch APS mode, a new heat-load chopper, and a new picosecond laser system with associated beam-delivery optics and synchronization electronics.

The new configuration extends the time resolution available for the successful nanosecond time-resolved crystallography user program at BioCARS into the sub-nanosecond time domain. Many challenging new areas of investigation become accessible, including studies of more-complex biological molecules, irreversible reactions, and important biological processes such as cooperativity, signal transduction, and catalysis.

The first experiments using the new configuration, completed in December 2007, were collaborations between NIH/NIDDK and the University of Massachusetts Medical School.

BioCARS is now welcoming new user groups interested in conducting time-resolved experiments on the upgraded beamline. Proposals can be submitted through the APS proposal system found here.

Contact Vukica Šrajer
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At the 14-ID-B dedication ceremony on April 18, 2008. Front row (l. to r.): James Viccaro, Executive Director of CARS; Argonne Associate Laboratory Director for Photon Sciences and APS Director Murray Gibson; Keith Moffat of The University of Chicago and principal investigator for BioCARS; Philip Anfinrud, collaborator, NIH/NIDDK; Timothy Graber, lead beamline designer for the upgrade, CARS. Back row (l. to r.): Zhong Ren, Shengyang Ruan, Yu-Sheng Chen, Frank Westferro, Robert Henning, Friedrich Schotte, Matti Meron, Vukica Šrajer and Guy Macha (all CARS, except Schotte, NIH/NIDDK). Not pictured: Harold Brewer (CARS), Hyun Sun Cho (NIH/NIDDK) and Naranbaatar Dashdorj (NIH/NIDDK).

A PERFECT CUT-AND-PASTE: THE MECHANISM OF A BACTERIAL GENE TRANSPOSITION

Transposons are mobile segments of genetic code that, with the aid of transposase enzymes, can move from one location in the genome to another. These movements frequently result in the proliferation of nonfunctional nucleotide sequences, exemplifying the “selfish gene” phenomenon. But transposable genetic elements have also been a force in evolution, because these transpositions may alter the functioning of affected genes. Understanding how transposons jump from one position in the genome to another clearly has great relevance to both basic science and medicine. In bacteria, the tiny transposons known as insertion sequences can facilitate the development of antibiotic resistance. Bacterial insertion sequences are among the simplest genetic transposition systems, making them valuable models for study. Now, researchers using an x-ray beamline at the APS have described the entire transposition cycle, from transposase activation to target site selection.

Originally identified in the gastric pathogen *Helicobacter pylori*, IS608 is a member of the IS200/IS605 family, which encodes the smallest DNA transposases discovered to date. Typically, insertion sequences code only for one or two proteins involved in transposition (primarily the transposase), and the coding region is usually flanked by inverted repeats. Those of the IS200/IS605 family are an exception, having imperfect palindromic sequences near their ends. Their transposase, TnpA, is only 155 amino acids in length, about half the length of most transposases, yet it can carry out all the steps of translocation. To discover how this small, single-domain molecule works, researchers from the National Institute of Diabetes, Digestive, and Kidney Diseases, National Institutes of Health; and the Laboratoire de Microbiologie et Génétique Moléculaires Centre, National de la Recherche Scientifique, crystallized and solved the three-dimensional structure of five different complexes of TnpA with DNA substrates of varying lengths by using the SER-CAT beamline 22-ID at the APS.

TnpA forms a homodimer in which each subunit contains a His-hydrophobic-His (HUH) motif and a mobile helix αD carrying a catalytic tyrosine. When properly aligned with the HUH motif, the tyrosine is able to cleave the transposon by attacking the phosphate backbone of the donor DNA.

The palindromic DNA sequences in IS608 are folded into two hairpin loops that serve as recognition sites for the transposase to find and bind the transposon ends. The additional binding of four nucleotides upstream of the hairpin causes a conformational change in the transposase. This change moves the mobile helix to realign important catalytic residues, including the tyrosine, so that the active site is now fully assembled and positioned to attack the phosphate bond (Fig. 1).

During transposition, the excised IS608 initially forms a single-strand circle in which the two ends are joined. IS608 is always taken from a transposon flanking donor sequence containing TTAC to a target sequence also containing TTAC, where it inserts exactly 3' to these four nucleotides. This nucleotide sequence is recognized not by TnpA itself but by base-pairing with the four-nucleotide extension of the left hairpin when it is bound to the activated transposase. The right end is also directed into the TnpA active site by means of internal DNA interactions. Other members of the IS200/IS605 family exhibit similar fidelity to a specific four- or five-nucleotide sequence.

Despite its small size, TnpA carries out its cut-and-paste operations with remarkable precision. Upon excision, the donor backbone is sealed without replication of the excised strand, and insertion takes place without target site duplication. The novel DNA self-recognition and single-strand transposition system revealed by this research may have applications in genomics and biotechnology. — *Carol Hart*

See: Orsolya Barabas[1], Donald R. Ronning[1], Catherine Guynet[2], Alison Burgess Hickman[1], Bao Ton-Hoang[2], Michael Chandler[2], and Fred Dyda[1]*, “Mechanism of IS200/IS605 Family DNA Transposases: Activation and Transposon-Directed Target Site Selection,” Cell **132(2)**, 208 (25 January 2008).
DOI: 10.1016/j.cell.2007.12.029

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22-ID • SER-CAT • Life science • Macromolecular crystallography, multi-wavelength anomalous dispersion • 3.3-cm Undulator A • Accepting general users

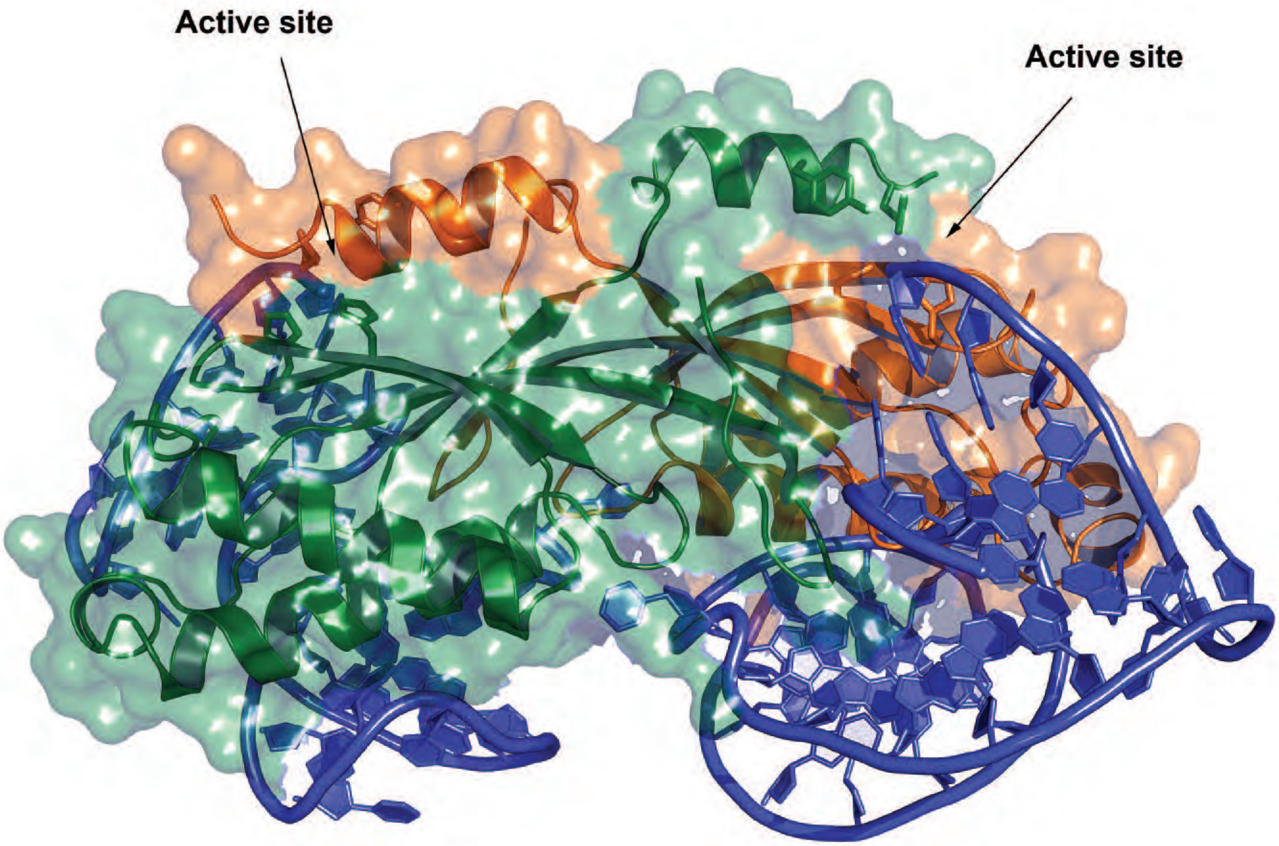

Fig. 1. Overall structure of TnpA bound to transposon end DNA.

A QuickTime movie from this research can be viewed here.

HOW DNA "SPELL CHECKERS" FIX MISSPELLED GENES

A recent study of a pair of DNA repair proteins is helping scientists to understand how living things fix genetic damage that would otherwise bring life on Earth to a grinding halt. University of Chicago researchers determined the first three-dimensional structure of the *E. coli* repair enzyme AlkB bound to a strand of DNA, where it corrects errors that could bring about mutation or cell death. The structure revealed an unusual mechanism for swapping out damaged segments of the DNA molecule. In a second finding, the investigators determined the structure of a related human enzyme, ABH2, which they say might help scientists design better chemotherapy treatments for cancer.

All cells contain a DNA genome, which encodes a set of instructions that tells the cell how to grow and reproduce. During reproduction, the cell makes a copy of the genome and gives the copy to its offspring cell. The copying process is never perfect, so the duplicate genome will have at least a few little changes, called mutations, which are the raw material of evolution. But if the mutations disrupt important genes, the offspring may be impaired or die. AlkB and ABH2 both counteract a common source of mutation, called methylation, in which methyl groups—small carbon molecules—are stuck at random to DNA.

The enzymes act much like word-processing software that automatically corrects a misspelled word, except the word is actually a sequence of DNA "letters" (called bases) that make up a gene. DNA consists of two strands wound together like a spiral staircase. Each "step" is made of a two bases, one from each DNA strand. To copy the genome, a cell must scan the bases on one strand of DNA. But methylation can cause the cell to misread the identity of the affected base.

To figure out how these protein machines physically excise methyl groups, the researchers mixed short, methylated DNA molecules with versions of the enzymes engineered to become stuck in place during the repair procedure. They then grew crystals from the enzyme-DNA mixtures and passed x-rays through each crystal to solve its atomic structure—work that was performed on the BioCARS 14-BM and SBC-CAT 19-BM beamlines at the APS.

The group found that AlkB had squeezed together the two bases flanking the methylated one and flipped around the damaged base so that it was buried in the enzyme, which could then strip away the methyl group (Fig. 1). Scientists have never seen an enzyme do that before, the team reported. Interestingly, ABH2 worked by quite a different mechanism. Instead of squeezing the DNA, it inserted a slim, finger-like part of itself into the DNA to wedge free the damaged base and fill its place during repairs (Fig. 1).

Biologists don't yet know exactly how enzymes like AlkB and ABH2 search through the billions of bases in a DNA molecule to find the damaged ones. But according to these researchers, a chemical strategy used in this study provides a powerful method for studying DNA repair enzymes. Human cells contain multiple enzymes similar to ABH2, one of which seems to play a role in obesity. Researchers believe ABH2 can help tumors withstand chemotherapy drugs, some of which work by methylating DNA to kill fast growing cells. The University of Chicago group notes that one application of its findings might be in designing drugs to make chemotherapy more effective by shutting off ABH2. — *JR Minkel*

See: Cai-Guang Yang, Chengqi Yi, Erica M. Duguid, Christopher T. Sullivan, Xing Jian, Phoebe A. Rice, and Chuan He*, "Crystal structures of DNA/RNA repair enzymes AlkB and ABH2 bound to dsDNA," Nature **452**, 961 (24 April 2008).
DOI: 10.1038/nature06889

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14-BM • BioCARS • Life science • Macromolecular crystallography, fiber diffraction, biohazards at the BSL2/3 level, subatomic (<0.85 Å) resolution • Bending magnet • Accepting general users

19-BM • SBC-CAT • Life science • Anomalous diffraction (MAD/SAD), ultra-low-temperature (15K) • Bending magnet • Accepting General Users

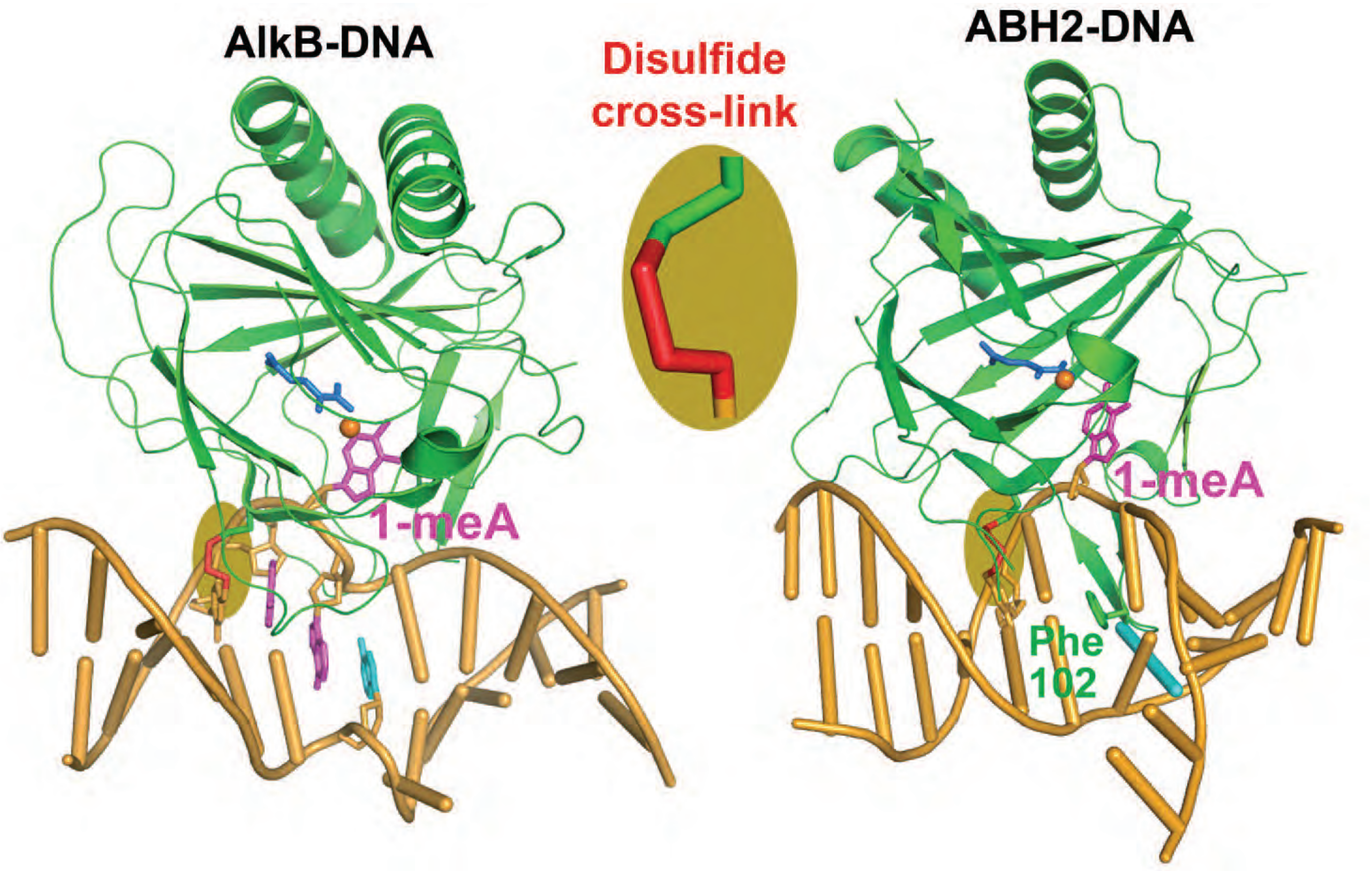

Fig. 1. Schematic structures of DNA repair enzymes (green) bound to double-stranded DNA (gold) containing a methylated base (pink; 1-meA) that would cause mutation if it were copied by the cell. Both enzymes disrupt stacking of DNA base pairs to get access to the damaged base, which is shown flipped away from the interior of the DNA molecule. The E. coli enzyme AlkB (left) is seen squeezing and distorting the surrounding bases (pink and light blue), whereas human ABH2 has inserted an amino acid (Phe 102) in place of the damaged base. The enzymes are held in this configuration by an engineered disulfide chemical bond (red and green; inset).

CYLINDRICAL COATS AND PICKET FENCES

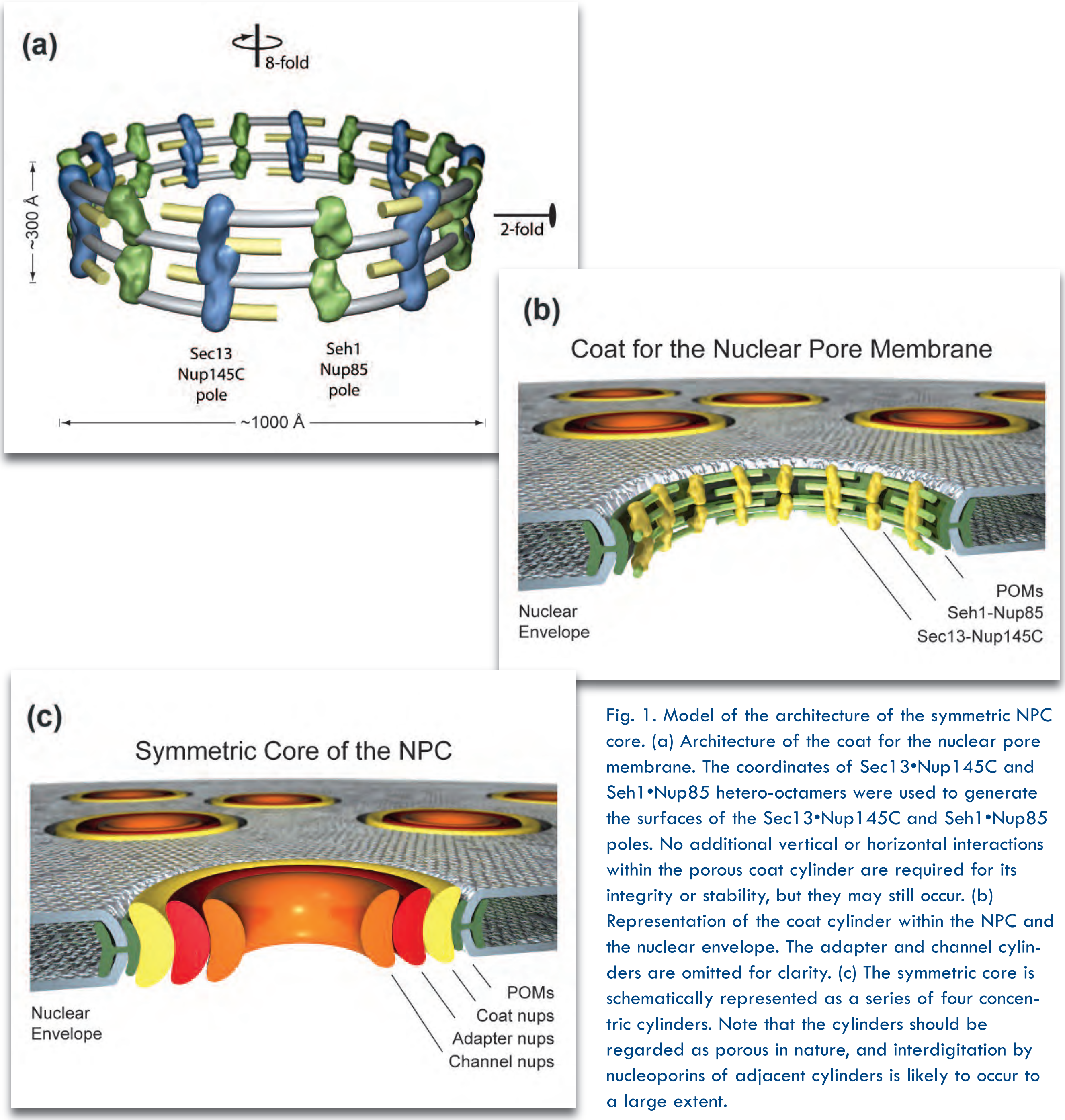

Fig. 1. Model of the architecture of the symmetric NPC core. (a) Architecture of the coat for the nuclear pore membrane. The coordinates of Sec13•Nup145C and Seh1•Nup85 hetero-octamers were used to generate the surfaces of the Sec13•Nup145C and Seh1•Nup85 poles. No additional vertical or horizontal interactions within the porous coat cylinder are required for its integrity or stability, but they may still occur. (b) Representation of the coat cylinder within the NPC and the nuclear envelope. The adapter and channel cylinders are omitted for clarity. (c) The symmetric core is schematically represented as a series of four concentric cylinders. Note that the cylinders should be regarded as porous in nature, and interdigitation by nucleoporins of adjacent cylinders is likely to occur to a large extent.

Eukaryotic cells, which are found in higher organisms, contain a nucleus surrounded by fluid called the cytoplasm. Large molecules must pass through the double membrane of the nuclear envelope to travel between the cytoplasm and the nucleus. They do so by way of unique portals called nuclear pore complexes (NPCs), which are embedded in the nuclear envelope, and which are crucial components in cell life. The NPC represents one of the largest protein structures in eukaryotic cells and is composed of multiple copies of 30 different types of nucleoporin proteins. It is the NPC's large size (relative to other protein structures) and its flexibility that have made it difficult for researchers to determine the structure, and hence the functioning, of this important protein assembly. X-ray diffraction data obtained by Rockefeller University Researchers at two APS x-ray beamlines, as well as two beamlines at the Advanced Light Source (ALS), have added important pieces to this puzzle.

The researchers determined a series of crystal structures of the nucleoporin pair Seh1•Nup85, which forms part of the cylindrical coat of the NPC (Fig. 1). The diffraction data were collected at the GM/CA-CAT 23-ID-D and NE-CAT 24-ID-C beamlines at the APS, and beamlines 8.2.1 and 8.2.2 at the Advanced Light Source at Lawrence Berkeley National Laboratory. Based on those data, the team was able to propose a structure for the cylindrical coat of the NPC, called the "NPC coat," and found similarities to other classes of membrane coats.

It had previously been determined that the NPC consists of a symmetric central core through which large molecules, such as proteins, pre-ribosomal particles, and messenger RNA, pass into and out of the nucleus. The NPC also contains cytoplasmic filaments extending into the cytoplasm and a "nuclear basket" on the other side of the central core in the nucleus. The structure of the NPC has remained largely unknown, partly because of the challenges involved in solving such a large and flexible protein assembly.

By determining multiple crystal structures of the Seh1•Nup85 nucleoporin pair, the researchers were able to draw several conclusions about the architecture of the cylinder-shaped NPC coat. They found that four copies of Seh1•Nup85 assemble into elongated, curved, 8-part (octamer) rods that bear striking similarities to those of another nucleoporin pair, Sec13•Nup145C, whose structure had been previously determined by the same researchers. Interestingly, although the configurations of the two nucleoporin pairs are distinct, both have similar overall dimensions and curvatures, suggesting closely related roles for the two octamers in the structure of the NPC.

The group proposed that in the NPC, the two nucleoporin octamers, Seh1•Nup85 and Sec13•Nup145C, are arranged in a structure that resembles a picket fence, consisting of 16 alternating vertical rods linked horizontally by three additional nucleoporins of the coat cylinder.

The NPC coat is similar in structure and function to another protein coat, COPII, which lines vesicles in the secretory pathway, suggesting that the NPC coat represents yet another class of membrane coats.

To reach these conclusions, the researchers used yeast proteins and crystallized the Seh1•Nup85 complex under three different conditions. Notably, similar assemblies were obtained in all three unrelated crystal forms. The finding that the lengths of the Seh1•Nup85 and Sec13•Nup145C complexes roughly correspond to the known height of the yeast NPC (approximately 300 Å), suggests that these rods may also occur in the assembled NPC in living cells.

The researchers gleaned insights into structural changes that may take place in Seh1•Nup85 during transport of large molecules through the NPC; Seh1•Nup85 may engage in a hinge-like motion during this process, providing the necessary flexibility of the NPC.

According to the researchers, more nucleoporin complex structures must be determined in order to resolve the final mysteries of one of the largest protein assemblies within eukaryotic cells. — *Emma Hitt*

See: Erik W. Debler, Yingli Ma, Hyuk-Soo Seo, Kuo-Chiang Hsia, Thomas R. Noriega, Günter Blobel**, and André Hoelz*, "A Fence-like Coat for the Nuclear Pore Membrane," Mol. Cell **32**, 815 (December 26, 2008).
DOI: 10.1016/j.molcel.2008.12.001

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23-ID-D • GM/CA-CAT • Life science • Macromolecular crystallography, microdiffraction, anomalous diffraction (MAD/SAD), subatomic (<0.85 Å) resolution • 3.0-cm undulator • Accepting general users

24-ID-C • NE-CAT • Life science • Microfluorescence (hard x-ray), tomography, microdiffraction • 3.3-cm Undulator A • Accepting general users

TARGETING ANTIBIOTIC-RESISTANT BACTERIA

Finding potent chemical agents to set against antibiotic-resistant bacteria continues to pose a very significant challenge for drug-discovery groups in the pharmaceutical industry and in academic laboratories. Effective therapies must find not only novel chemical entities, but also essential targets within the macromolecular machinery of the disease-producing pathogen—targets that are outside established therapies. The emergence of antibiotic-resistant bacterial strains has directed the attention of antibacterial strategists toward less conventional targets, such as tRNA synthetases, which are essential for protein synthesis, but are distinct from the ribosome, which serves to catalyze the translation of messenger RNA into an amino acid sequence. A research team using x-rays from the APS has obtained the first crystal structure of the enzyme that attaches the amino acid phenylalanine to the carrier transfer RNA (phenylananine tRNA synthetase, PheRS), a required step in protein synthesis. Their results hold promise for new pharmaceuticals based on this novel target in the bacterium *Staphylococcus haemolyticus* (*S. haemolyticus)* and other pathogens.

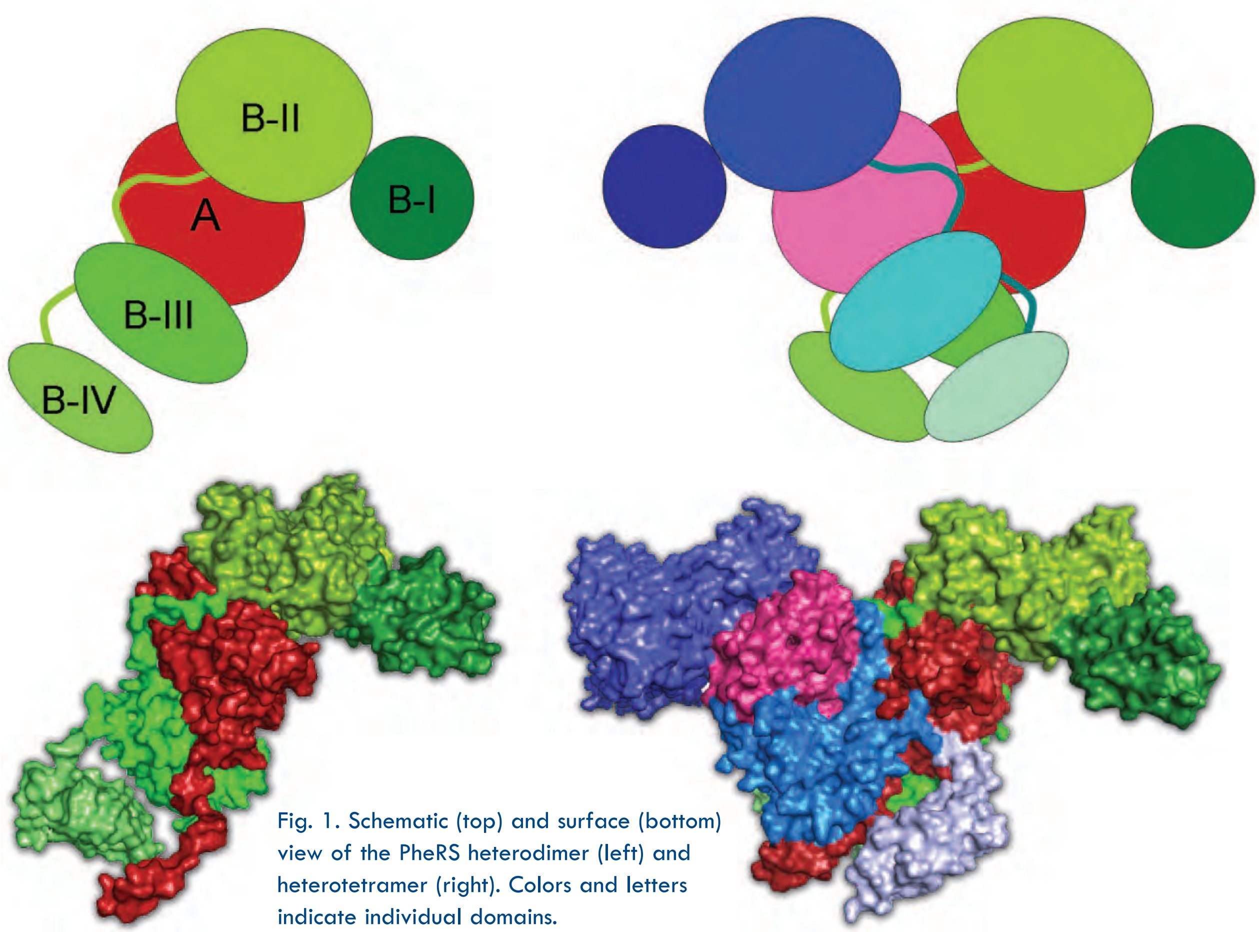

Fig. 1. Schematic (top) and surface (bottom) view of the PheRS heterodimer (left) and heterotetramer (right). Colors and letters indicate individual domains.

The researchers from Pfizer, Affinium Pharmaceuticals, and Blue Sky Biotech employed protein engineering and the IMCA-CAT 17-ID beamline. The IMCA-CAT facility is equipped for high-throughput robotic crystal screening, which proved to be essential for this result, as it greatly reduced the time required for crystal selection. Synchrotron x-ray diffraction data were collected at 17-ID using a wavelength of 1 Å.

The team captured, in a well-ordered lattice, the functional heterodimer of PheRS of SHA. The functional heterodimer assembles into an obligate heterotetramer $(\alpha\beta)_2$, making the crystal engineering even more difficult. The starting point was crystals of the native enzyme that diffracted only to approximately 3-Å to 5-Å resolution, not adequate for an extensive structure-based drug discovery effort of this target in complex with inhibitors that needed to be optimized. Available in the Protein Data Bank (www.rcsb.org/pdb/home/home.do) were several structures of the same protein from a non-pathogenic organism, *Thermus thermophilus* (TTH PheRS)—a more stable form of the enzyme coming from a thermophile that is not pathogenic.

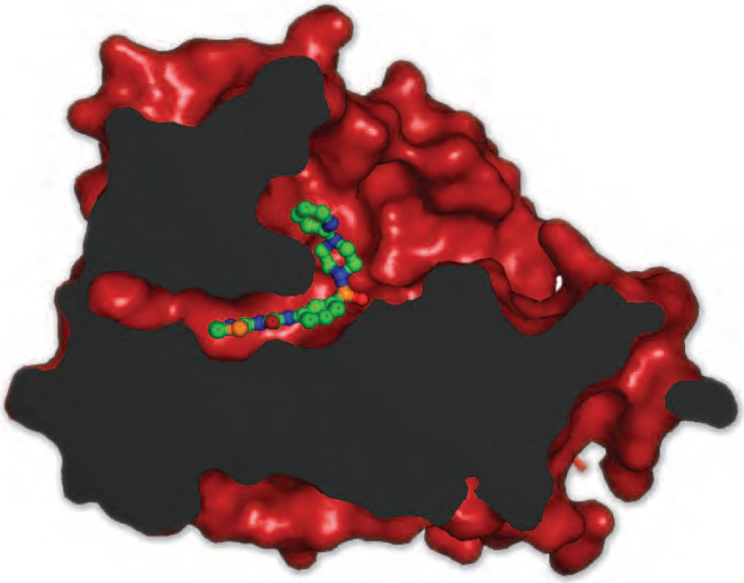

Fig. 2. Cutaway view of the SHA PheRS active site with the inhibitor molecule (Compound 1) shown as balls and sticks colored by element.

The expression and purification of the native protein was relatively easy, but obtaining high-quality crystals required a persistent and ingenious effort based on a rational protein engineering approach that had been used successfully before by this team. The strategy is focused on addressing the two main causes of inadequate diffraction in protein crystals: protein disorder and poor/inefficient crystal contacts. The application of this strategy to a protein of the size and complexity of SHA PheRS had not been done before.

The resulting structure of *S. haemolyticus* (SHA) PheRS revealed the atomic details of the 2300-amino acid enzyme at a resolution of better than 2 Å in complex with a number of synthetic inhibitors discovered by the high-throughput screening.

The multidomain structure of the target protein can be compared to a multi-segmented worm with flexible pieces, the key segment of which is the SysfA protein. The flexible segments are connected weakly with each other in the sequence: SyfB-IV:SyfB-III:SyfA:SyfB-II:SyfB-I (Fig. 1). In the end, only a combination of slightly modified protein (lacking the disordered N-terminal section of the small subunit) and a sequence differing in only three amino acids from the native enzyme in a non-critical area yielded the best diffracting crystals. Most important, the structure of the PheRS also revealed the binding mode of a key inhibitor (compound 1: a phenyl-thiazolylurea sulfonamide) bound in the active site and used in the crystallization process (Fig. 2). This class of compounds, as well as the ones from the ethanolamine family, represent *de novo* discovered chemical entities (as opposed to analogues of the phenyl-adenylate or phenylalanine) and open the path to subsequent optimization.

These results could lead to structure-based drug design on this novel and promising target across a range of pathogens.

— *Celerino Abad-Zapatero*

See: Artem G. Evdokimov[1]*, Marlene Mekel[1], Kim Hutchings[1], Lakshmi Narasimhan[1], Tod Holler[1], Teresa McGrath[2‡], Bryan Beattie[2], Eric Fauman[1], Chunhong Yan[1], Holly Heaslet[1], Richard Walter[1], Barry Finzel[1], Jeffrey Ohren[1], Patrick McConnell[1], Timothy Braden[1], Fang Sun[1], Cindy Spessard[1], Craig Banotai[1], Loola Al-Kassim[1], Weijun Ma[3], Paul Wengender[3], Denis Kole[3] Norman Garceau[3], Peter Toogood[1], and Jia Liu[1], "Rational protein engineering in action: The first crystal structure of a phenylalanine tRNA synthetase from *Staphylococcus haemolyticus*," J. Struct. Biol. **162**, 152 (2008).

DOI: 10.1016/j.jsb.2007.11.002

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Use of the IMCA-CAT beamline 17-ID at the APS was supported by the companies of the Industrial Macromolecular Crystallography Association through a contract with the Center for Advanced Radiation Sources at the University of Chicago. Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

17-ID • IMCA-CAT • Life science • Macromolecular crystallography, anomalous diffraction (MAD/SAD) • 3.3-cm Undulator A • Accepting general users

KNOWING WHEN TO STOP: VISUALIZING THE PROTEIN TERMINATION COMPLEX OF THE BACTERIAL RIBOSOME

In all living cells, from bacterial to human, protein production is the task of the ribosome. This highly conserved cellular machinery translates the instructions of the genetic code conveyed by messenger RNA (mRNA) into production of proteins necessary for the cellular function. There are structural differences between bacterial ribosomes and those of higher organisms, but the fundamental processes of protein synthesis are very similar throughout the tree of life. A team of researchers from the University of California, Santa Cruz (UCSC) using a GM/CA-CAT beamline at the APS has succeeded in describing the molecular structures involved in the concluding step of protein production in *Thermus thermophilus* (a species of bacteria that is a model organism for much research), bridging the transition from the "RNA world" to our familiar "protein world" at the beginnings of life on Earth. The experimentation is part of an ongoing endeavor by the Noller Lab at UCSC to crystallize ribosomal complexes at every stage of protein translation in order to achieve a full step-by-step visualization of how proteins are made by the ribosome.

Translation usually involves three stages: initiation of protein synthesis, elongation of the polypeptide chain, and termination [Fig. 1(a)]. Start and stop codons on the mRNA mark the beginning and end of a coding sequence, and elongation proceeds codon by codon as transfer RNA (tRNA) molecules bearing the appropriate amino acids enter the decoding center (A site) of the small subunit to the ribosome. The amino acids of the growing chain are linked by peptide bonds in the peptidyl transferase center (PTC) of the larger ribosomal subunit. Release factors are then required for the termination step, leading to dissolution of the peptidyl-tRNA bond. In bacteria, release factor 1 (RF1) recognizes the UAG and UAA stop codons, whereas release factor 2 (RF2) complexes with the UGA and UAA stop codons. The termination step of translation is remarkably precise, with an error rate between one in a thousand and one in a million; however, the mechanisms of stop codon recognition and termination had until now eluded definitive description.

The UCSC researchers succeeded in visualizing to a resolution of 3.2 Å the termination complex formed by the bacterial ribosome, an initiator tRNA bound to an AUG start codon, an mRNA bearing the stop codon UAA, and RF1 bound to the stop codon. Crystals of this complex were screened using beamlines at the Stanford Synchrotron Radiation Laboratory and the Lawrence Berkeley National Laboratory. X-ray diffraction data were then obtained using the GM/CA-CAT beamline 23-ID-D at the APS.

A key interaction of the ribosome and the release factor involves a "switch loop" connecting domains 3 and 4 of RF1 that moves to reach the ribosome's PTC and in so doing extends the α7 helix by two turns, forming a rigid connection between the ribosomal decoding site and domain 3 of RF1 [Fig. 1(b-e)]. This conformation of the switch loop is stabilized by interactions within a pocket formed between the ribosome and domain 2 of RF1, which is responsible for recognition of the UAA stop codon. The precision of termination appears to result from the synchronization and interdependence of RF1 binding, stop codon recognition, and the conformational changes that bring domain 3 of RF1 into contact with the ribosomal PTC, which cleaves the peptidyl-tRNA linkage, releasing the newly assembled polypeptide chain from the ribosome.

The ribosome is a mechanism of astonishing complexity, yet it, like all life, evolved from simpler molecules. In their analysis of the molecular structure of the termination complex, the researchers observed that the involvement of the polypeptide backbone of RF1 suggests the process might have originated in the interactions of RNA with simple peptides, thereby bridging the transition from the "RNA world" to our familiar "protein world" at the beginnings of life on Earth.

— *Carol Hart*

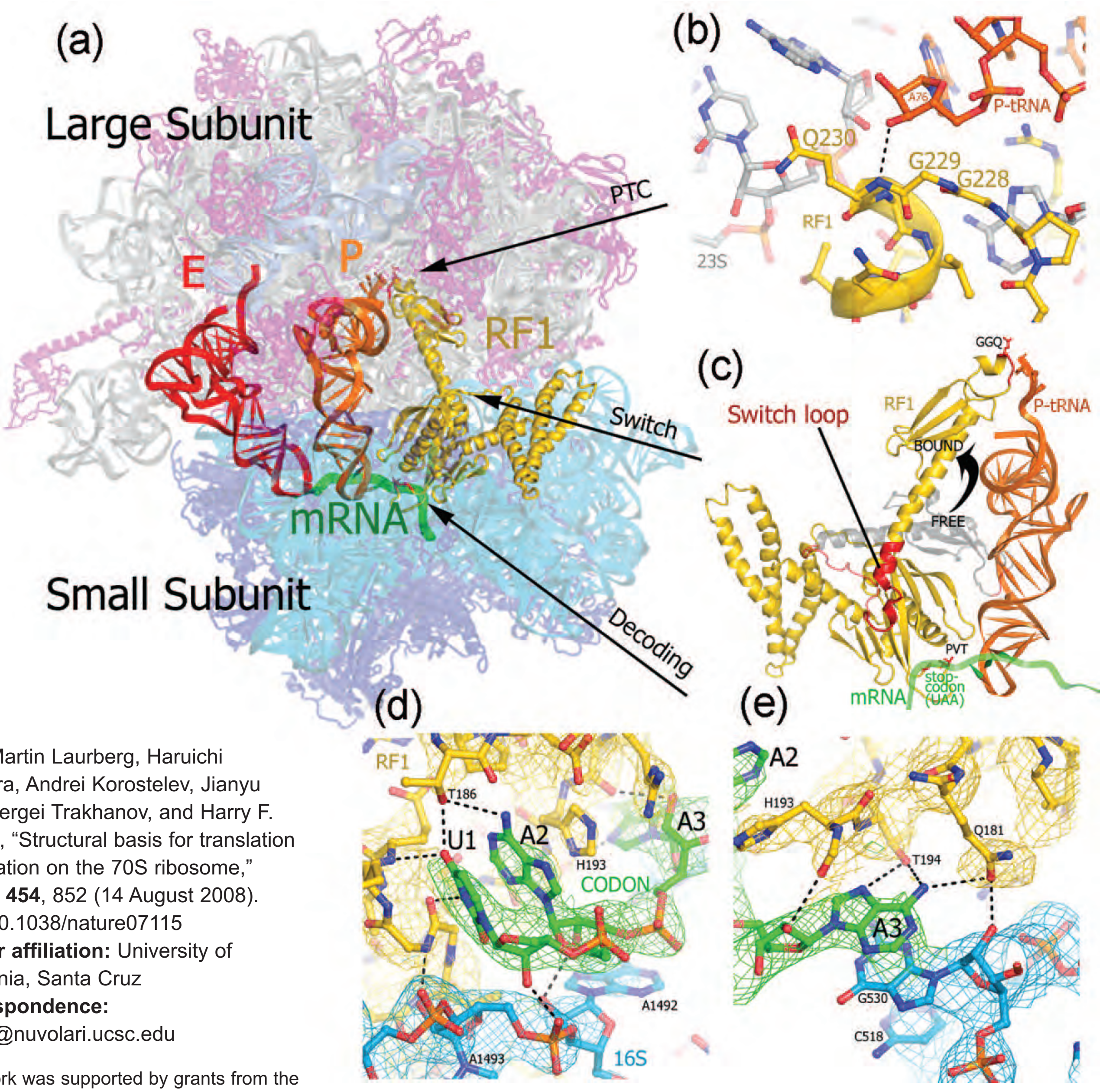

Fig. 1. The structure of the translation termination complex. (a) Overview of polypeptide elongation: the ribosome moves along the mRNA in a synchronized movement of mRNA and tRNAs between the A (aminoacyl), P (peptidyl) and E (exit) binding sites on the ribosome. (b) Interactions of the GGQ motif of RF1 (yellow) with the PTC, in which the polypeptide backbone (dotted line) is positioned to participate in catalysis. (c) Upon ribosomal binding and stop codon recognition, the switch loop (red) rearranges, moving the free form RF1 (gray) to dock the GGQ motif into the PTC. (d, e) Recognition of the UAA stop codon (green) by the RF1 decoding center in domain 2.

See: Martin Laurberg, Haruichi Asahara, Andrei Korostelev, Jianyu Zhu, Sergei Trakhanov, and Harry F. Noller*, "Structural basis for translation termination on the 70S ribosome," Nature **454**, 852 (14 August 2008). DOI: 10.1038/nature07115

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23-ID-D • GM/CA-CAT • Life science • Macromolecular crystallography, microdiffraction, anomalous diffraction (MAD/SAD), subatomic (<0.85 Å) resolution • 3.0-cm undulator • Accepting general users

HOW THE PROTEIN GOT TO THE OTHER SIDE – OF THE CELL MEMBRANE

A recent study by researchers using the APS may help explain how cells use molecular machinery to extrude proteins through tiny channels across a plasma membrane—a fatty layer that envelopes the cell and, in cells of higher organisms, breaks it up into separate compartments. The researchers from Harvard Medical School determined the three-dimensional structure of SecA, a protein that extracts chemical energy from small molecules in the cell, in contact with the SecY complex, a group of proteins that forms a channel across the plasma membrane of bacteria. They suggest that SecA acts like a miniature clamp and piston to export or translocate other proteins through the SecY channel.

Every protein is assembled as a string of amino acids, called a polypeptide, and the particular sequence of amino acids gives the protein its overall structure, which in turn determines its function. Most polypeptides destined for export have a short signal sequence of amino acids at their beginning that have an affinity for greasy environments such as the plasma membrane. In animals, cells ship immune system proteins from the interior to a special compartment that ferries them to the cell surface. Other cells secrete protein hormones or enzymes, in the case of plants and animals, or potent toxins in the case of molds and bacteria.

In bacteria, protein translocation begins when the peptide is ushered to the plasma membrane, where it encounters SecA, which is believed to unravel peptides tagged with a signal sequence and feed them through the SecY complex channel like thread through the eye of a needle. The channel that carries out translocation in other species is highly similar in amino acid sequence to SecY, suggesting it works in the same basic way. But until now researchers didn't know the specific mechanism by which SecA moves polypeptides through the channel.

Tthe Harvard team isolated SecA and SecY from *Thermotoga maritima*, a bacterium that grows near underwater volcanoes. They crystallized the two proteins together and then determined the microscopic structure of the crystal by measuring how x-rays were diffracted after they passed through the sample. The work was carried out on SBC-CAT beamline 19-ID and NE-CAT beamllne 24-ID-C at the APS, and beamline X29 at the National Synchrotron Light Source, Brookhaven National Laboratory.

According to the group's structural data, SecA has a "C" shape and sits on top of the hourglass-shaped SecY complex like a donut with a bite taken out of it (Fig. 1). SecY joined to SecA has a different structure than SecY alone. With SecA attached, the inner mouth of the channel is wider, facilitating peptide entry, and a piece of protein plugging the middle of the channel has partly cleared out.

The researchers propose that SecA works like a clamp, grabbing onto the polypeptide chain and positioning it on top of the channel. From there, insertion of the signal sequence into the channel wall would fully open the channel and allow the translocation of the polypeptide across the membrane.

One of SecA's jobs is to bind to a molecule called ATP, the universal source of energy in every cell. SecA releases the energy harnessed in ATP by breaking it into its component parts to push the polypeptide chain into the SecY channel. By repeated cycles of ATP binding and breaking, the protein can produce a series of coordinated movements, much like swiping fare cards through a subway turnstyle.

The team noted that SecA has a short, finger-like projection wedged between the clamp and the channel, pointing down toward the channel opening at a 45° angle. The team proposes that when SecA binds ATP, the peptide finger slides into the SecY channel, pressing down on the peptide lodged there.

If the sliding motion coincided with the SecA's clamp releasing its grip, the effect would be to push the peptide a small way through the channel. When SecA releases the broken ATP molecule, the piston could retract while the clamp reengaged, keeping the peptide in place. To finish translocation, simply repeat the process until the protein emerges from the other side.

— *JR Minkel*

See: Jochen Zimmer, Yunsun Nam, and Tom A. Rapoport*, "Structure of a complex of the ATPase SecA and the protein-translocation channel," Nature **455**, 936 (16 October 2008).
DOI: 10.1038/nature07335

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This work was supported by a National Institutes of Health grant. T.A.R. is an HHMI investigator. Y.N. is supported by the Damon Runyon Cancer Research Foundation (DRG-#1953-07). Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

19-ID • SBC-CAT • Life science • Anomalous diffraction (MAD/SAD), subatomic (<0.85 Å) resolution, ultra-low-temperature (15K) • 3.3-cm Undulator A • Accepting general users

24-ID-C • NE-CAT • Life science • Microfluorescence (hard x-ray), tomography, microdiffraction • 3.3-cm Undulator A • Accepting general users

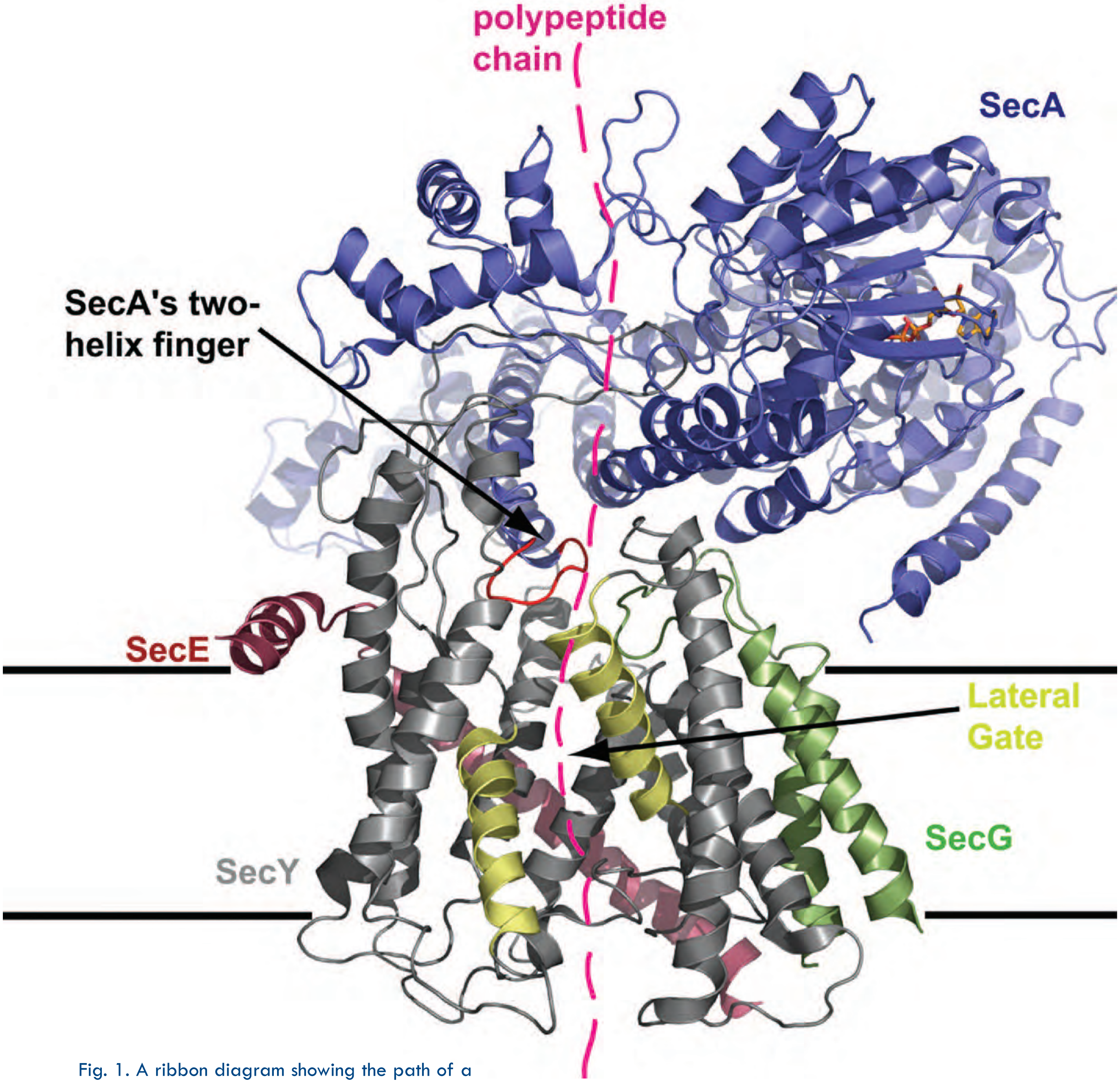
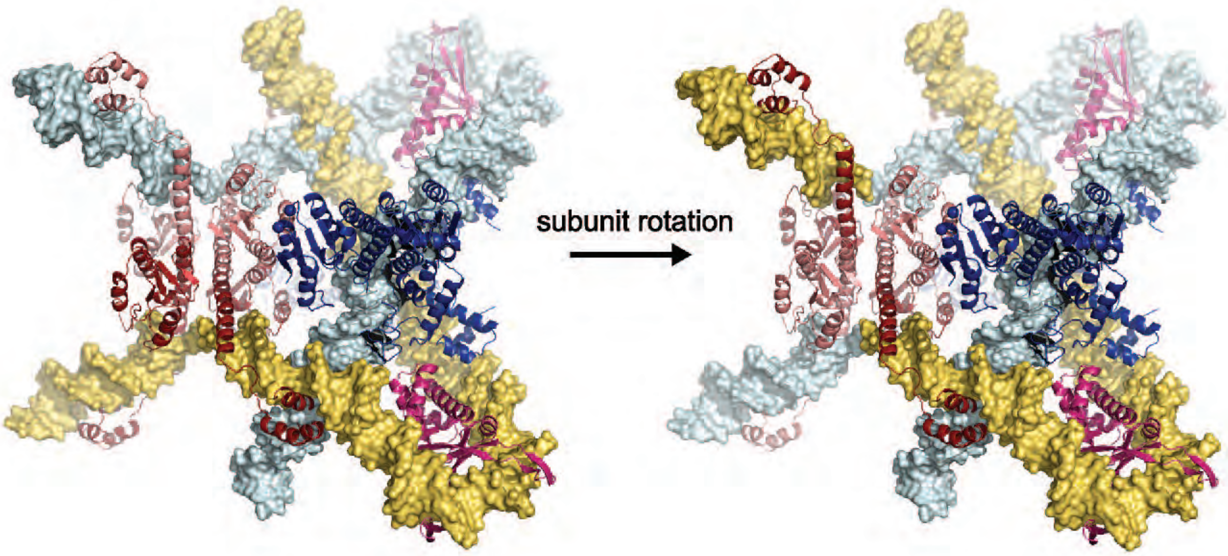


Fig. 1. A ribbon diagram showing the path of a polypeptide chain (marked in pink) destined for export across a plasma membrane (horizontal black lines) through the SecY channel complex. According to an interpretation of recent structural data, SecA (blue) clamps the polypeptide in place and breaks an ATP molecule (orange; partially obscured in the upper right) to inch the protein along.

A three-dimensional structure from this research can be viewed here

RESOLVING DNA RECOMBINATION

When it comes to resembling either one of our parents, we may be described as a chip off the old block, but our cells actually contain a mix of DNA from both parents. The process that adds this healthy variety to our gene pool, involving the chopping up and exchanging of pieces of DNA, is known as genetic recombination. Recombination can also be site-specific—occurring between short, defined sequences within two double-stranded DNA molecules. The latter type of recombination occurs only in simple organisms such as bacteria and yeast. For example, site-specific recombination enables bacteria to develop resistance to multiple antibiotics; it is also used as the basis for many genetic engineering tools, allowing researchers to insert and express genes in various cell types. Site-specific recombination takes place with the help of a group of enzymes known as recombinases, which includes a family of enzymes called resolvases. Researchers from The University of Chicago used two APS beamlines to understand more about one member of the resolvase family, a four-piece molecule known as Sin. By doing so, they hoped to gain a better understanding of the mechanisms at play during this important process.



A QuickTime movie from this research can be viewed here

Fig. 1. The Sin-site II synaptic tetramer can be docked with existing crystal structures of the $\gamma\delta$ resolvase-site I tetramer and IHF-DNA complexes to create a model of the synaptic complex. Recombination is achieved by subunit rotation within the site I tetramer.

During site-specific recombination, molecules such as Sin, along with other proteins, form a complex that binds to strands of DNA and enables the strands to join together and exchange segments of DNA. It was already known that Sin consisted of two complexes, a catalytic and a regulatory, and that Sin forms a catalytic complex when bound to one type of DNA site, and a regulatory complex when bound to a different DNA site. The catalytic complex of Sin spurs the chemical reactions that take place during recombination. By contrast, the regulatory complex, as its name suggests, regulates the catalytic complex. The regulatory complex is very important because it ensures that Sin rearranges pieces of DNA only when and where appropriate.

In this study, the researchers tried to clarify some additional features of the Sin molecule and determined three new findings: (1) how two Sin subunits join together to form a regulatory complex, (2) how the catalytic and regulatory complexes join to form the Sin tetramer (a four-piece molecule), and (3) how the regulatory complex helps control the catalytic complex.

To explore these aspects of Sin,

"Resolving" continued on page 104

Hot Dogs and Healthy Bones: The Parathyroid Hormone-Receptor Complex

Parathyroid hormone (PTH) is the key regulator of calcium and phosphate balance and has stimulatory effects on bone, acting overall to increase bone mass. Its significance to bone health has attracted much research interest for decades; the crystal structure of the hormone has been described, but purifying and crystallizing its receptor presented special challenges. Using the LS-CAT 21-ID-D beamline at the APS, researchers from the Van Andel Institute in Michigan solved the structure of the binding domain of the parathyroid hormone–receptor complex to a resolution of 1.95 Å. A recombinant (genetically engineered) form of parathyroid hormone is currently approved for patients with osteoporosis who are at high risk for fracture. But the medication requires daily injections and is associated with significant risks and adverse effects. Understanding the structure of hormone-receptor interaction may lead to strategies for the development of more tolerable and convenient therapies for osteoporosis and other bone disorders.

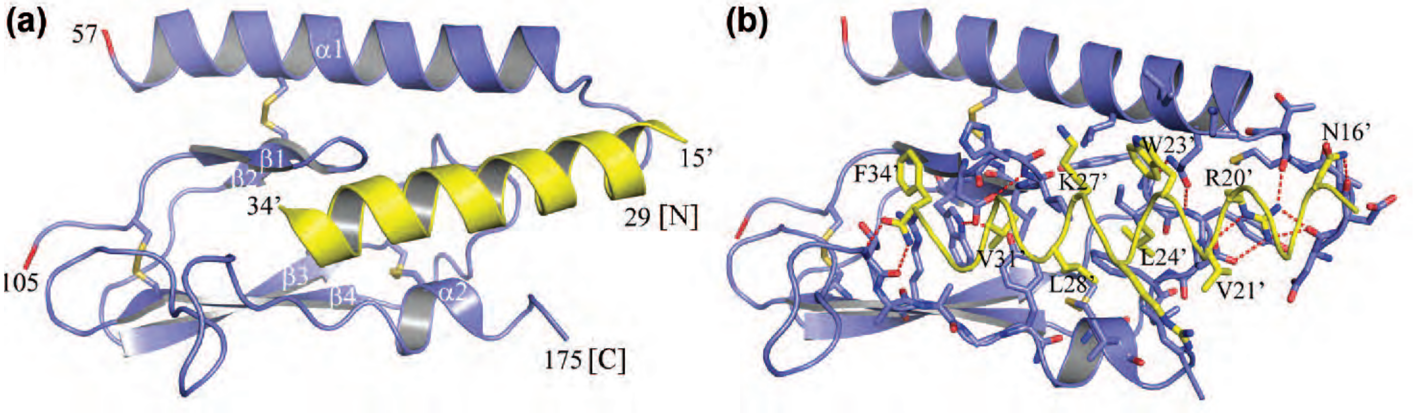


Fig. 1. (a) Ribbon diagram showing the extracellular domain (ECD) of the human parathyroid hormone receptor (slate blue) in complex with a synthetic PTH fragment, residues 15-34 (yellow). The positions of the N- and C-terminus of the ECD are indicated along with secondary structure elements. Residues 58-104 of the ECD were disordered. PTH residues are designated with a prime to distinguish them from receptor residues. (b) Detailed view of the interface between PTH and the ECD of its receptor. Selected side chains are shown in stick representation and the red dashes indicate hydrogen bonds.

Parathyroid hormone is a polypeptide of 84 amino acids that is secreted by the parathyroid gland in response to low circulating levels of calcium. Its primary receptor, type 1 PTH receptor (PTH1R), belongs to the class B G protein-coupled receptor (GPCR) family. GPCRs constitute a large, diverse group of cell surface receptors that transmit hormonal and other extracellular signals across signalling pathways to trigger the appropriate cellular response. In kidney cells expressing PTH1R, activation by the hormone increases calcium retention, while in bone PTH1R activation triggers an immediate release of calcium, accompanied by longer-term changes in calcium metabolism that stimulate bone production.

The overall structure of the extracellular domain of PTH1R, where hormone binding takes place, consists of two α-helices and four β-strands. These are arranged as three layers: an extended α helix, a middle layer of β strands, and a bottom layer of β strands, with one looping to join the second α-helix—all held in place primarily by disulfide bonds. Parathyroid hormone docks as a single continuous α-helix within a central hydrophobic groove formed by these three layers—

"Hot Dogs" continued on page 104

"Hot Dogs" *from page 103*

yielding a "hot dog on a roll" structure (Fig.1). Shape correlation statistical analysis shows a high degree of surface topology matching at the hot dog and roll interface. Interestingly, the residues forming the PTH-binding groove are not conserved in the class B GPCRs (with the exception of type 2 PTH receptor), suggesting that the hormone receptors in this class have distinct ligand-binding topologies within a conserved hot dog structure for hormone-receptor interaction.

Cell membrane receptors are challenging subjects for structural studies, because both production of the purified protein and its crystallization present complex problems. The approach developed by the Van Andel Institute researchers included the use of affinity tags at both termini of the molecule: a maltose-binding protein at the N-terminus and a hexahistidine at the C-terminus. An affinity tag is a short amino acid sequence fused to a protein (usually to a terminus) to aid in its purification (and often its crystallization as well). As an additional step, overnight incubation with a bacterial enzyme that promotes disulfide bond formation (bacterial protein disulfide isomerase) greatly reduced protein misfolding.

The method, the researchers say, is flexible, and should be adaptable for use in structural studies of other class B GPCRs. In addition to PTH, the class B GPCRs bind such pharmaceutically important molecules as glucagon, calcitonin, growth hormone-releasing hormone, and corticotrophin-releasing factor. A procedure for purifying and crystallizing the receptor-hormone complex thus has great significance for both basic research and therapeutics in a wide range of disorders. — *Carol Hart*

See: Augen A. Pioszak and H. Eric Xu*, "Molecular recognition of parathyroid hormone by its G protein-coupled receptor," PNAS **105**, 5034 (1 April 2008). DOI: 10.1073/pnas.0801027105

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21-ID-D • LS-CAT • Life Sciences • Macromolecular crystallography, anomalous diffraction • U33S undulator • Accepting general users

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"Resolving" *from page 102*

the researchers pieced together structural data that were already available and came up with a model that effectively supported what was already known about the function of Sin during site-specific recombination. They also defined the structure of the regulatory portion of Sin by using x-ray crystallography at the BioCARS 14-BM and SBC-CAT 19-ID beamlines at the APS and compared it with information available about a catalytic complex similar to the one in Sin, from a protein called γδ resolvase.

Several differences were noted between Sin's regulatory and catalytic complexes. An important one was that the regulatory complex was catalytically inactive in contrast to the catalytic complex. In fact, the differences between the catalytic and regulatory complexes were unexpectedly striking; that the protein structure changed to such a great extent when bound to different DNA sites was highly unusual.

The researchers also determined that two regulatory complexes of Sin joined together entirely through contacts between their DNA-binding domains to form the Sin tetramer. This hypothesis contrasted with existing models of Sin and other resolvases, but it was strongly supported by results they obtained by using mutated versions of the Sin protein, a method that could determine which amino acids were necessary for an interaction and which were not.

Piecing together their information, the researchers generated a model of the synaptic complex formed when Sin participates in site-specific recombination. This information, along with other insights into the resolvases, may ultimately enhance the understanding of site-specific recombination and even aid in the development of more effective tools for genetic engineering.
— *Emma Hitt*

See: Kent W. Mouw[1], Sally-J. Rowland[2], Mark M. Gajjar[1,‡], Martin R. Boocock[2], W. Marshall Stark[2], and Phoebe A. Rice[1]*, "Architecture of a Serine Recombinase-DNA Regulatory Complex," Mol. Cell **30**, 145 (April 25, 2008). DOI: 10.1016/j.molcel.2008.02.023

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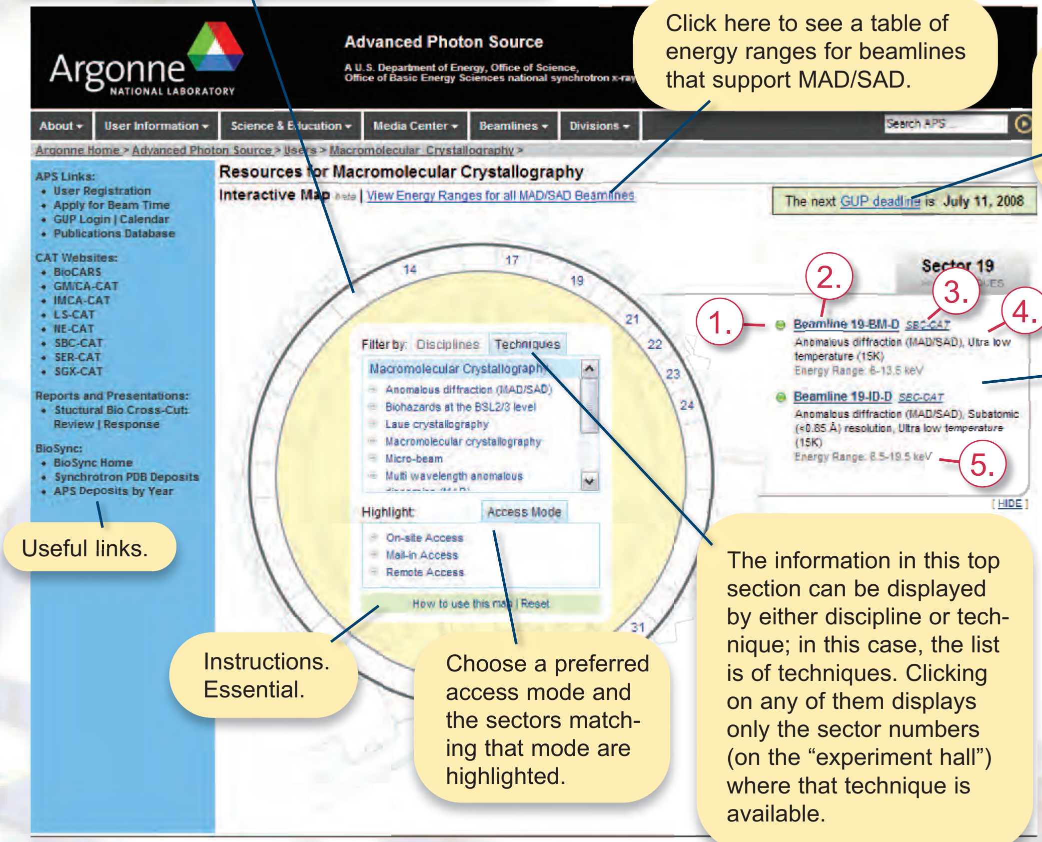
14-BM • BioCARS • Life science • Macromolecular crystallography, fiber diffraction, biohazards at the BSL2/3 level, subatomic (<0.85 Å) resolution • Bending magnet • Accepting general users

19-ID • SBC-CAT • Life science • Anomalous diffraction (MAD/SAD), subatomic (<0.85 Å) resolution, ultra-low-temperature (15K) • 3.3-cm Undulator A • Accepting general users

A NEW INTERFACE FOR MACROMOLECULAR CRYSTALLOGRAPY AT THE APS

In 2007, the APS Scientific Advisory Committee (SAC) conducted a cross-cut review of macromolecular crystallography (MX) at the APS. Among their recommendations was “that APS enhance the ease of access to details of MX activities at the APS” by creating a prominent direct link to those activities from the APS Web site.

The response to the SAC recommendation, as developed by Jonas Downey (APS Engineering Support Division [AES]), the APS Webmaster; Xuli Wu (AES); Susan Strasser (X-ray Science Division); and Robert Fischetti (Biosciences Division and GM/CA-CAT) with feedback from many members of the APS MX community, is shown below in an annotated screen shot of the actual page (credit to *Harper’s Magazine* for the annotation idea). The page, which helps MX users find a beamline at the APS that matches their research interests, can be found here.



Resources for Macromolecular Crystallography

Interactive Map beta | View Energy Ranges for all MAD/SAD Beamlines

The next GUP deadline is **July 11, 2008**

Beamline 19-BM-D *SBC-CAT*
Anomalous diffraction (MAD/SAD), Ultra low temperature (15K)
Energy Range: 6-13.5 keV

Beamline 19-ID-D *SBC-CAT*
Anomalous diffraction (MAD/SAD), Subatomic (<0.85 Å) resolution, Ultra low temperature (15K)
Energy Range: 6.5-19.5 keV

A plan view of the APS experiment hall provides the foundation for information display.

Click here to see a table of energy ranges for beamlines that support MAD/SAD.

The current deadline for general-user proposals (GUPs), and a link to the GUP proposal system, are prominently displayed.

Click on a visible MX sector number on the experiment hall planview...
...and this pane appears. This is the main source of information for each sector:
1. A status indicator. Green = operational/accepting general users.
2. This links to information in the APS Beamline Directory).
3. Click here to be directed to the operator’s Web site.
4. Techniques supported at the beamline.
5. Source energy range for this beamline.

Useful links.

Instructions. Essential.

Choose a preferred access mode and the sectors matching that mode are highlighted.

The information in this top section can be displayed by either discipline or technique; in this case, the list is of techniques. Clicking on any of them displays only the sector numbers (on the “experiment hall”) where that technique is available.

Marine Sediments Have an Apatite for Diatomaceous Polyphosphate

Phosphorus is an essential nutrient for life. Levels of atmospheric carbon dioxide, a greenhouse gas, are directly related to the growth and productivity of marine life, which is a function of phosphorus availability. A team of scientists using an APS beamline has identified a process by which marine organisms influence the amount of atmospheric carbon the sea absorbs. A greater understanding of how phosphorus uptake, metabolism, and sequestration occur within marine organisms could provide clues to how carbon uptake and sequestration take place in the ocean and affect the global carbon balance.

Understanding the sources and sinks of phosphorus in systems like the ocean relates directly to understanding the controls on marine productivity.

Calcium phosphate deposited in marine sediments is a major sink for phosphorus in the form of the mineral apatite, but the mechanism by which apatite forms and is buried is unknown. One key step in the formation of marine apatite may involve polyphosphate bodies formed in common marine organisms. Polyphosphate generated by living cells has not been considered important in marine phosphorus cycl-ing. But recent advances in high-resolution spectromicroscopy led to a re-evaluation of this thinking. The re-search team, with members from the Georgia Institute of Technology, the University of South Carolina, Argonne National Laboratory, the Skidaway In-stitute of Oceanography, and the Aus-tralian Synchrotron found that polyphosphate from marine diatoms and mineral apatite derived from these polyphosphates represent a significant sink of phosphate. Marine sediments collected off the coast of British Columbia were analyzed using scanning x-ray microscopy (SXM) at XOR beamline 2-ID-B with a spatial resolution of ~60 nm and were found to have significant levels of polyphosphate and apatite derived from polyphosphate (Fig. 1).

In order to analyze polyphosphate levels in marine samples collected during the spring bloom (when organisms might be expected to accumulate polyphosphate), investigators performed bulk 31P nuclear magnetic resonance spectroscopy. The measurements indicated that polyphosphate constituted 7% of the surface water biomass, but it did not alter the normal carbon/nitrogen/phosphate composition of the samples. Polyphosphate constituted 11%, 7%, and 8% of dissolved matter, sinking particles, and surface sediment, respectively. High-resolution spectromicroscopy supported the hypothesis that the polyphosphate found in these samples originated from diatoms because the size (0.5 μM to 3 μM) of the polyphosphate fragments found in each sample type were comparable to those found in diatoms.

Further x-ray spectromicroscopic analysis revealed information about the next step in the sedimentation process: the transition of polyphosphate into mineral apatite. In sediment samples, the investigators were able to detect polyphosphate, apatite, and also some distinct particles that had spectral properties representing materials that could be considered transitional between the two. This finding suggests that polyphosphate from diatoms provides sites for nucleation of the geologically stable mineral phase—apatite—in marine sediments.

The researchers concluded that polyphosphate from diatoms could represent an important sink of phosphate that is globally important because of the widespread abundance of these planktonic organisms.

Thus, a clearer understanding of the dynamics of phosphate deposition and sequestration by diatoms may broaden our understanding of both modern and ancient climate change.

— *Sandy Field*

See: Julia Diaz[1], Ellery Ingall[1]*, Claudia Benitez-Nelson[2], David Paterson[3†], Martin D. de Jonge[3‡], Ian McNulty[3], and Jay A. Brandes[4], "Marine Polyphosphate: A Key Player in Geologic Phosphorus Sequestration," Science **320**, 652 (2 May 2008). DOI: 10.1126/science.1151751

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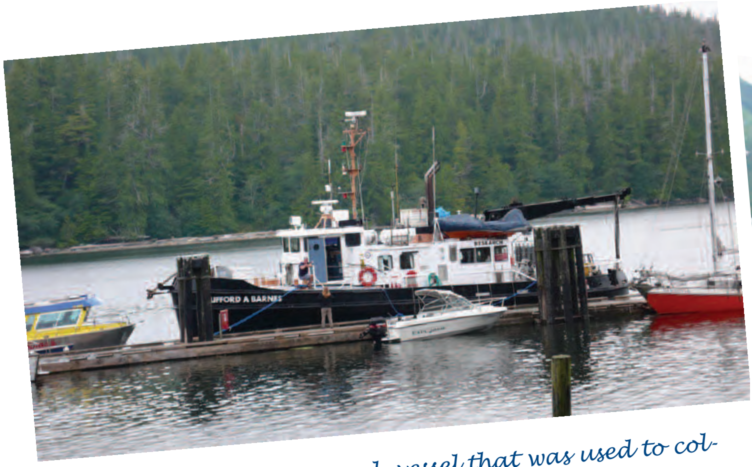
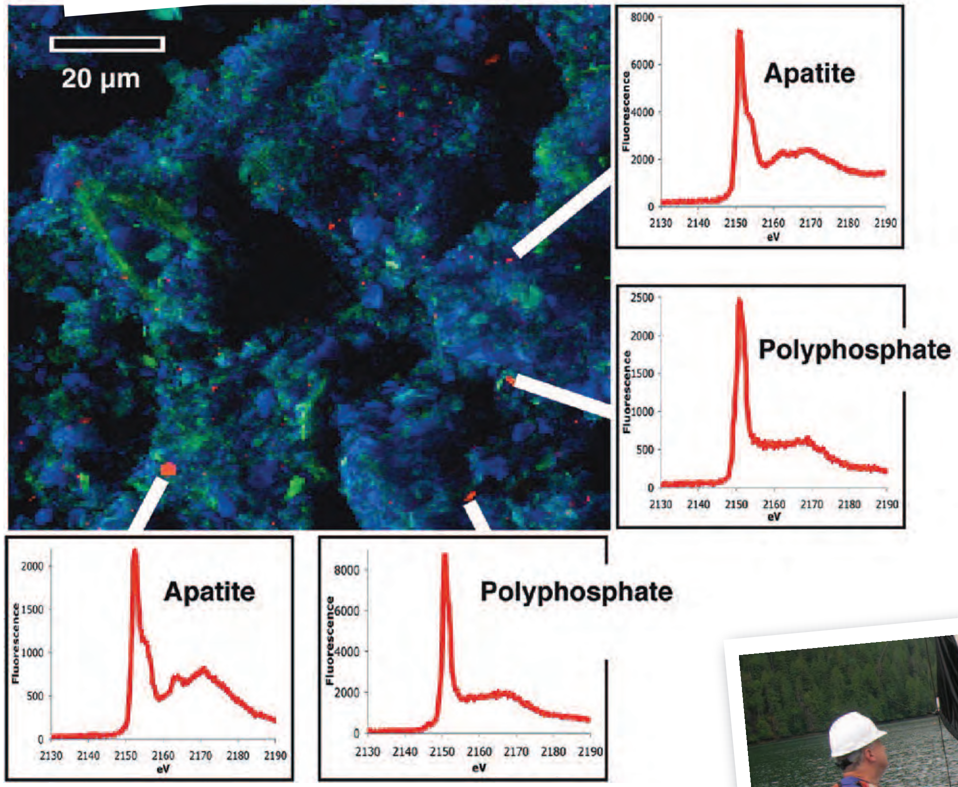
This material is based on work supported by the National Science Foundation under grant 0526178. Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357).

2-ID-B • XOR • Materials science, environmental science, physics • Coherent x-ray scattering (soft x-ray), microfluorescence (soft x-ray) • 5.5-cm undulator • Accepting general users



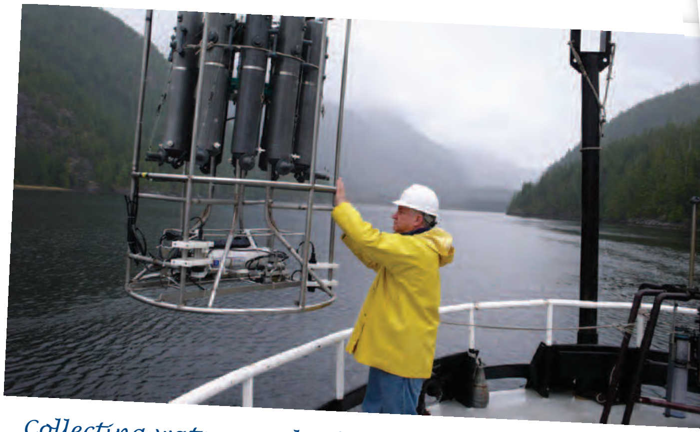
The RV Barnes, the research vessel that was used to collect samples in Effingham Inlet, British Columbia, houses all of the equipment needed to collect water, plankton, and sediment samples

Processing a sediment core



< Fig. 1. X-ray fluorescence micrograph and fluorescence spectra of phosphorus-rich regions in Effingham Inlet sediment. Sedimentary phosphorus (red) appears as distinct, heterogeneously distributed submicrometer-sized particles against a comparatively uniform background of sedimentary aluminum (blue) and magnesium (green). On the basis of high-resolution x-ray spectroscopic characterization, about half of the 147 phosphorus-rich regions examined were found to be polyphosphate, whereas the other half were classified as apatite. (© 2008 American Association for the Advancement of Science. Reprinted with permission.)

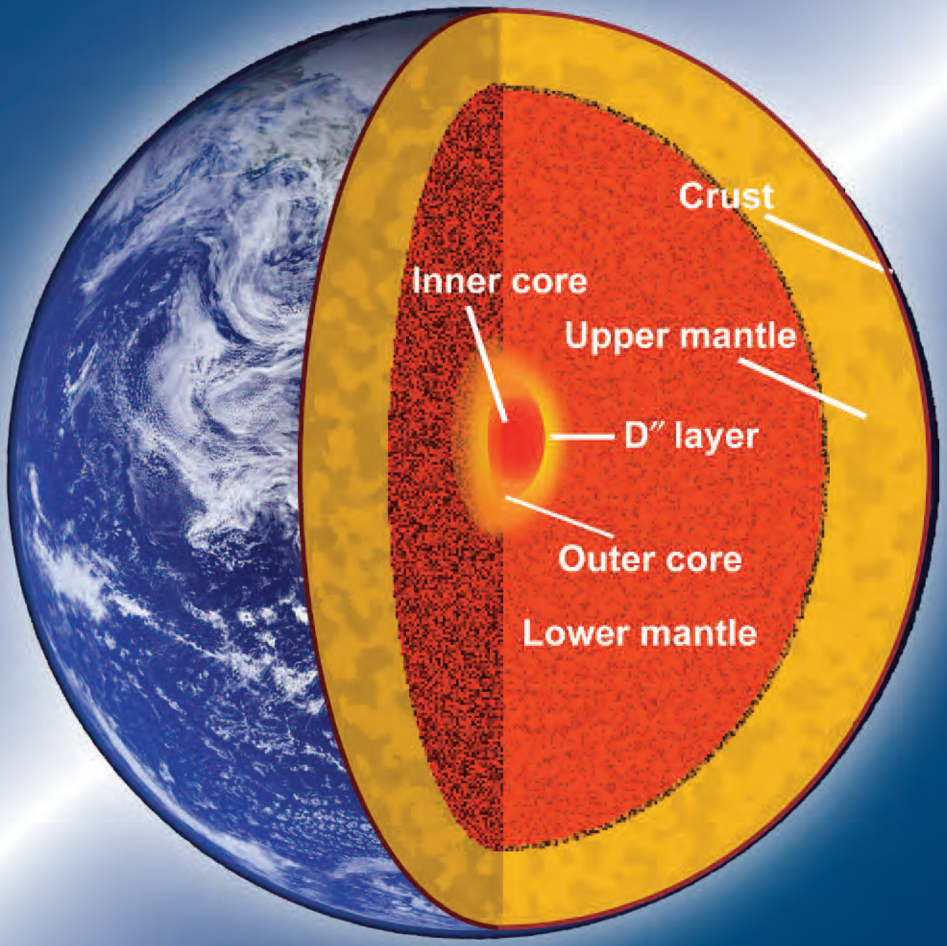
Rinsing particle samples aboard the research vessel



Collecting water samples from aboard the RV Barnes in Effingham Inlet, British Columbia

MOLTEN GLASS IN THE EARTH'S INTERIOR

Modeling the structure and dynamics of the Earth's interior requires a greater understanding of how Earth materials behave at the incredibly high pressures and temperatures deep inside our planet. As part of this quest for knowledge, researchers used an APS x-ray beamline to gain new information about the properties of $MgSiO_3$ glass, a model system for molten liquids at the temperatures and pressures that exist in the transition zone and the core-mantle boundary near the core of the Earth. $MgSiO_3$-rich silicate melts are important not only because of their suggested presence in those places, but also because their composition is believed to be similar to the Earth's early magma ocean and so may hold clues to the planet's evolution. These studies suggest that, under intense pressure, oxygen triclusters formed in the melt, thus enhancing density, viscosity, and crystal-melt partitioning, as well as reducing element diffusivity in the deeper part of the Earth's lower mantle. (Earth photo courtesy of NASA/JPL-Caltech)



The researchers used the GSECARS 13-ID and the HP-CAT 16-ID-B and -D beamlines at the APS, and beamline BL12-XU of the SPring-8 light source in Japan to examine the $MgSiO_3$ glass with high-pressure x-ray Raman spectroscopy technique. They studied the glass in a diamond anvil cell up to pressures of 39 GPa. Beyond 20 GPa the K-edge spectra features began to show a peak at 544 eV to 545 eV, representing a pressure-induced, structural change in the glass. This is believed to be due to the formation of triclustered oxygen (that is, oxygen atoms surrounding—and linking—three silicon (Si) atoms). Triclusters had been predicted, but never experimentally.

At low pressure, oxygen typically coordinates with two cations, not three. To show that the spectral feature was truly due to a change in coordination number—as opposed to a change in some other structural adjustment such as bond angle or distance—the researchers measured the spectra in a variety of other crystalline phases. Features arising from the edge-sharing oxygen or oxygen linking two, six-coordinated silicon atoms, for example, would show a spectra peak at a slightly lower voltage. Since phases, with their associated different atomic structures, did not show the special spectra peak, a change in coordination remains the best possible cause. The x-ray Raman scattering spectrum feature shown at 545 eV can best be attributed to the formation of triply-coordinated oxygen and changes in atomic arrangement in medium-range order, including the formation of a three-member ring, an increase in bond length, and a decrease in bond angle. This experimental data is the first to strongly suggest that at high pressures, oxygen can coordinate with three silicon cations.

The researchers concluded that including the formation of oxygen triclusters into models of the Earth's structure and formation is crucial. Possible effects from the triclusters include causing a denser $MgSiO_3$ melt in the Earth's mantle; an explanation for the atomistic origin of the high-density Mg-silicate melts at the core-mantle boundary; a decrease in the volume available for other elements, thus inhibiting such elements as radioactive nuclides and significantly affecting the process of chemical differentiation in the Hadean magma oceans; and an explanation for the transport properties including viscosity and diffusivity toward the deeper part of the Earth's lower mantle. — *Karen Fox*

See: Sung Keun Lee[1]*, Jung-Fu Lin[2]**, Yong Q. Cai[3], Nozomu Hiraoka[3], Peter J. Eng[4], Takuo Okuchi[5], Ho-kwang Mao[6]***, Yue Meng[6], Michael Y. Hu[6], Paul Chow[6], Jinfu Shu[6], Baosheng Li[7], Hiroshi Fukui[8], Bum Han Lee[1], Hyun Na Kim[1], and Choong-Shik Yoo[9], "X-ray Raman scattering study of $MgSiO_3$ glass at high pressure: Implication for triclustered $MgSiO_3$ melt in Earth's mantle," Proc. Nat. Acad. Sci. USA **105**(23), 7925 (June 10, 2008).
DOI: 10.1073pnas.0802667105

Author affiliations: [1]Seoul National University, [2]Lawrence Livermore National Laboratory, [3]National Synchrotron Radiation Research Center, [4]The University of Chicago, [5]Nagoya University, [6]Carnegie Institution of Washington, [7]Stony Brook University, [8]Okayama University, [9]Washington State University Present addresses: ‡Brookhaven National, Laboratory, †SPring-8

Correspondence: *sungklee@snu.ac.kr, **afu@jsg.utexas.edu, ***h.mao@gl.ciw.edu

GSECARS is supported by the U.S. Department of Energy, Basic Energy Sciences (DOE-BES), Geosciences; the National Science Foundation (NSF) Earth Sciences; and the State of Illinois. HP-CAT is supported by the DOE-BES, Materials Science; the DOE National Nuclear Security Administration; the Carnegie Institution of Washington (CIW)/DOE Alliance Center; the NSF; and the W.M. Keck Foundation (CIW). This work was supported by the Korea Science and Engineering Foundation Grant 2007-000-20120-0 (to S.K.L.) through the National Research Laboratory Program, a Lawrence Livermore Fellowship (to J.F.L.), and the 21st Century Center of Excellence program of the Institute for Study of the Earth's Interior (H.F.). Use of the Advanced Photon Source at Argonne National Laboratory was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

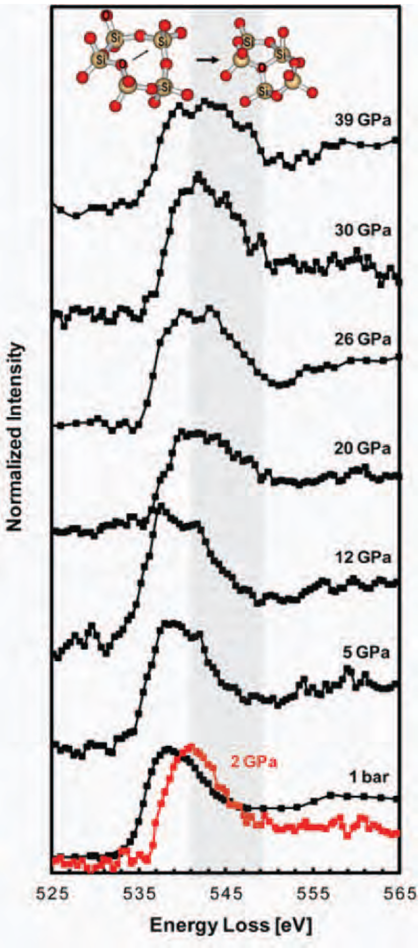


Fig. 1. (A). Oxygen K-edge x-ray Raman spectra for $MgSiO_3$ glasses at high pressures (plotted as energy loss [incident energy–elastic energy] vs. normalized scattered intensity). Gray area represents energy range from 543 eV to 551 eV. Schematic local structure for the formation of the oxygen tricluster is also shown. Red and yellow spheres denote oxygen and silicon atoms, respectively.

13-ID • GSECARS • Geoscience, environmental science • Microfluorescence (hard x-ray), x-ray absorption fine structure (XAFS), microdiffraction, micro-XAFS, high-pressure diamond anvil cell, high-pressure multianvil press, inelastic x-ray scattering • 3.3-cm Undulator A • Accepting general users

16-ID-B • HP-CAT • Materials science, geoscience • Microdiffraction, powder diffraction, single crystal diffraction • 3.3-cm Undulator A • Accepting general users

16-ID-D • HP-CAT • Materials science, geoscience, physics • Nuclear resonant scattering, inelastic x-ray scattering, x-ray Raman scattering, x-ray emission spectroscopy • 3.3-cmr Undulator A • Accepting general users

HEAT IN THE ARCHAEAN MANTLE

For scientists pursuing an understanding of the Earth's evolution, one clue lies in komatiites, a type of igneous rock—most of which are billions of years old—containing crystals of the mineral olivine. These rocks formed from magmas produced in one of two ways: partial melting of the Earth's mantle when it was much hotter than today, or partial melting at comparable temperatures to today, but with a great deal of water. (Indeed, Earth science is split in two between the “hot or not’ state of our planet's interior over the first few billion years of its history.) Determining which environment did indeed produce komatiites would help explain the Earth's thermal evolution. So far, the lack of a sample of the original komatiite magma has hindered the possibility of such studies. Now, researchers using the APS have achieved the first studies of a komatiite melt, preserved as inclusions in olivine. Their work shows that little to no water was involved in its formation, implying it formed under very hot conditions.

The researchers, who represent Imperial College London, the University of Tasmania, The Australian National University, and The University of Chicago, studied an unusually pristine, 2700-million-year-old komatiitic magma sample from Belingwe, Zimbabwe, preserved as inclusions in olivine (Fig. 1). The team measured water in the komatiite inclusions using infrared spectroscopy. The results showed just 0.18% to 0.26% water by weight, far less than the 3% to 5% by weight that would be required by the wet-melting model.

This lack of current water in the sample, however, did not rule out water having been present in the past, so the crux of their research was to explore this possibility. Melt inclusions that lose water after entrapment show physical, visible structures that the researchers did not observe. Even more likely, however, is that water may have been reduced to H_2 and diffused out of the sample, leaving behind oxygen, which would in turn have oxidized the iron, essentially creating rust.

To examine this possibility, the group used the synchrotron x-ray technique iron K-edge x-ray absorption near-edge structure spectroscopy at the GSECARS 13-ID beamline at the APS to record spectra of the sample. The results were referenced to recently prepared standards of the oxidation state of iron in mid-ocean-ridge basalt, a rock with similar composition, which could be used for comparison. The iron would be fully oxidized if only 1.5%-by-weight water had been lost; instead, only about 10% of the iron was oxidized.

Fig. 1. An olivine grain from the Belingew komatiite containing melt inclusions. The melt inclusion in the centre of the image contains quenched melt (glass) and a dark shrinkage bubble. The inclusion is approximately 50 μm across.

These results are consistent with the “anomalously hot mantle” model for the formation of the Belingwe komatiite, suggesting that 2.7 billion years ago, the Earth’s mantle was ~500° C hotter than it is today.

— *Karen Fox*

See: Andrew J. Berry[1]*, Leonid V. Danyushevsky[2], Hugh St C. O’Neill[3], Matt Newville[4], and Stephen R. Sutton[4], “Oxidation state of iron in komatiitic melt inclusions indicates hot Archaean mantle,” Nature **455**, 960 (October 2008). DOI:10.1038/nature07377

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13-ID • GSECARS • Geoscience, environmental science • Microfluorescence (hard x-ray), x-ray absorption fine structure (XAFS), microdiffraction, micro-XAFS, high-pressure diamond anvil cell, high-pressure multianvil press, inelastic x-ray scattering • 3.3-cm Undulator A • Accepting general users

CARBON IN THE EARTH'S INNER CORE?

Ever since the Earth's solid core was first discovered in 1936, scientists have sought to understand its composition—a tough job considering its inaccessibility. It is generally accepted that the core is made largely of iron, similar to iron meteorites, but determining which additional elements are present remains challenging. Iron carbide (Fe_3C) has been nominated as one possibility, though some studies have suggested it is too light to match the inner core density. In this 2008 study, researchers used nuclear resonant inelastic x-ray scattering at the APS to show that although iron carbide is indeed too light, the addition of carbon to an iron-nickel alloy may be a viable candidate as another element at the core. Determining the composition of the Earth's inner core can help science learn how the Earth was formed and set the boundaries for theories of the Earth's history and the mechanisms behind the Earth's magnetic field.

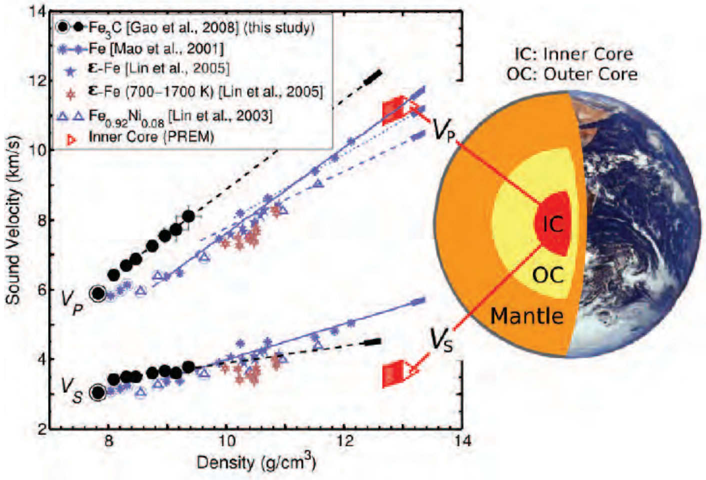

Fig. 1. A comparison of compressional and shear velocities versus density between iron carbide and other iron-rich alloys. All data are at 300K unless otherwise marked. Low-pressure magnetic phases are marked by the outer circles.

This study was performed on the XOR 3-ID beamline at the APS by researchers from the University of Illinois at Urbana-Champaign, Argonne, the Carnegie Institution of Washington, and Indiana University. The team used synchrotron Mössbauer spectroscopy (SMS) to measure the magnetic properties of the carbide sample and nuclear resonant inelastic x-ray scattering to measure the phonon density of states and derive the compressional and shear velocities of the material.

The SMS results showed that while iron carbide is ferromagnetic at atmospheric air pressure, the sample lost its magnetism between 4.3 GPa and 6.5 GPa. The team derived a compressional velocity (kilometers per second) of iron carbide expressed as a function of density, ρ, to be $-3.99 + 1.29\,\rho$ (g/cm^3) and the shear wave velocity (in kilometers per second) to be $1.45 + 0.29\,\rho$ (g/cm^3) (Fig. 1).

The study also showed that at an average inner core pressure of 338 GPa and a likely inner core temperature of 5300K, the estimated density of iron carbide is 2.4% smaller than that of the inner core, whereas the density of iron alone is 3% higher. Clearly, neither iron carbide nor iron alone is the perfect candidate for the inner-core material. On the other hand, a combination of iron and iron carbide may match the density of the Earth's inner core.

Plus, the addition of carbon to an iron-nickel alloy brings the compressional and shear wave velocities closer to those seen in the inner core. So it is reasonable to think that carbon might be present in the inner core.

The total concentration of carbon, however, would have to be lower than that found in iron carbide, namely lower than 6.7%. And, of course, there is no reason yet to completely rule out other light elements, such as hydrogen, oxygen, silicon, and sulfur, as a possibility in the inner core. Other iron carbide compounds, including Fe_7C_3, should be studied as well.

Since knowledge of the composition of the Earth's inner core holds clues as to how the Earth formed, determining the materials therein will provide important constraints on theories of the Earth's history. The addition of carbon might also put constraints on theories behind the mechanisms behind the Earth's magnetic field.

— *Karen Fox*

See: Lili Gao[1,2]*, Bin Chen[1], Jingyong Wang[1], Esen E. Alp[2], Jiyong Zhao[2], Michael Lerche[2,3], Wolfgang Sturhahn[2], Henry P. Scott[4], Fang Huang[1], Yang Ding[3,4], Stanislav V. Sinogeikin[4], Craig C. Lundstrom[1], Jay D. Bass[1], and Jie Li[1], "Pressure-induced magnetic transition and sound velocities of Fe_3C: Implications for carbon in the Earth's inner core," Geophys. Res. Lett. **35**, L17306 (2008). DOI:10.1029/2008GL034817

Author affiliations: [1]University of Illinois at Urbana-Champaign, [2]Argonne National Laboratory, [3]Carnegie Institution of Washington, [4]Indiana University
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3-ID • XOR • Physics, geoscience, life science, chemistry, materials science • Nuclear resonant scattering, high-pressure diamond anvil cell, inelastic x-ray scattering • 2.7-cm undulator • Accepting general users

ARSENIC AND WHOLE RICE

Arsenic is a recognized human carcinogen, and rice takes it up more readily from polluted soil and water than do other grains. Inorganic chemical forms of arsenic pose a greater health hazard than organic forms, and studies have suggested that brown rice contains more arsenic than polished or white rice from which the outer husk has been removed. Using beamline 20-ID (XOR/PNC) at the APS, researchers have mapped the location of organic and inorganic arsenic in brown and white rice grains from different parts of the world. They found that arsenic indeed concentrates in the husk, and that rice from Southeast Asia has predominantly inorganic arsenic whereas in rice from the U.S. it is mostly organic. Their results are important in understanding the dangers of arsenic for populations that consume large amounts of rice.

The researchers, from the University of Aberdeen, the U.S. Environmental Protection Agency (U.S. EPA), the University of Copenhagen, the Chinese Academy of Sciences, and Bangladesh Agricultural University, studied four rice samples. They obtained brown rice from a paddy field in the U.S., where arsenic contamination often derives from pesticides used in prior cultivation of cotton, and from a Chinese paddy field known to be polluted by a nearby metal mining operation. A third sample of brown rice came from plants grown for the study in Bangladesh using water tainted with arsenic to mimic known field conditions. The fourth sample was commercial white rice of U.S. origin.

X-ray fluorescence analysis of halved rice grains yielded cross-sectional maps, with approximately 10-μm resolution, of the location of arsenic. Figure 1 (top) shows that arsenic in a Bangladeshi rice grain concentrates at the surface, specifically along the grain's longitudinal groove. Fluorescence studies also revealed the location of other elements: iron, zinc, manganese, and copper collected in roughly the same location as the arsenic, whereas cadmium and nickel were distributed throughout the bulk of the grain, in the starchy component known as the endosperm (Fig. 1, middle). In contrast, a fluorescence map of a white rice grain from the U.S. (Fig. 1, bottom) shows that arsenic is spread through the endosperm.

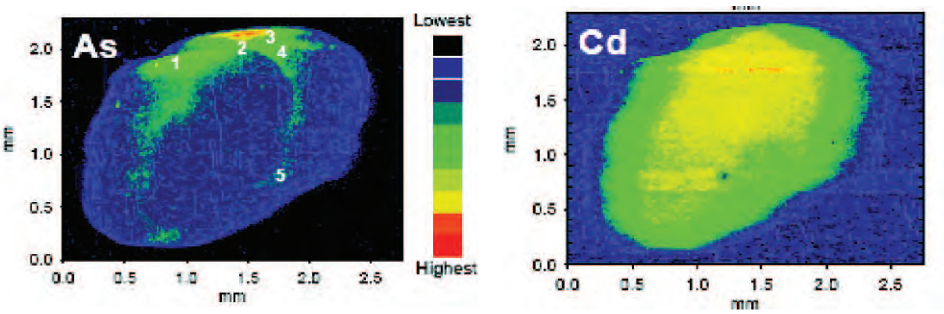
Using two different chemical extraction methods followed by mass spectroscopy, the researchers assayed the total amounts of arsenic in the rice and its differentiation into inorganic (mostly arsenite and arsenate) and organic (mostly dimethyarsinic acid [DMA]) forms. Bangladeshi rice had the highest total concentration, at 0.61 mg of arsenic per kilogram. Brown rice from the U.S. and China contained 0.44 mg/kg and 0.36 mg/kg, respectively, while U.S. white rice contained 0.28 mg/kg. The Chinese rice, however, had the highest proportion of inorganic versus organic arsenic—almost 60%. That proportion ranged from about 40% to 45% in the other samples.

Because these measurements provided no information about the location of the different arsenic species, the researchers examined a number of 10-μm spots on bisected rice grains using the x-ray absorption near-edge structure (XANES) technique. In this technique, ejection of a core electron by an x-ray is followed by emission of photons as other electrons in the arsenic-containing molecule lose energy to fill the vacancy. The XANES analysis showed that up to 80% of the arsenic in the outer layers of brown rice was inorganic, while arsenic in the endosperm of white rice was fairly

evenly split between organic and inorganic forms.

People in Southeast Asia overwhelmingly prefer to eat white rice; the market for brown rice is among Western consumers who believe it offers health benefits. However, bran from the brown rice polishing process ends up in other products, particularly rice milk and fiber supplements. The researchers say that while arsenic in drinking water is regulated, arsenic intake from food may pose a greater danger to some populations and warrants closer attention and investigation.

— David Lindley



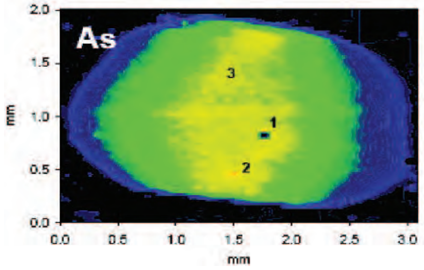


Fig. 1. Synchrotron x-ray fluorescence maps of bisected rice grains reveal the presence of arsenic in the outer layers of a brown rice grain from Bangladesh (above), while cadmium is spread through the interior (above right), as is arsenic in a white U.S. grain (right).

See: Andrew A. Meharg[1]*, Enzo Lombi[2], Paul N. Williams[1], Kirk G. Scheckel[3], Joerg Feldmann[1], Andrea Raab[1], Yongguan Zhu[4], and Rafiql Islam[5], "Speciation and Localization of Arsenic in White and Brown Rice Grains," Enviro. Sci. Tech. **42**, 1051 (2008). DOI: 10.1021/es702212p

Author affiliations: [1]University of Aberdeen, [2]University of Copenhagen, [3]U.S. Environmental Protection Agency, [4]Chinese Academy of Sciences, [5]Bangladesh Agricultural University

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Use of the APS was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract DE-AC02-06CH11357. E.L. was supported by the CSIRO Emerging Science Initiative on Synchrotron Science: Extreme Chemistry and Environmental Science.

20-ID • XOR/PNC • Materials science, environmental science, chemistry, geoscience • Microfluorescence (hard x-ray), x-ray absorption fine structure (XAFS), surface diffraction, micro-XAFS, x-ray Raman scattering, time-resolved XAFS • 3.3-cm Undulator A • Accepting general users

EVENTS

SHAKEN BUT NOT STIRRED

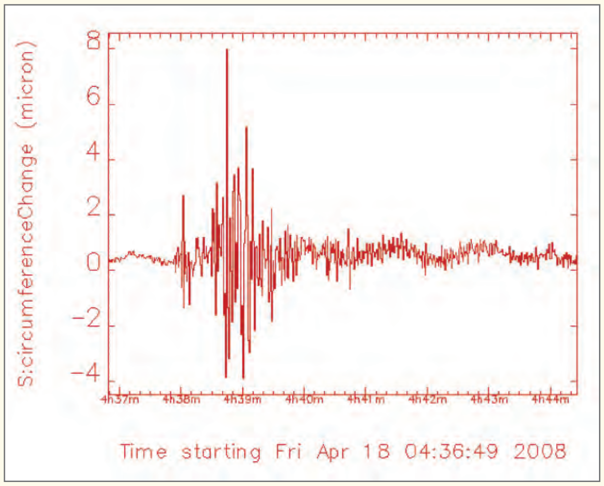

Fig. 1. Variation of the APS storage ring circumference in microns during an earthquake event in southern Illinois. The data was calculated using horizontal particle beam position monitor data from the ring.

The magnitude-5.2 earthquake that occurred in Illinois' Wabash Valley fault system on Friday, April 18, 2008, could have caused a fault of different kind—a system fault interrupting delivery of x-ray beams to APS users. But thanks to the technology in use at the APS, much of it developed at Argonne, experimenters taking data at the APS when the earthquake occurred at 4:36 a.m. (DST) were continued their research uninterrupted.

When tremors from the quake reached the Argonne site, the earthquake was "detected" by the beam position monitors in the APS storage ring (Fig. 1). The electron beam in the storage ring remained on course with no noticeable adverse effects while the entire ring shifted back and forth a maximum of 12 *μ*m. The x-ray beam position monitors assured that x-ray beams continued to illuminate experiment samples.

According to the Associated Press, there were no immediate reports of significant injuries or damage resulting from the quake, which was felt as far away as southern Ontario, Canada. A second, smaller quake, measured at 4.5 on the Richter scale, struck several hours later.

Compensating for Earth- (and Moon-) related influences on the APS accelerator complex is fairly routine for the Diagnostics Group in the Accelerator Systems Division. The radio frequency in the accelerator is routinely changed to compensate for Earth tides. The storage ring moves 37 *μ*m over a roughly 12-h period as the Moon travels from one side of the Earth to the other.

Contact Glenn Decker (decker@aps.anl.gov)

DNA DIRECTS NANOPARTICLE ASSEMBLY

Making something smaller—for instance, shrinking a computer from room size to palm size—requires that the tools doing the work shrink along with the item being downsized. So it is in nanotechnology, which is the future of biomedical applications, electronics, and nearly every other imaginable science and engineering frontier. A team of researchers from Northwestern University and Argonne National Laboratory has produced a system that can be used to guide the assembly of colloidal crystals—a material widely used in photonics and electronics, among other areas. Their discovery holds promise for advances in the development of optics, medical diagnostics, catalysis, and separations.

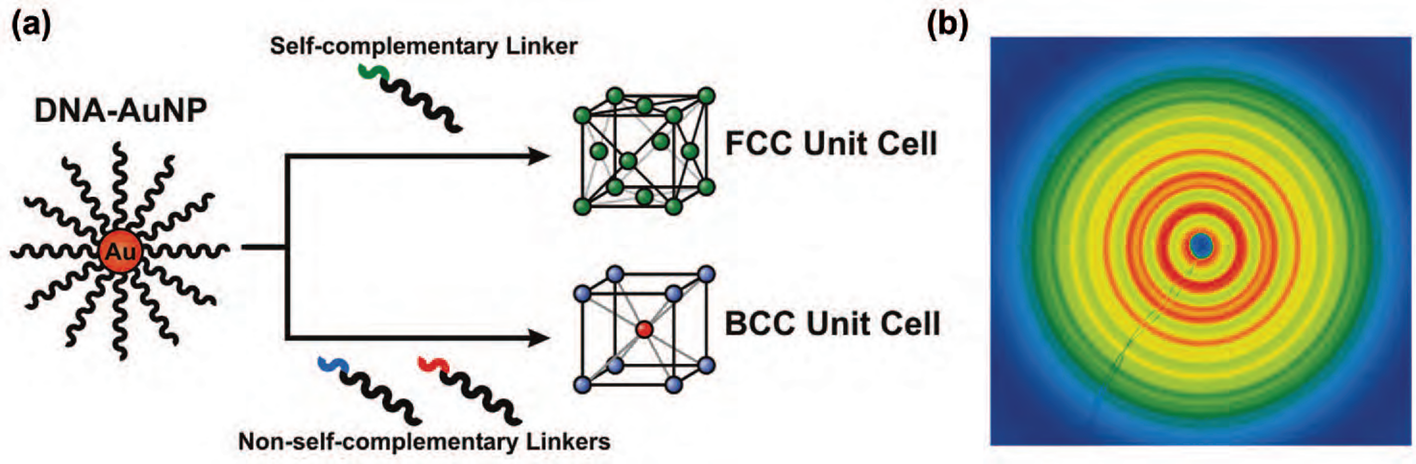

Fig. 1. DNA-driven nanoparticle crystallization: (a) Utilizing the same DNA-functionalized nanoparticle core, face-centered cubic and body-centered cubic lattices can be created with the addition of complementary linking sequences. (b) The two-dimensional, SAXS pattern corresponding to a DNA-AuNP FCC structure, taken at the DND-CAT beamline.

The seed for this research was planted in 1995, when comparisons between nanoparticles and atoms began to emerge, along with the idea that nanoparticles could be used to build molecules in the same way that atoms form molecules. The search for a synthetically programmable material to carry out this task led to DNA as a good candidate. Taking their quest into the laboratory, the researchers in this study, with the help of the DND-CAT 5-ID and the XOR 12-ID beamlines at the APS, have shown how DNA can be used to guide the assembly of three-dimensional nanoparticles. In particular, two-dimensional small-angle x-ray scattering (SAXS) data collected at the APS allowed the scientists to clearly model the formation of molecules from nanoparticles under the direction of DNA.

The basic idea behind using DNA as the assembler of nanoparticles is as simple and elegant as the structure of DNA first reported by Watson and Crick in 1953, and it takes advantage of the same base-pairing rules. In the work done by the research team in this study, single strands of DNA were attached to gold spheres and, when the complementary DNA sequences found each other and paired according to Watson and Crick base-pairing rules, the DNA became double-stranded and brought along the gold. By changing the length and sequence of the DNA strands, including a non-bonding single base that serves as a flexor, and adjusting the reaction temperature, the scientists were able to control the identity of the final three-dimensional product, thus turning DNA into a programmer of colloidal crystallization (Fig. 1).

The main thrust of the research demonstrates a very fundamental capability: the ability to guide the organization of nanoscale building blocks into preconceived architectures. The goal is to elucidate the rules for making any structure and allow the design of materials from the bottom up with any sort of physical and chemical property needed for an application.

One set of reaction conditions produced a crystal lattice of gold spheres and DNA linkers called a "body-centered cubic crystal," which is the same crystal structure as cesium chloride; this arrangement allowed for the maximum number of interactions. A face-centered crystal resulted from another set of experiments that used a different linker type and length.

This study demonstrates ways of

"DNA" continued on page 116

PROOF OF MESOSCOPIC MISFIT IN NANOSIZED METALLIC ISLANDS

As technology advances and nano-sized metallic interfaces become more and more readily available for design and application, there is an increasing demand for a detailed understanding of what happens to the structural, magnetic, optical, and chemical properties of a sample as its size decreases and more atoms begin to experience reduced coordination compared with a sample of the same material in bulk. A group of researchers using an APS x-ray beamline has obtained direct experimental proof for the theoretical prediction of mesoscopic relaxation in nanoislands.

It is well known that the atomic rearrangement of samples plays a key role in determining all of their physical properties. These atomic rearrangements are usually predicted on the basis of macroscopic lattice mismatch. Common macroscopic systems used to investigate these changes are heteroepitaxial metals, characterized by layers of atoms overlying the crystal surface (adlayers) whose island sizes can span hundreds of nanometers. However, for samples with nanoislands consisting of tens of atoms, a new concept is needed to adequately explain structural rearrangements resulting from stress and strain fields near the metallic islands.

The important structural changes caused by giant atomic relaxations have been predicted theoretically. For example, it has been shown, using molecular dynamics (MD) simulations, that in the case of cobalt islands spanned by fewer than 100 atoms overlying on Cu(001), the average interatomic bond length is significantly reduced compared with its value in bulk. This phenomenon is called mesoscopic lattice mismatch. A direct observation of mesoscopic lattice mismatch had so far proven elusive, however, in part because the nanoislands lack both a well-defined interatomic distance and long-range order and because scanning tunneling microscopy (STM) lacks the required resolution in real space. However, researchers from Max-Planck-Institut für Mikrostrukturphysik, Argonne National Laboratory, and the University of Illinois at Urbana-Champaign used surface x-ray diffraction (SXRD) experimental techniques to probe the local structure of the adatoms relative to the substrate (1 × 1)-surface unit cell to obtain direct experimental proof for the theoretical prediction of mesoscopic relaxation in nanoislands.

The locations of the adatoms relative to the underlying surface were ascertained by using a static Gaussian displacement distribution function for the cobalt atoms that lie outside the hollow sites of the Cu(001) substrate lattice. The relevant measurements were performed *in situ* under ultra-high vacuum conditions at both the XOR/UNI 33-ID beamline at the APS and the ID03 beamline at the European Synchrotron Radiation Facility (ESRF) in Grenoble, France. The intensity distribution along the crystal truncation rods (CTRs) was used to identify the locations of the adatom adsorption sites relative to the substrate (1 × 1)-unit cell by looking at the interference between the substrate structure factor (F_{sub}) and the structure factor of the adsorbate (F_{ad}). A precise calibration of the amount of cobalt present was obtained by observing the intensity oscillations at the (hkl) = (1 0 0.1) reflection, close to the (100) anti-phase condition along the (10l) CTR. The amount of cobalt deposited could be determined to within 10% to 15% accuracy.

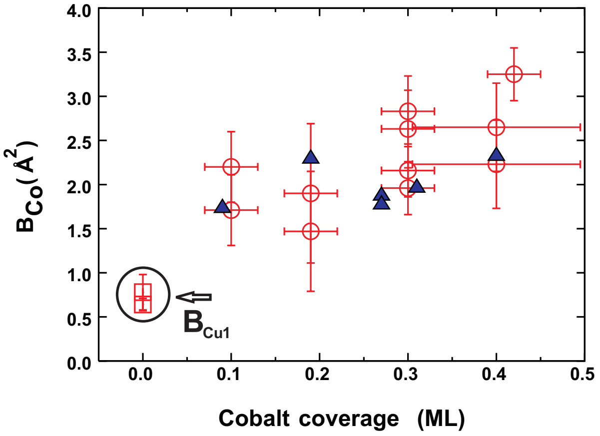

Fig. 1. Experimentally derived Debye parameters of cobalt (open circles) as a function of cobalt coverage. Triangles represent simulated data based on MD calculations. Experimental Debye parameters for first layer copper atoms for uncovered Cu(001) are plotted as squares at zero coverage. (© 2008 The American Physical Society)

When the Debye parameter (B) for cobalt was plotted against the concentration of cobalt deposited (Fig. 1), it was found to potentially be as large as 3.2 Å^2, with an average value of 2.5 Å^2, corresponding to a root mean

“Islands” continued on page 116

“Islands” from page 115

square (rms) displacement of 0.18 Å. Such values of B cannot be due to thermal vibrations, for which B is typically less than 1 Å^2. The team concluded that the SXRD data provide strong evidence that cobalt atoms deposited on the Cu(001) substrate formed nanosized islands with unusually large disorder, corresponding to static displacements.

The next step in this study was to compare these measurements with results obtained by using MD simulations (Fig. 2). Excellent agreement was found between the experimental and theoretical results obtained from MD fits, providing further proof that the enhanced Debye parameter is directly related to mesoscopic relaxations.

This work has given experimental verification to the new paradigm of mesoscopic lattice mismatch, which is expected to play a central role in advancing the understanding of the structure and physical properties of nanoislands in general. — *Luis Nasser*

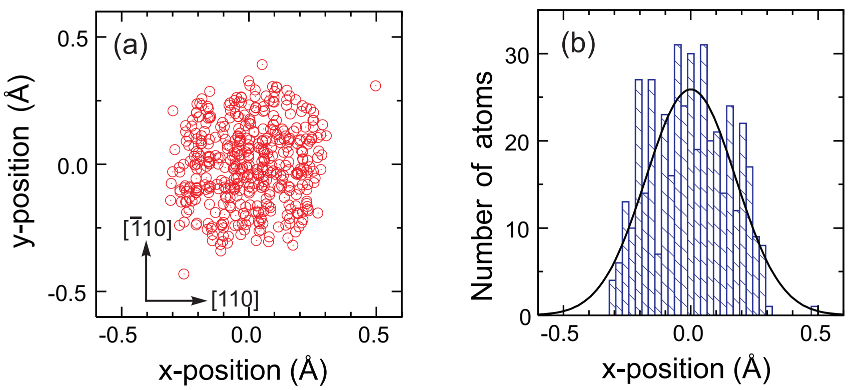

Fig. 2. MD calculation for 0.3 ML Co/Cu001. (a) Positions of cobalt atoms within Cu(001)-surface unit cell. (b) Distribution projected to a axis together with Gaussian fit (solid line). (© 2008 The American Physical Society)

See: O. Mironets[1], H.L. Meyerheim[1]*, C. Tusche[1], V.S. Stepanyuk[1], E. Soyka[1], P. Zschack[2], H. Hong[3], N. Jeutter[4], R. Felici[4], and J. Kirschner[1], “Direct Evidence for Mesoscopic Relaxations in Cobalt Nanoislands on Cu(001),” Phys. Rev. Lett. **100**, 096103 (7 March 2008). DOI: 10.1103/PhysRevLett.100.096103

Author affiliations: [1]Max-Planck-Institut für Mikrostrukturphysik, [2]Argonne National Laboratory, [3]University of Illinois at Urbana-Champaign & ESRF

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Use of the Advanced Photon Source was supported by the US Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

33-ID • XOR/UNI • Materials science, physics, chemistry • Anomalous and resonant scattering (hard x-ray), diffuse x-ray scattering, x-ray reflectivity, surface diffraction, x-ray standing waves, general diffraction • 3.3-cm Undulator A • Accepting general users

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“DNA” from page 114

achieving two different products, and points to the day when DNA can be used to assemble just about any desired nanoparticle configuration. There is now ample evidence and knowledge to proceed in the use of DNA for directed assembly of crystalline nanoparticles, instead of the amorphous complexes that have been reported until now.

The particles created by the research group have spectacular optical and catalytic properties. The group has already used DNA-modified gold nanoparticles in the development of many high-sensitivity biodetection assays. Although such gold nanoparticles have already entered commercial application, the structures produced in the present study exist only in solution. Once certain technical problems are solved, the structures will be ready for use in many applications, such as optics, medical diagnostics, catalysis, and separations. The research group describes the structures as highly porous and tailorable networks, bringing to fruition the idea of using DNA to direct assembly of nanoparticles.

— *Mona Mort*

See: Sung Yong Park[1‡], Abigail K.R. Lytton-Jean[1]*, Byeongdu Lee[2], Steven Weigand[1], George C. Schatz[1], and Chad A. Mirkin[1]*, “DNA-programmable nanoparticle crystallization,” Nature **451**, 553 (31 January 2008). DOI:10.1038/nature06508

See also: Haley D. Hill[1], Robert J. Macfarlane[1], Andrew J. Senesi[1], Byeongdu Lee[2], Sung Yong Park[1,‡], and Chad A. Mirkin[1], “Controlling the Lattice Parameters of Gold Nanoparticle FCC Crystals with Duplex DNA Linkers,” Nano Lett. **8**(8), 2341 (2008). DOI: 10.1021/nl8011787

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5-ID • DND-CAT • Materials science, polymer science • Powder diffraction, x-ray reflectivity, small-angle x-ray scattering, surface diffraction, wide-angle x-ray scattering, x-ray standing waves, x-ray optics development/techniques • 3.3-cm Undulator A • Accepting general users

12-ID • XOR/BESSRC • Chemistry, physics, materials science • Small-angle x-ray scattering, wide-angle x-ray scattering, grazing incidence small-angle scattering • 3.3-cm Undulator A • Accepting general users

STUDYING PHASE CHANGES IN LIQUIDS

A solid can have different crystal arrangements that give it different properties. At certain temperatures and pressures, one crystalline state can abruptly change to another. The difference between phases is not quite the same as the difference between crystalline arrangements. The density and entropy in each phase is distinct. We tend to think of liquids, as homogenous fluids, capable of only one phase. That, it turns out, is not entirely true. Researchers using the APS and the Synchrotron Radiation Source at Daresbury Laboratory have demonstrated that two different liquid phases can separate. They also detected the variables that define the transition from one phase of a liquid to another in supercooled yttria-alumina melts. This is the first time the phenomenon has been seen in any liquid at any temperature. The non-contact method that they developed could also be used to explore instabilities in other liquids.

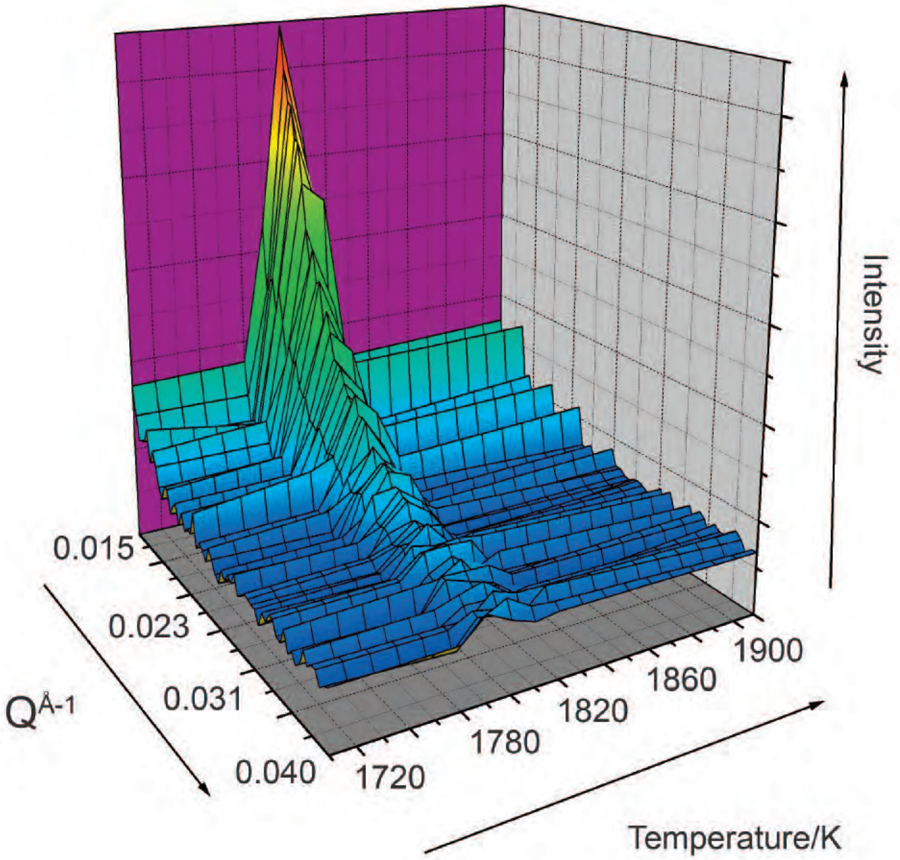

Fig. 1. A sharp peak in the intensity of scattered x-rays, at about 1800K, indicates the transition between two liquid phases in a yttria-alumina melt.

There is growing evidence that a liquid can have more than one phase, and that the phase transitions occur at characteristic temperatures and pressures, like changes between states of matter. Common sense suggests that a liquid mixes over time, resulting in a homogenous single-phase material. But unlike crystals, liquids fluctuate in density in over space and time. The changes in density could be the start of self-assembled areas of lower and higher density phases. If that is possible, then there should be a critical point, at some characteristic temperature and pressure, where both phases can coexist.

Actually catching liquids when they unmix, however, is difficult. Except for liquid phosphorous and yttria-alumina melts, researchers have not seen macroscopic separation of liquids into two phases. The evidence for the separation in yttria-alumina was based on examining rapidly-quenched glasses, which also suggests that the phase transition conditions are close to the material's glass transition from a liquid to a solid.

The researchers from Aberystwyth University, Ecole Nationale Supe'rieure de ChimiedeParis, Argonne, Materials Development, and Daresbury Laboratory investigated supercooled liquid yttria-alumina compounds, levitated on a stream of gas to keep them from contacting solid surfaces that would cause them to crystallize.

They designed a furnace that levitates a droplet, while also allowing the droplet to be probed by synchrotron-generated x-rays produced by the Daresbury Laboratory Synchrotron Radiation Source station 6.2 and XOR beamline 11-ID-C at the APS. They detected information about the structure from scattered x-rays, using both small-angle x-ray scattering (SAXS)

“Phase” continued on page 123

SQUEEZING SOLID OXYGEN TO REVEAL ITS INNER SECRETS

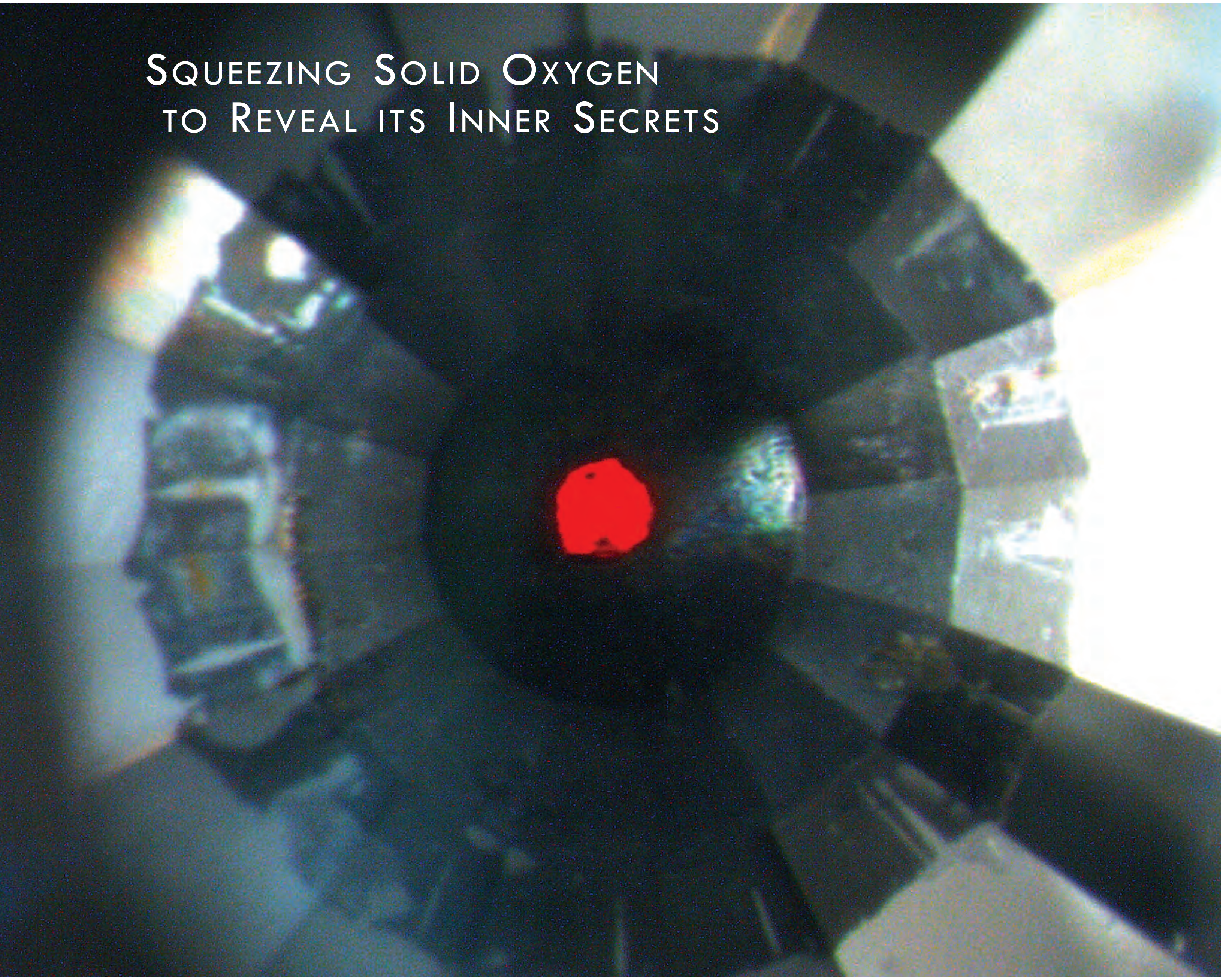

Fig. 1. Solid oxygen phases display spectacular colors. The figure shows the red epsilon phase under 38 GPa of pressure in a diamond anvil cell.

Subjected to enormous pressures, oxygen transforms from a gas into a liquid and then from a liquid into a solid. But solid oxygen is not a simple thing. Under increasing pressure, its molecular structure changes as it goes through a series of distinct solid phases. It eventually becomes metallic and, at sufficiently low temperatures, superconducting. Using the GSECARS 13-ID and HP-CAT 16-ID-D beamlines at the APS, scientists have detailed some of the changes in molecular bonding that occur as oxygen molecules link up into the different geometrical arrangements corresponding to these phases. In particular, they find a mechanism that explains how four oxygen molecules form stable molecular clusters associated with one of the phases.

Oxygen solidifies at a pressure of 5.5 GPa, equivalent to about 55,000 times normal atmospheric pressure. The O_2 molecules cohere into an orderly geometric lattice—the rhombohedral beta phase—that transforms at a pressure of 9.6 GPa into the orthorhombic delta phase. At 10 GPa, the monoclinic epsilon phase appears, which is modified at 96 GPa into the zeta phase. X-ray diffraction studies recently revealed the presence of box-like molecular clusters, consisting of four O_2 molecules lined up at the corners of a square, in the epsilon phase. How these clusters form, and the nature of the chemical bonds that hold them together, was not understood.

Researchers from the Carnegie Institution of Washington, Argonne, The University of Chicago, the University of Saskatchewan, and Brookhaven National Laboratory used inelastic x-ray scattering from oxygen samples compressed in a diamond anvil cell (Fig. 1) to investigate these structural changes. In this technique, a form of Raman scattering, x-rays bouncing off a molecular structure sometimes lose a little energy to electrons that jump from one orbital to another. By tracking how that energy loss spectrum changed in a sample of oxygen under steadily increasing pressure, the researchers could determine how oxygen's bonds shifted in energy as the molecules were squeezed closer together, and thus infer changes in bond structure and characteristics.

From the liquid through the solid beta and delta phases, the inelastic x-ray scattering data revealed a gradual shift in the energy of certain molecular orbitals, indicating that the increasing proximity of other oxygen molecules was perturbing but not disrupting those orbitals. At a pressure of 10 GPa, however, when oxygen switches from the delta to the epsilon phase, the researchers found abrupt, discontinuous changes in orbital energies, suggesting a transformation in the character of the orbitals.

It is well known in organic chemistry that empty orbitals of neighboring molecules can accept otherwise nonbonding electrons to form intermolecular bonds that keep a larger structure together. By similar reasoning, the researchers in this study argue that certain oxygen bonds can transform, when O_2 molecules are sufficiently close, into extended orbitals that serve to maintain $(O_2)_4$ clusters in a specific geometrical arrangement. The estimated energy levels of these intermolecular bonds, in relation to the O_2 bonds they derive from, fit with the changes in electron orbital energies seen in the x-ray scattering data.

At the highest pressure achieved in these experiments, 38 GPa, the x-ray data hint at further changes in bonding structure that could presage the formation of the metallic, and indeed superconducting, zeta phase of solid oxygen near 100 GPa. Conducting similar x-ray scattering experiments all the way to the zeta phase is feasible, although getting to higher pressures requires working with smaller samples and overcoming a number of technical challenges.

— *David Lindley*

See: Yue Meng[1,2]*, Peter J. Eng[2,3], John S. Tse[4], Dawn M. Shaw[4], Michael Y. Hu[1,2], Jinfu Shu[1], Stephen A. Gramsch[1], Chichang Kao[5], Russell J. Hemley[1]**, Ho-kwang Mao[1,2], "Inelastic x-ray scattering of dense solid oxygen: Evidence for intermolecular bonding," Proc. Nat. Acad. Sci. USA **105**, 11640 (2008).
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13-ID • GSECARS • Geoscience, environmental science • Microfluorescence (hard x-ray), x-ray absorption fine structure (XAFS), microdiffraction, micro-XAFS, high-pressure diamond anvil cell, high-pressure multianvil press, inelastic x-ray scattering • 3.3-cm Undulator A • Accepting general users

16-ID-D • HP-CAT • Materials science, geoscience • Nuclear resonant scattering, inelastic x-ray scattering, x-ray Raman scattering, x-ray emission spectroscopy • 3.3-cm Undulator A • Accepting general users

CRYSTALLIZING SELENIUM UNDER HIGH PRESSURE

Researchers from Harbin Institute of Technology, Argonne, Harvard University, and the Carnegie Institution of Washington combined x-rays from the APS, time-resolved diamond anvil cell (DAC) x-ray diffraction (XRD), and a novel DAC microtomography technique of their design to reveal that amorphous selenium (a-Se) undergoes an unexpected two-stage crystallization process that is accompanied by an unusual volume expansion when the material is subjected to a pressure of 10.4 GPa. Amorphous selenium is valuable for modeling pressure effects in group IV elements and amorphous materials because of its wide range of structural and bonding properties. The new technique employed in this research holds promise for accurate determinations of the equations of state of glasses and melts up to megabar pressures, which are crucial to many problems in Earth, planetary, and materials sciences.

The high-pressure DAC microtomography technique, which permits direct measurement of the equation of state of the amorphous phase, was developed and applied at the XOR 2-BM beamline at the APS, while the DAC XRD experiments were conducted at the HP-CAT 16-ID-B beamline, also at the APS.

Previous investigations suggested that a-Se formed a trigonal structure (t-Se) when it crystallized at a pressure of about 10 GPa, which failed to explain why the electrical resistance during crystallization initially dropped to a value that was 2 to 3 orders of magnitude smaller than that of t-Se. Nor did it account for the electrical resistance spontaneously increasing as the crystallization process continued under constant pressure.

In situ XRD patterns taken using a finely focused synchrotron x-ray beam revealed that Se first crystallized to the monoclinic phase (*m*-Se), which persisted from 20 min to hours at different locations in the sample before gradually converting to the trigonal phase. Because *m*-Se is metallic, and thus has a relatively low resistance, its presence explains the structural origin of the seemingly anomalous changes in electrical resistance that occurred during the crystallization process.

The density of the a-Se sample was measured throughout the crystallization process by using the high-pressure computed microtomography technique, in which numerous two-dimensional radiographic images (exposure time: 120 msec per image) of the sample were recorded at 0.125° rotation angle increments and then reconstructed as a sequence of three-dimensional tomographic images (Fig. 1). The technique allowed a precise measurement of the pressure-volume EOS of a-Se with a $\Delta V/V_p$ precision of 0.45% at the highest pressure conditions.

The results indicate the importance of using time- and spatially-resolved high-pressure x-ray diffraction and imaging techniques to understand the kinetics of structural transformations in materials under extreme conditions. They also demonstrate the utility of the new microtomographic technique for determining the equations of state of amorphous materials at extreme pressures and temperatures, and suggest the use of pressure to control and directly monitor the relative densities and energetics of phases to create new phases from highly metastable states.

The new microtomographic technique could find widespread use in making accurate determinations of the equations of state of glasses and melts up to megabar pressures, which are crucial to many problems in Earth, planetary, and materials sciences.

— *Vic Comello*

See: Haozhe Liu[1]*, Luhong Wang[1], Xianghui Xiao[2], Francesco De Carlo[2], Ji Feng[3], Ho-kwang Mao[4], and Russell J. Hemley[4]*, “Anomalous high-pressure behavior of amorphous selenium from synchrotron x-ray diffraction and microtomography,” Proc. Nat. Acad. Sci. USA **105**(36), 13229 (2008).
DOI: 10.1073pnas.0806857105

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2-BM • XOR • Physics, life science • Phase-contrast imaging, tomography, microdiffraction, general diffraction • Bending magnet • Accepting general users

16-ID-B • HP-CAT • Materials science, geoscience • Microdiffraction, powder diffraction, single crystal diffraction • 3.3-cm Undulator A • Accepting general users

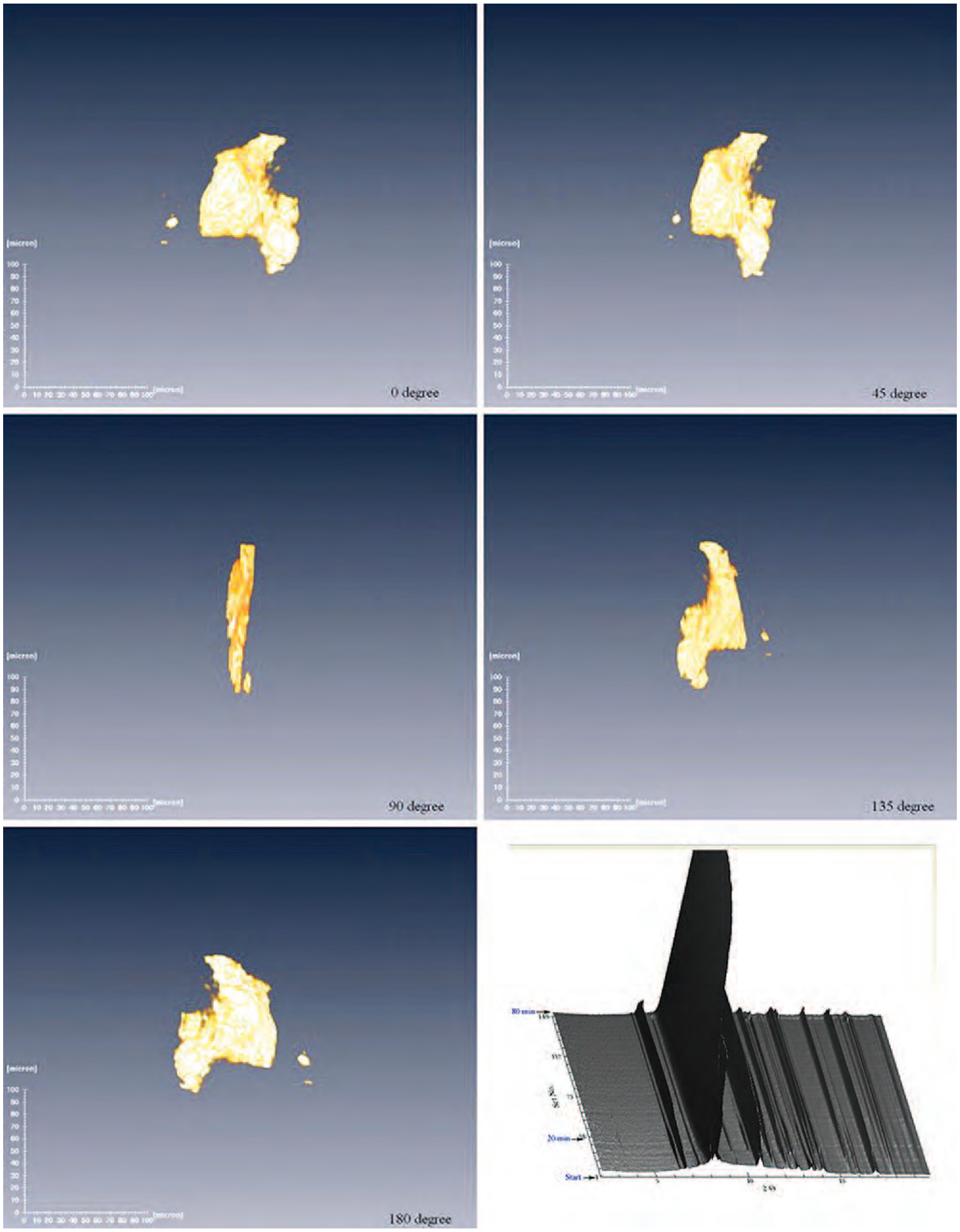

Fig. 1. Snapshots from three-dimensional imaging movie of an a-Se sample in a DAC at ~10.7 GPa, and corresponding time-resolved XRD data. (Note: The movie can be viewed here.

A RADICAL SOLUTION

Understanding how highly reactive chemicals known as inorganic radicals behave in water is key to understanding a wide range of phenomena, from ozone depletion in the upper atmosphere to the effects of climate change on the oceans. Unfortunately, because inorganic species, such as hydrated halogen atoms, tend not to produce strong colors under ultraviolet light, it is difficult to study their structure and reactions using conventional spectroscopic methods. Researchers from Argonne, however, have turned to transient x-ray absorption spectroscopy (XAS) to investigate the hydration of short-lived radicals, such as the bromine atom, with atomic resolution. A hydrated bromine radical forms when a bromide ion in water loses an electron. Utilizing the laser pump x-ray probe capabilities of XOR beamline 7-ID at the APS, the Argonne researchers have obtained new experimental evidence for the behavior of hydrated bromine radicals, which could open up studies of other inorganic species of relevance to atmospheric and oceanic science, in interstellar chemistry, as well as general inorganic chemistry research.

The hydration of a simple-seeming chemical species, the bromine atom, Br^0, would at first sight appear to be a straightforward case of surrounding the bromine with water molecules in aqueous solution. However, scientists know little about the precise details of hydration of bromine, or indeed any of the other halogen atoms, including chlorine, fluorine, and iodine. All of these elements are, in one way or another, closely tied to environmentally important processes that affect the whole planet. Volatile organic compounds containing halogen atoms, for instance, can break down to release radicals and other chemical species that react, under the intense ultraviolet light from the sun, with ozone in the upper atmosphere.

This study used x-ray pulses from the APS in conjunction with amplified ultraviolet pulses from a titanium-sapphire laser to reveal details of the water structure around reactive bromine radicals. The laser pulse removed the electron from negatively charged bromide anions and the x-ray pulse probed the neutral atom. By synchronizing the laser pulses with the synchrotron using a feedback loop and overlapping the beams at an angle of 4° in the sample, the researchers fine tuned the relative delay between laser and x-ray pulses electronically. This allowed them to measure the time-dependent change of the sample as the atoms react.

The sample itself is a 100-μm-thick jet of sodium bromide solution. The researchers employed selenium filters to block elastically scattered x-rays and detect the bromine K_α fluorescence using gated avalanche photodiode detectors on each side of the liquid jet. By recording fluorescence for two consecutive x-ray pulses right after the laser fired, they obtained spectra at each relative delay time. The first x-ray pulse probed the short-lived Br atoms and the second probed the reaction product Br_2^-.

Crucially, the difference between studies involving the simple

“Radical” continued on page 123

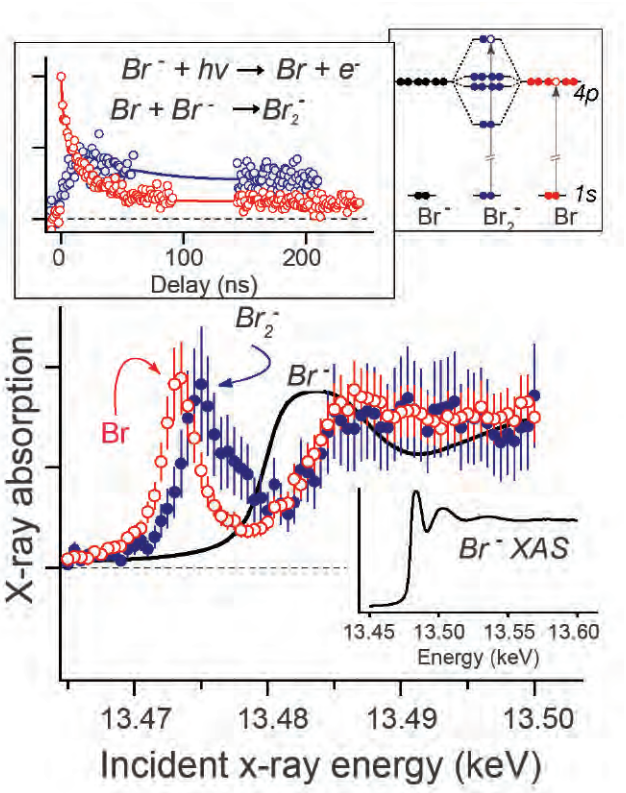

Fig. 1. Time-resolved XAS probes the hydration structure of reactive bromine radicals (red) and di-bromide anions (blue) after an ultraviolet laser pulse removes an electron from the bromide anion. Differences in the x-ray absorption spectrum reveal details of the electronic and atomic structure of each species. The lifetime of neutral bromine atoms is only about 17 nsec.

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halide ions and halogen radicals is one of the latter being water repellant—hydrophobic—as opposed to the water-loving, hydrophilic ions. This means that whereas the halide ions form strong but transient hydrogen bonds with water molecules, the halogen radicals sit in a solvent cavity. Within this cavity the atom weakly interacts with only a single water molecule in the first layer, rather than interacting with several water molecules through relatively strong hydrogen bonds.

Other researchers had used XAS to investigate the case of I^0 and gleaned some intriguing information about the behavior of this chemical species. However, the Argonne researchers point out that the interpretation of the spectra for the hydrated I^0 species is complicated by its reaction with iodide ions in the solution. These must be present in excess amounts to allow the XAS experiments to be carried out. The result is that they can form substantial amounts of di-iodide and tri-iodide, containing two and three iodine atoms, respectively.

In contrast, the researchers explain, bromine produces a much stronger absorption than iodine and so only dilute solutions are required for the equivalent studies, which slows down the reaction to form di-bromide and tri-bromide chemical species and allows the spectra of those species to be measured separately.

The team's findings suggest that XAS is well suited to observing adducts formed between water molecules and radicals, such as the bromine atom. The work could open up studies of other inorganic species of relevance to atmospheric and oceanic science, in interstellar chemistry, as well as general inorganic chemistry research.

— *David Bradley*

See: Christopher G. Elles*, Ilya A. Shkrob, Robert A. Crowell, Dohn A. Arms, and Eric C. Landahl, “Transient x-ray absorption spectroscopy of hydrated halogen atom,” J. Chem. Phys. **128**, 061102 (2008).
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Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

7-ID • XOR • Materials science, atomic physics, chemistry • Time-resolved x-ray scattering, radiography, time-resolved x-ray absorption fine structure • 3.3-cm Undulator A • Accepting general users

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“Phase” from page 117

and wide-angle x-ray scattering (WAXS) techniques. Because different phases have different densities (and entropies), they scatter x-rays differently, so these methods let the researchers probe both the nanoscale structure and atomic structure of a droplet over a temperature range of hundreds of degrees, all the way down into the supercooled regime.

The researchers detected nanoscale density inhomogeneities in droplets made of slightly different compositions of yttrium-alumina using SAXS. In general, the small-angle scattering increased with temperature, but one melt contained a distinctive feature: a narrow peak just below 1800K due to nanostructural changes that occured in the density fluctuations. The WAXS data showed a change in the inter-atomic polyhedral packing pattern of the melt at the same temperature (Fig. 1).

They were able to link theSAXS peak to a phase change between low-density and high-density liquids. The peak’s narrowness and reversibility are hallmarks of a first-order phase transition in liquid (according to the “two-state” model), and unlike the alternative hypothesis that liquid phase changes occur gradually through incremental metastable states for high- and low-density amorphous transitions.

Moreover, around this point the temperature of the droplet changed, creating a repetitive pattern. When the group employed video imaging, they saw that the droplet fliped bottom-side-up at the beginning of each cycle. The phenomenon carried on for over an hour, and resumed after re-melting. The speed of rotation and the temperature change yielded the density and entropy differences between the two phases.

The researchers’ ability to detect the transition was enabled by the design of the contactless furnace that incorporated probes for *in situ* data gathering. This design should allow further experiments with other liquids at ambient pressure. One intriguing possibility is exploring instabilities in supercooled water. — *Yvonne Carts-Powell*

See: G.N. Greaves[1], M.C. Wilding[1], S. Fearn[1], D. Langstaff[1], F. Kargl[1], S. Cox[1], Q. Vu Van[1], O. Majérus[2], C.J. Benmore[3], R. Weber[4], C.M. Martin[5], and L. Hennet[6], “Detection of First-Order Liquid/Liquid Phase Transitions in Yttrium Oxide-Aluminum Oxide Melts“ Science **322**, 566 (24 October 2008).
DOI: 10.1126/science.1160766
Author affiliations: [1]Aberystwyth University, [2]Ecole Nationale Supérieure de Chimie de Paris, [3]Argonne National Laboratory, [4]Materials Development, [5]Daresbury Laboratory
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11-ID-C • XOR/BESSRC • Materials science, geoscience, physics, chemistry • Diffuse x-ray scattering, high-energy x-ray diffraction, pair distribution function • 2.3-cm ndulator • Accepting general users

NEW RESOLUTION WITH THE FULL-FIELD HARD X-RAY TRANSMISSION MICROSCOPE AT 32-ID

A full-field x-ray transmission microscope (TXM) at the XOR 32-ID microscopy beamline of the APS is now capable of providing the best reported lateral resolution for Fresnel zone plate (FZP) hard-x-ray microscopy. Tests performed on a variety of specimens with 8-keV to 10-keV photons have found that the first-order lateral resolution is below 40 nm, based on the Rayleigh criterion, and similar resolution levels were found in the 7-keV to 18-keV photon energy range.

The microscope system can also operate in a Zernike phase contrast imaging mode, which increases the contrast for fine features of most materials in the hard x-ray spectral region, especially materials consisting of low atomic number elements. For these elements, the contrast can increase by two orders of magnitude, which is particularly important for organic and biological specimens. When used in the phase contrast mode, the TXM enables viewing of features in the 30-nm range, as shown by a Zernike phase contrast image of a 180-nm-thick Siemens star test pattern with 30-nm minimum separation at the center (Fig. 1).

Thanks to the extraordinary brightness of the APS and the TXM's optimized, elliptically shaped glass capillary condensers, good-quality images can be obtained at excellent imaging throughput of 50-msec-per-frame with ~1×10^4 charge-coupled-device counts per pixel. These results were obtained using a state-of-the-art FZP structure with an outmost zone width of 45 nm, a diameter of 80 μm, and an aspect ratio of ~20 (thickness of 900 nm). The structure was made of gold on a silicon nitride membrane.

The imaging results illustrate a few of the many opportunities that can now be exploited because of the new resolution levels in x-ray microscopy. Besides subcellular imaging studies in the life sciences, these capabilities can be used, for example, to image nanostructures of interest in nanoscience and nanotechnology. And this is only the beginning. The researchers, from Argonne; Academia Sinica; National Tsing Hua University; National Taiwan Ocean University; Xradia, Inc.; Pohang University of Science and Technology; Ecole Polytechnique Fédérale de Lausanne; the National Synchrotron Radiation Research Center; and the National Health Research Institutes estimate that an outermost FZP zone width of 30 nm will be feasible in the near future, which should enable additional improvements in resolution. Tthe very high flux achieved at the 32-ID microscopy beamline makes the practical use of FZPs in the third (or higher) order feasible, with a better resolution even before improvements in hardware are made. Resolution levels approaching 10 nm can be foreseen.

Combined with the high penetration of hard x rays, such resolution levels can open amazing new opportunities for nondestructive, three-dimensional imaging of objects on the nanometer scale. — *Vic Comello*

See: Y.S. Chu[1], J.M. Yi[1], F. De Carlo[1], Qun Shen[1], Wah-Keat Lee[1], Hung-Jen Wu[2], C.L. Wang[2], J.Y. Wang[2], C.J. Liu[2], C.H. Wang[2], S.R. Wu[2,3], C.C. Chien[2,3], Yeukuang Hwu[2,3,4,5]*, Andrei Tkachuk[6], W. Yun[6], M. Feser[6], K.S. Liang[5], C.S. Yang[7], J.H. Je[8], and G. Margaritondo[9], "Hard-X-ray Microscopy with Fresnel Zone Plates Reaches 40 nm Rayleigh Resolution," Appl. Phys. Lett. **92**, 103119 (2008).

DOI:10.1063/1.2857476

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32-ID • XOR • Materials science, life science • Phase-contrast imaging, ultra-small-angle x-ray scattering, radiography • 3.3-cm Undulator A • Accepting general users

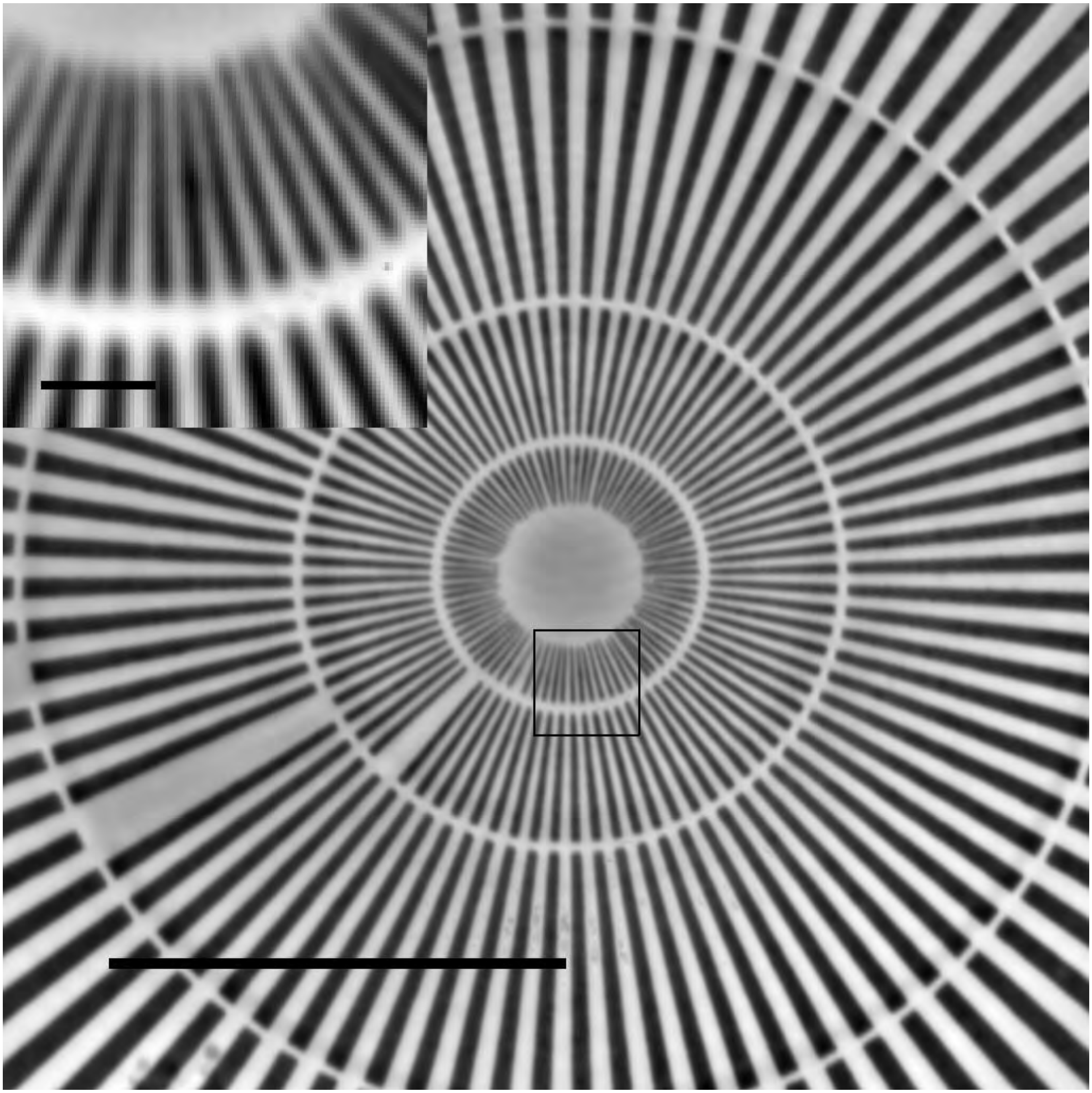

Fig. 1. An 8-keV x-ray micrograph of an Au Siemens star test pattern. Bar in full image is 5 μm. Bar in inset (box region) is 300 nm.

USING X-RAY CALORIMETRY TO PROBE PHONONS

Phonons—the vibrations in crystalline materials—can reveal otherwise-hidden aspects of materials. Sound, heat, and electrical conduction depend on phonon activity. The way phonons travel in a material (in other words, how waves of vibrations propagate) illuminates information about the forces that bond atoms together. Researchers from the University of Illinois at Urbana-Champaign and Argonne used an APS x-ray beamline in their development of a new, direct method of mapping phonon dispersion relations, which relate the frequency of a phonon to its wave number (or momentum) that should prove useful for studies of phonons and quantum phase transitions in solids and thus further the field of materials physics.

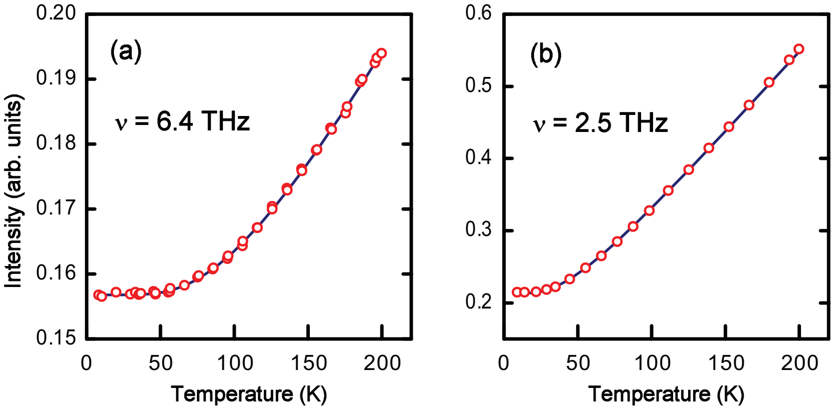

Fig. 1. Temperature dependence of x-ray thermal diffuse scattering intensities from copper at (a) (2.65, 0, 0) and (b) (1.1, 1.1, 1.1) in momentum space. The circles are data points. An increasing phonon population at higher temperatures causes the x-ray scattering intensity to increase in each case. A model analysis yields the curves, and the phonon frequencies are determined to be (a) 6.4 THz and (b) 2.5 THz, respectively.

Detecting phonon dispersion relations is difficult. Several methods exist, but each has limitations. Inelastic neutron scattering can measure phonon dispersions if one has a large single crystal, and if the material does not absorb many neutrons. Inelastic x-ray scattering (IXS) is limited mainly by its slow data acquisition rate. A third option, x-ray thermal diffuse scattering (TDS), is an indirect method that can introduce systemic errors based on which model is used to fit data.

The new method developed by the researchers in this study is similar to TDS, but provides direct measurement of phonon energies. The group measured the temperature dependence of the x-ray scattering intensity at a number of points in momentum space. Because the variation in intensity depends on the phonon populations, the researchers could determine the phonon energies at these points.

The sample (in this case, a copper single crystal) was bombarded with a 0.5 × 0.5 mm^2 beam of 8.0-keV x-rays at XOR/UNI beamline 33-ID. Variables included the temperature of the sample (which was held at different temperatures from 10K to 200K), the angle of the diffractometer, and the orientation of the sample. The researchers controlled the temperature of the copper carefully, and adjusted for the thermal expansion of the system.

The x-ray intensity depended strongly on the temperature (Fig. 1). At low temperatures, the intensity stayed flat, because the phonons were frozen out. As the temperature increased, the material passed a threshold at which the intensity increased. Because this threshold depends on the phonon frequency, it enabled the measurement of phonon frequency.

The researchers obtained first-order results with higher-order correction and determined methods of dealing with longitudinal- and transverse-mode phonons. When they compared their results against those from prior neutron measurements, the results agreed well.

The new method is similar to inelastic x-ray scattering, but because it measures heat content in the sample (rather than energy, as in IXS), it can gather data faster. This method should also be applicable to studies of quantum phase transitions in solids.

— *Yvonne Carts-Powell*

See: Ruqing Xu[1], Hawoong Hong[2], Paul Zschack[2], and T.-C. Chiang[1]*, “Direct Mapping of Phonon Dispersion Relations in Copper by Momentum-Resolved X-Ray Calorimetry,” Phys. Rev. Lett. **101**, 085504 (22 August 2008).
DOI: 10.1103/PhysRevLett.101.085504

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33-ID • XOR/UNI • Materials science, physics, chemistry • Anomalous, resonant, and diffuse x-ray scattering, x-ray reflectivity, surface diffraction, x-ray standing waves, general diffraction • 3.3-cm Undulator A • Accepting general users

HIGH-RESOLUTION CHEMICAL IMAGING USING SCANNING TUNNELING MICROSCOPY

Argonne researchers are exploring a radically new concept that promises to provide nearly atomically resolved chemical information about solid surfaces. The approach uses a scanning tunneling microscope (STM) for lensless imaging of electrons emitted when samples are illuminated with monochromatic x-rays (Fig. 1). The ejected electrons carry valuable chemical information about their originating environments, and electronic and magnetic information as well. The technique could revolutionize the study of chemically active surfaces.

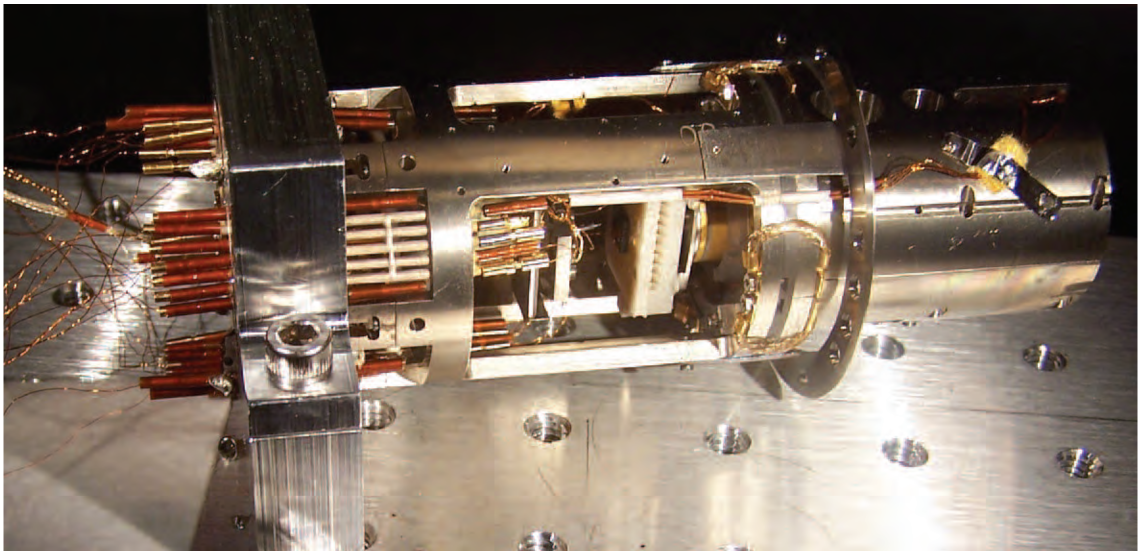

Fig. 1. The STM used in the experiment. The compact design of the microscope allows easy adaptation at different beamlines.

The researchers' experiments were performed at XOR beamline 4-ID-C at the APS using a focused x-ray beam 100 × 100 μm^2 in size. Samples were irradiated at an angle of 10° with respect to the sample surface, and emitted electrons were detected at an STM tip made of polished $Pt_{90}Ir_{10}$ wire having a diameter of 250 μm. The tips used were coated with boron nitride, producing an insulating layer everywhere except at the very point of each tip. This drastically reduced the unwanted background of nonresonant photoejected electrons. The total electron yield (TEY) also was measured directly from the sample, which consisted of a patterned Cu (3-nm)/NiFe (5-nm) multilayer film fabricated on a silicon wafer. X-ray-generated electrons due to photoelectric absorption both at the tip and at the sample were studied to determine how well the desired resonant currents and the unwanted background currents could be controlled by small biases applied between the sample and the tip. The currents were studied in the far field (400-nm to 1600-nm tip/sample separation), where quantum mechanical tunneling does not occur.

The TEY current peaks due to the metallic Ni *L* absorption edges were clearly visible at 852.4 eV and 869.6 eV with biases between -5 and +5 V (Fig. 2a). Splitting of the *L* edges was also visible, indicating a slight oxidation of the sample. The intensity of the Ni L_3 peak decreased for increasing bias from -5 to +5 V. Relative to its value at -5 V, the intensity fell to about 70% at 0 V, and was present at about the 30% level at 5 V. The bias dependence of the Ni L_2 peak exhibited a similar decrease of the intensity. The intensity ratio of the Ni L_2 to Ni L_3 peak amounted to 0.19 ±0.01, independent of the applied bias. This value is in good agreement with calculations of the expected Ni *L* peak ratio.

The corresponding tip current spectra (Fig. 2b) measured at the same time indicated that only about 40% of the initial intensity of the Ni L_3 peak remains without bias relative to its value at -5 V. With a bias of 5 V, the peak-to-peak intensity dropped to less

"Imaging" continued on page 128

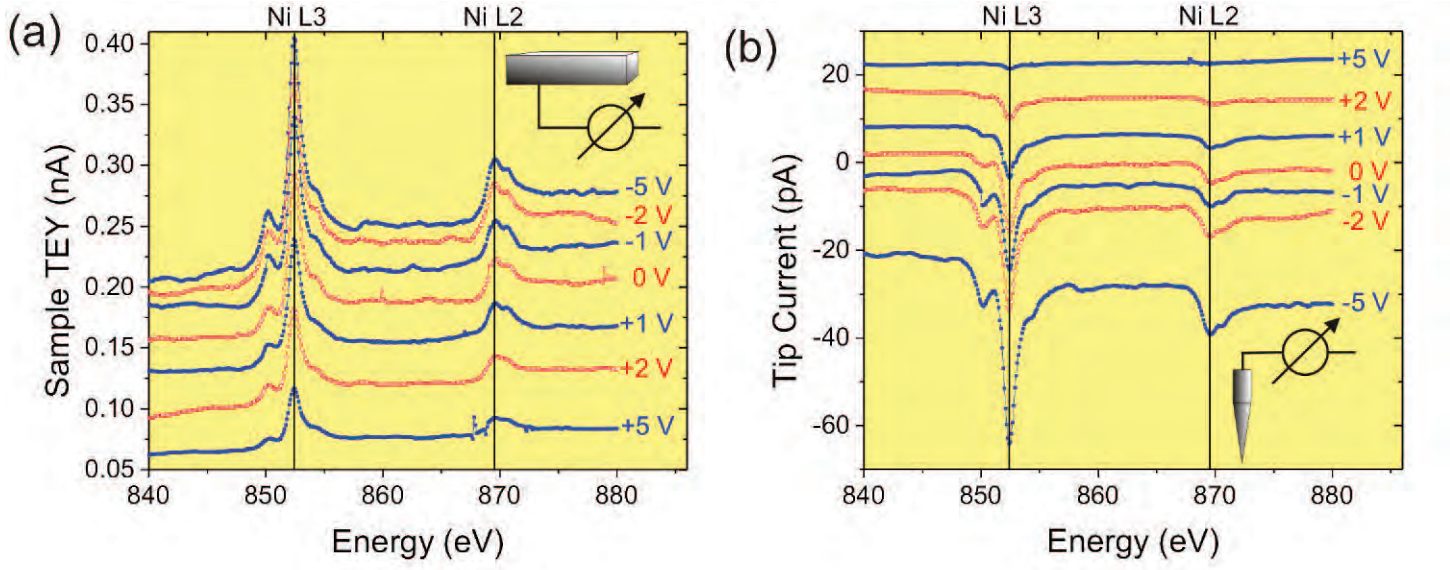

Fig. 2. (a) TEY of a NiFe sample with x-ray excitations between 840 and 880 eV as a function of sample bias. (b) Tip current recorded with a tip/sample separation of 1600 nm.

"Imaging" from page 127

than 4%. The intensity ratio of the Ni L_2 to Ni L_3 peak was 0.20 ±0.03 at the tip, reflecting the ratio measured by TEY. Each TEY-current and tip-current spectra also exhibited a characteristic offset as a function of the applied sample bias.

Data obtained with tip/sample separations of 400 nm, 800 nm, and 1600 nm could be fitted using one linear function. For these tip/sample separations, typically around 12% of resonant ejected electrons are detected at the tip, a percentage that can be doubled by applying a sample bias value of -5 V. Thus, a small bias between the tip and sample allows an accurate and effective control of the desired currents obtained at the absorption edges, as well as the background currents.

The researchers conclude that the ability to detect photoejected electrons via an experimental combination of monochromatic x-rays and STM could lead to high-resolution microscopy with chemical sensitivity. — *Vic Comello*

See: V. Rose*, J.W. Freeland, K.E. Gray, and S.K. Streiffer, "X-ray-excited photoelectron detection using a scanning tunneling microscope," Appl. Phys. Lett. **92**, 193510 (2008).
DOI: 10.1063/1.2936083

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4-ID-C • XOR • Physics, materials science • X-ray photoemission electron microscopy, x-ray photoemission spectroscopy, magnetic circular dichroism (soft x-ray), x-ray magnetic linear dichroism, magnetic x-ray scattering, anomalous and resonant scattering (soft x-ray) • Circularly polarized undulator • Accepting general users

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A HOME-GROWN PLATINUM SAXS DETECTOR

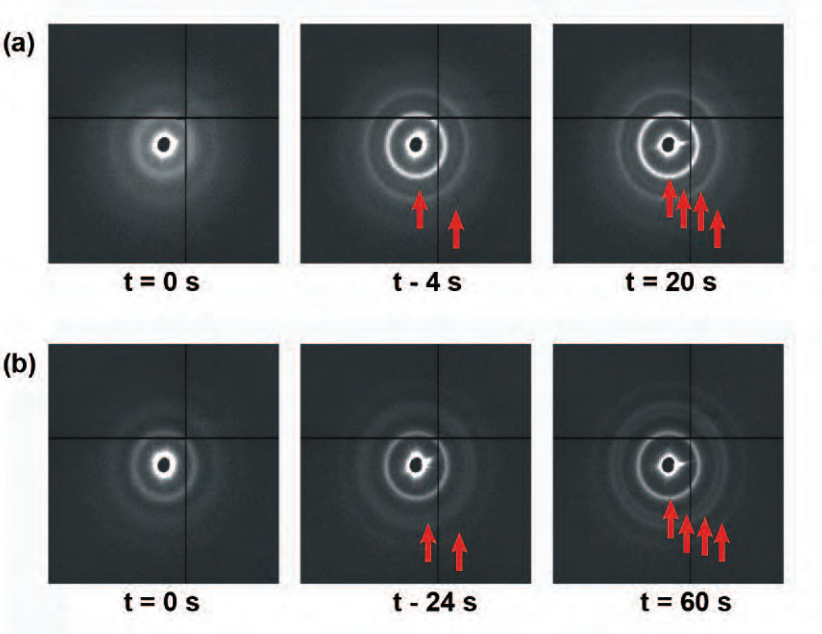

Fig. 1. Time-resolved two-dimensional SAXS images of crystal formation. The progression of images shows the formation disordered DNA-AuNP aggregates (t = 0 s) to highly-ordered BCC (a) and FCC (b) crystals. The arrows in each series of images indicate the initial appearance and subsequent sharpening of x-ray scattering peaks (BCC = q_0, $(\sqrt{2})q_0$, $(\sqrt{3})q_0$, (2)q0, $(\sqrt{5})q_0$; FCC = q_0, $(\sqrt{8/3})q_0$, $(\sqrt{11/3})q_0$, $(\sqrt{20/3})q_0$) corresponding to well-formed crystalline domains.

Detectors play a critical role in planning for renewal of the APS. The article in *APS Science 2007* on “XSD Technical Support” (ANL-07/25, pg. 154) made note of the high-sensitivity, charge-coupled device (CCD) detector being developed by the Beamline Technical Support (BTS) Group in the Argonne X-ray Science Division (XSD). Two of these detectors—now called Platinum detectors—for small angle x-ray scattering (SAXS) have been produced by BTS. One is installed and taking data at XOR/BESSRC beamline 12-ID-C, while the second has joined the BTS detector pool.

Science performed with the Platinum system includes an *in situ* study of crystal growth for DNA-AuNPs. Taking advantage of the Platinum’s speed, personnel at beamline 12-ID-C have used the detector to follow the four-step process of initial DNA-AuNP aggregation; localized restructuring into small, well-ordered crystalline domains; small crystal-crystal aggregation; and subsequent rearrangement forming large crystal systems with significant long-range order. Figure 1 shows SAXS data tracking the growth of these crystals.

The Platinum detectors feature a single-CCD prototype system and a 2 × 2 Mosaic CCD system. Both of these systems, which are optimized for sensitivity, utilize a front-illuminated Kodak KAF-4320E CCD coupled to a low-demagnification fiber-optic taper to allow for excellent sensitivity to light; as well as custom mechanical hardware, electronics, and software developed at Argonne. The CCD can be run in 1 × 1, 2 × 2, or 4 × 4 binned mode to trade-off resolution for frame rate. For the quad-CCD system, the image size varies from 1024 × 1024 pixels to 4096 × 4096 pixels. With 4 × 4 binning, the detector produces five frames per sec.

The Platinum detector software was developed by the BTS group during 2007-2008. This software controls the detector, saves data, interfaces to the Experimental Physics and Industrial Control System and applies all necessary calibrations to the data.

The Platinum detector was delivered to the 12-ID-C beamline in January 2008 and was first used for experiments during the summer 2008 user-beam run. The BTS group supplied technical support to fix problems that arose during the use of the new detector. By the fall 2008 run, the Platinum system had become the principal detector at the 12-ID-C beamline.

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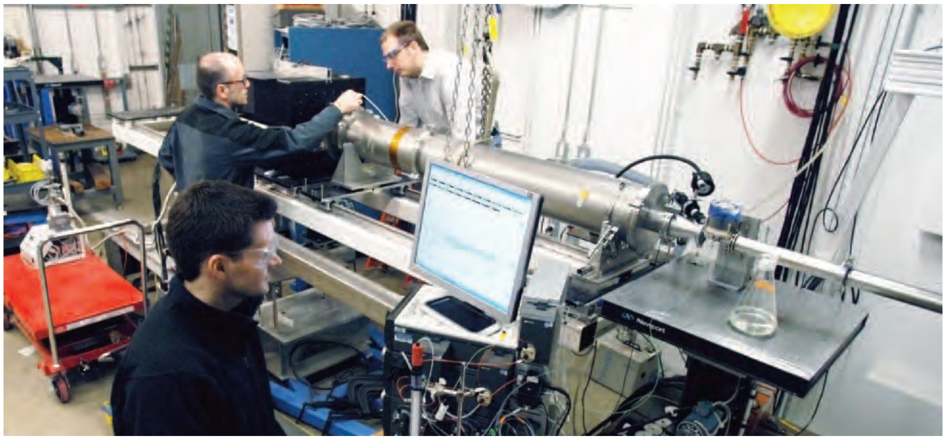
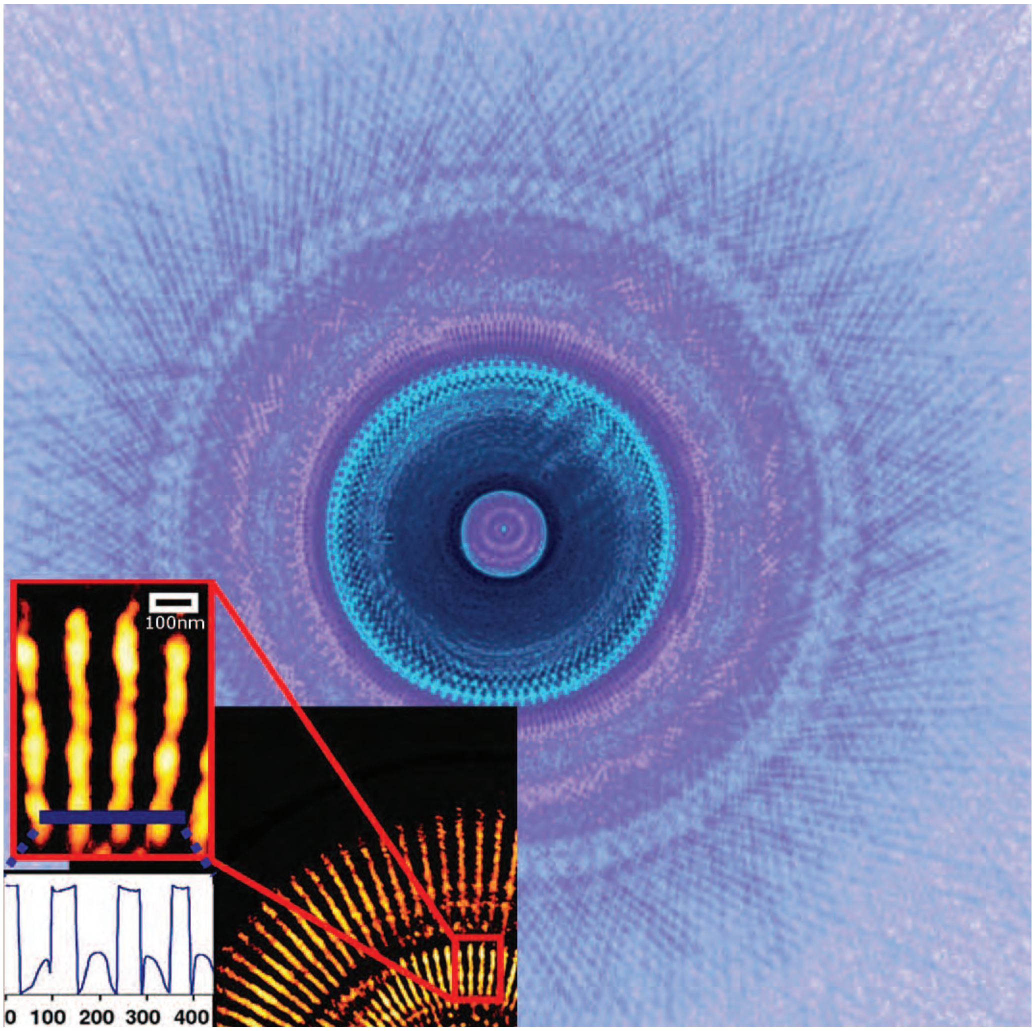


Evan Small (foreground) of the University of Illinois at Chicago (UIC), Sonke Seifert (behind Small) of XSD, and Andrew Mesecar (UIC) in the XOR/BESSRC 12-ID-C research station. The Platinum CCD detector is the black box visible immediately behind Seifert. The UIC researchers were at the APS to do SAXS studies on a complex of proteins related to cancer chemoprevention.

EXTENDING THE USEFULNESS OF COHERENT DIFFRACTION IMAGING

Coherent diffractive imaging (CDI) is a method for determining nanoscale two- or three-dimensional structural information. In CDI, a coherent beam of radiation interacts with a sample, yielding a diffraction pattern containing high-angle information. Then, computational iterative techniques reconstruct an image of the sample. Traditionally, because CDI requires that the diffraction be properly sampled, it can deliver this information only from isolated objects. To expand the applicability of CDI, Australian and U.S. researchers used a variation on CDI called Fresnel CDI (FCDI). Working at an APS beamline they have executed what they call “keyhole coherent diffractive imaging,” or keyhole CDI. This new technique promises to open the door to myriad new applications across a broad range of scientific disciplines.



Promising advances, such as the accurate imaging of a single quantum dot or a small virus, are likely

By using a finite, diverging illumination, the researchers were able to reconstruct small regions within extended objects and determine the phase shift that the x-rays had undergone. The new, more widely applicable method was demonstrated by imaging objects with radiation in the visible-light and x-ray ranges. An optical lens or Fresnel zone plate was used to create an effectively finite, diverging illumination on the sample, thereby isolating a small region within the larger object. X-ray diffraction from one sample region was measured, resulting in an image with 20-nm spatial resolution. The researchers found that the method relies on *a priori* knowledge of the illuminating beam, which is determined separately by using a similar technique. Important for further advances, their work removes the requirement for an isolated sample that previously limited the applicability of CDI. At the same time, FCDI retains the advantages of reconstructing the sample by using iterative algorithmic methods, which enables high-resolution imaging of a wide variety of samples within difficult-to-analyze environments.

< Fig. 1. A false-color image of the Fresnel far-field diffraction pattern from a selected region of a large sample. When FCDI is used, a diverging beam illuminates only a selected subsection of the sample and, through a computational method, provides an image of it at 20-nm spatial resolution. In this way, FCDI provides an escape from the "isolated-object" requirement of traditional CDI, while retaining most of the desired characteristics of that method. Inset: Inset: A portion of the reconstructed test object. Although the object is larger than the illumination spot, FCDI is sensitive only to contributions from within a selected region. The line-out demonstrates the high spatial resolution of the image.

The flexibility of the new technique also facilitates the study of weakly scattering targets for which a large flux density is required to image selected areas, and it avoids direct damage to neighboring regions of the sample.

Fresnel coherent diffractive imaging takes its name from the equivalence of far-field diffraction, with a divergent illumination, to “Fresnel” diffraction, with a planar one; that is, numerical Fresnel propagation, rather than Fourier, is necessary. The divergent wave front illuminating the sample also encodes spatial information into the diffraction, leading to less ambiguous object reconstructions and faster convergence of the iterative algorithm (Fig. 1). The interaction of such an illumination and the sample is guaranteed to provide a far-field diffraction pattern with a unique phase distribution. A high-quality focusing optic accurately defines a region of interest because the illumination rapidly decreases around its edges to a negligible value. Because the same geometry is used to determine the illuminating beam, its reconstruction is achieved at a resolution equal to that of the sample image.

The x-ray data that supported this study were collected at XOR beamline 2-ID-B of the APS. Measurements of the data occurred over the central region (the region that would be measured in a holographic experiment) and the high-angle scatter region (where the signal is measured beyond the aperture of the lens). Therefore, while FCDI requires a lens, the resolution of the resultant images is limited not by the lens aperture, but by the aperture of the detector.

The collaborators demonstrated that the illumination in the plane of the sample is a valid CDI constraint when phase-curved incident illumination is used. Consequently, the researchers retain the desirable high resolution of CDI, while still being able to image an object that extends well beyond the illuminating beam.

The researchers are confident that with the use of keyhole coherent diffractive imaging, many new applications in a wide range of scientific fields are possible. Promising advances, such as the accurate imaging of a single quantum dot or of a small virus, are likely because the size of the illumination spot in the sample plane adjusts easily with a quick modification to the sample’s defocus position.

— *William Arthur Atkins*

See: Brian Abbey[1], Keith A. Nugent[1], Garth J. Williams[1]*, Jesse N. Clark[2], Andrew G. Peele[2], Mark A. Pfeifer[2], Martin De Jonge[3], and Ian McNulty[3], “Keyhole coherent diffractive imaging,” Nat. Phys. **4**, 394 (May 2008). DOI: 10.1038/nphys896

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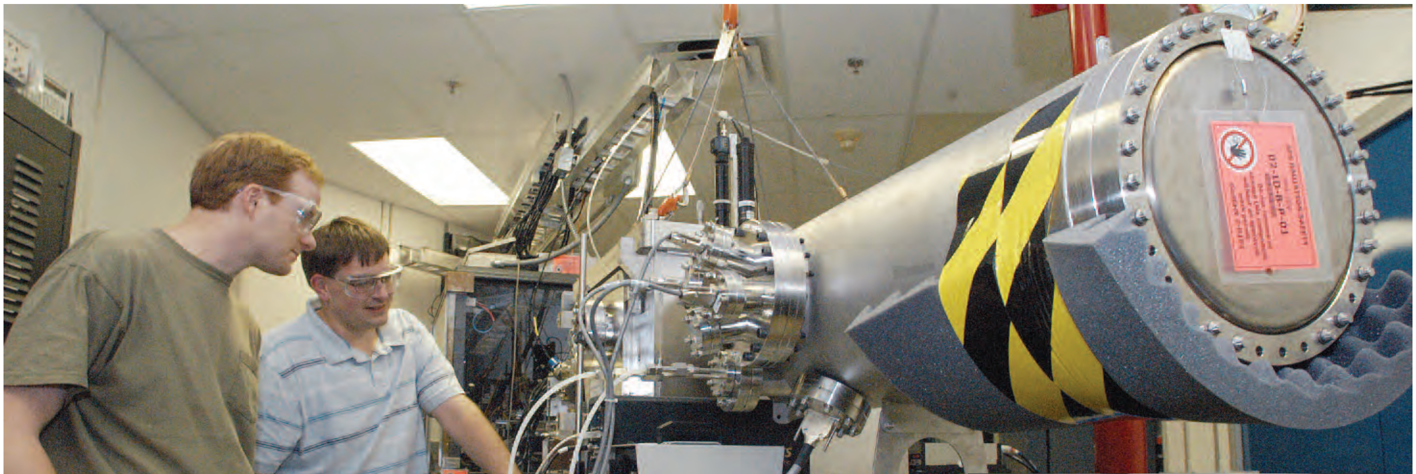
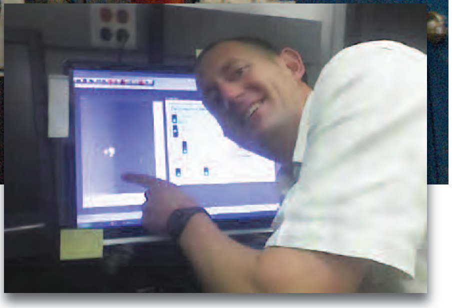
2-ID-B • XOR • Materials science , environmental science, physics • Coherent x-ray scattering (soft x-ray), microfluorescence (soft x-ray) • 5.5-cm undulator • Accepting general users

FRESNEL COHERENT DIFFRACTION IMAGING AT BEAMLINE 2-ID-B



Mark Pfeifer (left) of La Trobe University and Garth Williams of The University of Melbourne inspecting the coherent x-ray diffraction microscope.



Andrew Peele (La Trobe University) celebrates first light to the new x-ray diffraction microscope.

A new, three-dimensional coherent x-ray diffraction microscope, unique in the world, collected first light from the APS at 4:00 a.m. on Saturday, July 12, 2008. The event capped three months of installation and two days of commissioning at XOR beamline 2-ID-B by personnel from the La Trobe and Melbourne universities; Xradia, Inc. (the co-designer—with La Trobe—and manufacturer of the device); and the APS.

The new microscope is optimized for Fresnel coherent diffraction imaging and uses interferometric stabilization of the optics and sample down to 2 nm. Fresnel coherent diffraction imaging, which was developed by the major partners in this microscope, is a novel approach to coherent diffraction imaging in which the illuminating wavefront contains a spherical curvature. The method, based on an idea proposed by David Sayre and demonstrated experimentally by Miao and collaborators in 1999, was enhanced with the curved-wave approach by Nugent and collaborators in 2003. The technique and microscope are now available to APS users.

Fresnel coherent diffraction imaging provides reliable and unambiguous image reconstruction; an established spatial resolution better than 20 nm, with expected sub-5-nm resolution; a dose efficiency comparable to that of scanning x-ray microscopy (SXM); quantitative phase measurement; the ability to image any region within a sample with no need for exotic sample preparation; and an experimental configuration that is essentially identical to that of SXM. These are unique capabilities that combine the advantages of SXM for the study of "extended" specimens (samples that are not isolated in an otherwise empty field) and the high-resolution imaging capability of coherent diffraction imaging. The 2-nm precision and stability of the instrument is more than an order of magnitude higher than achieved in a coherent diffraction x-ray microscope. Given the sensitivity of coherent diffraction methods to structural detail at size scales beyond that accessible with x-ray lenses, it is anticipated that the exceptional stability of the new instrument will enable it to deliver images of nanomaterials and biological specimens with dramatically improved quality.

The ability to study extended samples opens the door to study many types of real-world samples such as magnetic films, biological tissues, intracellular structures, buried domains in ordered nanomaterials, and multicomponent organic electronic devices. *Contact Keith A. Nugent (Uk.nugent@physics.unimelb.edu.au), Andrew G. Peele (a.peele@latrobe. edu.au), and their collaborators, including Leann Tilley (L.Tilley@latrobe. edu.au), Garth J. Williams (garthw@ unimelb.edu.au), Mark A. Pfeifer (m.pfeifer@latrobe. edu.au, Mau-Tsu Tang (autsu@nsrrc. org.tw), Ting-Kuo Lee (tklee@phys. sinica.edu.tw), Ian McNulty (mcnulty@ aps.anl.gov), and Qun Shen (qshen@ bnl.gov)*

Development and fabrication of the microscope was funded by the Australian Research Council Centre of Excellence for Coherent X-ray Science. Use of the Advanced Photon Sourc is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

LIGHTING UP THE LINAC COHERENT LIGHT SOURCE

It was the shot that resonated around the accelerator world. On Saturday, December 13, 2008, a bunch (or "shot") of electrons was monitored, steered, guided, and accelerated by Argonne designed and produced technology as it traversed the 440-ft length of the U.S. Department of Energy's Linac Coherent Light Source (LCLS) free-electron laser at the SLAC National Accelerator Laboratory.

As related by John Galayda, Project Director for the LCLS, "A single, low-charge bunch of 13.6-GeV electrons was injected into the LCLS undulator system. The beam got 1/4 of the way along the undulator line. Upstream radio-frequency beam position monitors responded, giving enough information to make a steering correction upstream of the undulator. A second bunch of electrons was injected, and it passed through the entire channel to the beam dump. A million things had to be done perfectly in order to get to this point."

Keeping track of the "million things" being done for LCLS at Argonne fell to Geoff Pile of the Accelerator Systems Division (ASD). Pile's achievement was recognized with a special award from Argonne Director Robert Rosner and Murray Gibson, Argonne Associate Laboratory Director for Photon Sciences and Director of the APS. "The approach we took was that we had to deliver," said Pile, "just like any manufacturing company. I worked with three talented technical leads: Josh Stein (APS Engineering Support Division [AES]) for the undulator control system; Marion White (ASD) for undulators, magnets, and support and motion systems; and Dean Walters (Argonne Nuclear Engineering Division) for vacuum and diagnostics; and of course our colleagues at SLAC, as well as private industry."

Argonne's work on the LCLS undulator system began in 1999 under the guidance of Efim Gluskin, ASD Director. Steve Milton, then with ASD, served as LCLS undulator systems project director for the Argonne work until he took a new position with the Fermi project at Ellettra Sincrotrone. At that point, Pile stepped in.

"The LCLS could not have gotten here without the innovation and care that the Argonne LCLS team contributed to the effort," said Galayda.

^ Murray Gibson (l.) and Steven Richardson, Argonne Deputy Director for Operations/ Chief Operating Officer (r.) present a special award to Geoff Pile for managing the Argonne LCLS effort.

> One of the LCLS controls racks, crated, loaded, and given a send-off by the Argonne team that saw the project through: (l. to r.) Richard Voogd (Technical Services Division), Reggie Gilmore (AES), Peter Fuesz, Ray Davis, Eric Norum (all AES), Stan Pasky (ASD), Sharon Farrell, Josh Stein, Steve Shoaf, Rich Diverio, and Bob Laird (all AES).

^ The final five LCLS vacuum chambers, surrounded by (l. to r.) Pat Den Hartog, Emil Trakhtenberg, Loretta Cokeley (all AES), Efim Gluskin (ASD), Keith Knight (AES), Bill Ruzicka (Director, AES), Russ Otto, Kevin Knoerzer, Mark Martens, Mark Erdmann, Joe Gagliano, Tom Barz, Wayne Michalek, Horst Friedsam, Soon Hong Lee, Paul Aguirre, Aaron Lopez, Daniela Capatina, Kris Mietsner, Greg Wiemerslage, Dan Nocher, Mike Bosek (all AES), and Murray Gibson.

^ L. to r.: Joseph Xu (AES), Marion White, Isaac Vasserman, Emil Trakhtenberg, Robert Lill, and Efim Gluskin (all ASD) in the Long-Term Test Facility (LCLS undualtor, girder, and component mockup) in the APS experiment hall.

R&D PROGRESS ON AN X-RAY FREE-ELECTRON LASER OSCILLATOR

The recently proposed x-ray free-electron laser oscillator (XFELO) [1] is based on an ultra-low-emittance electron beam and a low-loss x-ray cavity using high-reflectivity crystal mirrors [2]. This novel x-ray source is expected to open unprecedented scientific opportunities due to its unique characteristics: peak brightness similar to, and average brightness much higher than, the self-amplified spontaneous emission (SASE) from high-gain FEL sources, and extremely narrow bandwidth. The low XFELO pulse intensity should avoid the violent sample disintegration possible in the case of the intense SASE pulses. Table 1 summarizes XFELO performance compared to that of SASE. An XFELO is recognized as a serious contender for use as a future light source in the recent white paper prepared by Argonne, Brookhaven National Laboratory, Lawrence Berkeley National Laboratory (LBNL), and the SLAC National Accelerator Laboratory [3]. An XFELO would be a strong candidate for the APS upgrade. A feasibility study for an XFELO, funded by Argonne, was carried out in 2008.

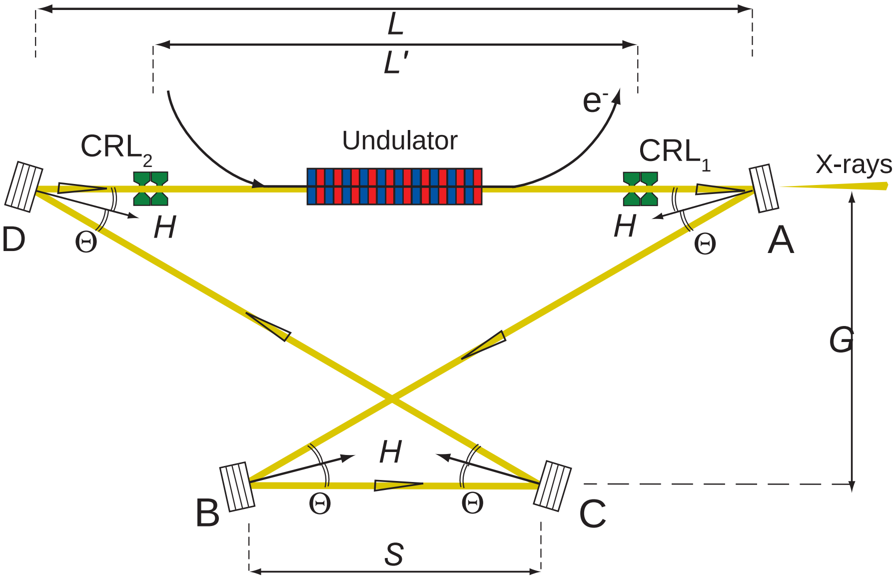


Fig.1. Schematic of a four-crystal x-ray optical cavity allowing a broad range of energy tuning.

A basic limitation of the x-ray cavity scheme in the original proposal [1] was the fact that the photon energy was not tunable. A new scheme making use of four Bragg crystals was developed, as illustrated in Fig. 1. The crystal orientation is such that the Bragg condition for a given wavelength is satisfied for each crystal [4]. With this scheme, a broad range of tuning can be achieved by a coordinated change of the distance G and S, and the crystal orientation. Another significant advantage of the scheme is the fact that the choice of crystal can now be made independent of wavelength consideration, so that diamond crystals with the highest reflectivity and optimum thermomechanical properties can be employed.

An analytical and numerical understanding of the FEL mode growth from initial noise and mode competition at saturation was developed [5]. The simulation of XFELO beam dynamics, taking into account the crystal responses, was made more efficient by modifying the GINGER code developed at LBNL [6]. The code was used to perform an extensive parameter study of an XFELO [7].

The x-ray cavity for an XFELO should have focusing elements for controlling the transverse mode profile. In Fig. 1, the focusing elements are indicated to be paraboloidal compound refractive lenses (CRLs). However, the polycrystalline CRLs currently employed at synchrotron radiation facilities are not suitable for an XFELO, because small-angle scattering from the boundaries of the Be microcrystals results in significant losses in reflectivity. Another option using grazing-incidence ellipsoidal mirrors as focusing elements is being studied, taking into account the mirror surface roughness [8]. The effect of the peak and average thermal loading on the reflectivity of the diamond crystals is also being studied.

Table 1. X-ray performance of XFELO and SASE sources. The spectral brightness is in the usual units: number of photons per second per (mm-mrad)^2 per 0.1% BW.

	SASE	XFELO
Wavelength	1.5 Å	1 Å
Electron energy	15 GeV	7 GeV
No. of photons/pulse	10^{12}	10^{9}
Pulse length (FWHM)	160 fs	2.5 ps
Bandwidth	0.3×10^{-3}	0.7×10^{-7}
Temporal coherence	Partially coherent (5.1×10^{-3})	Fully coherent
Intensity fluctuation	7% (classical)	~3×10^{-5} (quantum)
Transverse coherence	Fully coherent	Fully coherent
Rep rate	120 Hz	1 MHz
Peak spectral brightness	1.5×10^{33}	2.5×10^{33}
Average spectral brightness	3.0×10^{22}	6.0×10^{27}

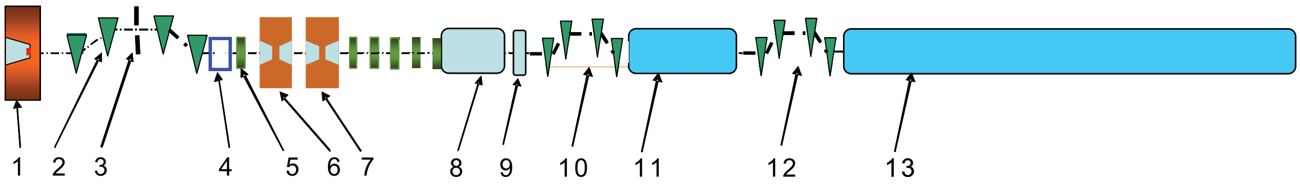


Fig. 2. General layout of the linac for an XFELO. 1: Rf cavity with thermionic cathode, 100 MHz, 1 MV. 2: Chicane and slits (3 total) as an energy filter. 4: Quadrupole triplet. 5: Focusing solenoid. 6: Monochromator of the beam energy f = 600 MHz. 7: Buncher, f = 300 MHz. 8: Booster linac section, f = 400 MHz. 9: Rf cosine-chopper to form rep rate of 1 MHz to 100 MHz. 10: Bunch compressor – I. 11: SC linac section, 460 MeV, f = 1300 MHz. 12: Bunch compressor – II. 13: Initial section of the SC linac, f = 1300 MHz.

Components of the x-ray optical cavity must be kept aligned to within very tight tolerances for stable operation of an XFELO. However, various destabilizing factors can occur, such as variations in the heat load and mechanical instabilities. A suitable feedback should be developed such that the Bragg angles of diffracting crystals are automatically adjusted to compensate for instabilities and maximize the XFELO output. The most promising scheme appears to be the null-detection technique, in which the Bragg angle is modulated and the resulting periodic variations in the output x-ray intensity is detected via a lock-in amplifier. The technique is routinely employed at the Laser Interferometer Gravitational Wave Observatory project [9]. We have implemented and tested a null-detection hardware feedback in the high-energy resolution beamline at the XOR/IXS 30-ID beamline at the APS [10]. The test was successful; the output intensity of the double-crystal monochromator was quickly adjusted to its maximum as the heat load on the crystal was changed. The setup was capable of stabilizing the crystal orientations to 50 nrad. This is an encouraging first step toward achieving the angular stability of about 10 nrad required for XFELO application [11].

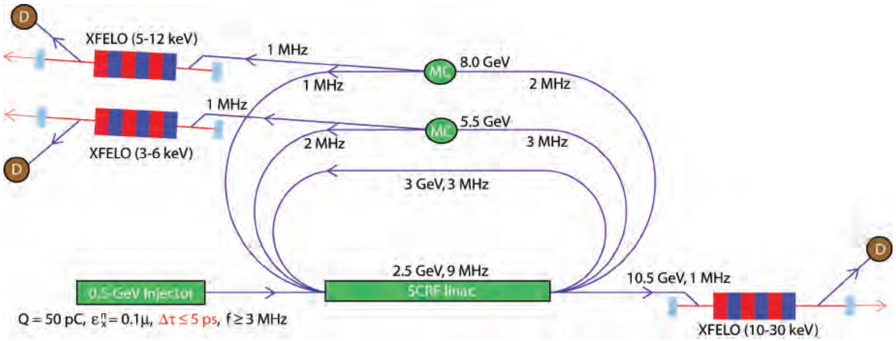


Fig. 3. A possible layout for an XFELO-based future light source facility. Three XFELOs are shown for clarity. However, many more FELs (up to two dozen) can be accommodated.

The injector is a critical element in the accelerator complex for XFELOs. A concept for an ultra-low-emittance injector, shown schematically in Fig. 2, is under study. The injector is based on a thermionic cathode in a 1-MV, 100-MHz, room-temperature cavity. The beam then passes through a chicane and slits to form a short ~0.5-nsec bunch; a buncher to form low longitudinal emittance of the bunched beam; an accelerating section to ~20 MeV using higher harmonic cavities; and a radio-frequency (rf) cosine-wave chopper to form any required bunch repetition rate between 1 MHz and 100 MHz. The results of initial optimizations of the beam dynamics are very promising [12].

The beam from the injector can be accelerated to the high energy necessary for XFELO operation by a superconducting (SC) linac. To save cost and space, recirculating loops can be introduced. An example layout is shown in Fig. 3, in which 0.5-GeV beam from the injector is accelerated by a 2.5-GeV superconducting linac with three recirculation paths to a final energy of 10.5 GeV. Three XFELOs are shown in Fig. 3. However, a larger number of XFELOs, probably up to two dozen, can be accommodated. A design of the recirculation arcs based on a theoretical minimum emittance lattice has been developed, showing that the small emittances and momentum spread that are needed for XFELO operation can be preserved by employing an optics module that exchanges the emittances between the horizontal and vertical planes [13]. *Contact Kwang-Je Kim (kwangje@aps.anl.gov)*

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APS LIGHT SOURCE OPERATIONS, CY 2008

In 2008, the APS operated with exceptional reliability and availability, continuing the stellar performance of the previous years. No changes were made in fill patterns in '08, and the APS operated in its three standard patterns (in order of most time spent using the fill pattern): 24 singlets, 324 singlets, and hybrid fill. The APS storage ring was operated using the standard and reduced horizontal beamsize (RHB) lattices.

Table 1. Availability statistics for CY 2007 (totals) and CY 2008 (by run).

	CY2007	CY2008			
	Totals	Run 08-1	Run 08-2	Run 08-3	Totals
Scheduled hours (h)	4840	1727	1284	1649	4660
Available for users (h)	4770.6	1622	1244	1605	4521
Beam availability (%)	98.57	96.8	96.9	97.4	95.9
Total downtime (h)	69.4	50	40	44	134
Number of faults	47	13	21	18	52
Mean time between faults (h)	101.5	128.6	59.2	97.4	86.0
Mean time to recovery (h)	1.48	4.2	1.9	2.4	2.9
Injector availability (%)	98.7	95.8	95.6	99.0	96.9

BEAM AVAILABILITY & MTBF

In calendar year (CY) 2008, the APS scheduled 4660 h for user operations and delivered 4521 h, for an x-ray availability of 95.9% for the year, slightly lower than CY 2007. The mean time between faults (MTBF) was 86 h, 10% lower than CY 2007. Injector availability remained high at 96.9%, providing reliable beam for top-up. Table 1 shows detailed statistics for CY 2008.

The APS is continuing a period of mature, stable operation characterized by unparalleled reliability. Indeed, the last run of 2008 was the 16th consecutive run for which the MTBF exceeded 48 h. The lowest MTBF during that 13-run period was 55.9 h, which is already very good.

FILL PATTERNS

The APS ring has the flexibility to support different fill patterns and lattices to serve special needs. The fill patterns used in CY 2008 were the same as those used in CY 2007. The standard average beam current for all operating modes is 100 mA.

- 24 uniformly-spaced bunches in top-up mode, used 56% of the time. This is the most common fill pattern, also called 24 singlets, and features 24 equally-populated bunches separated by 154 ns. The bunch length is 40 ps rms. This bunch pattern is a good compromise between the needs of timing users, who benefit from the bunch separation, and flux-hungry users, who require 100 mA but do not have requirements for the bunch distribution. Bunch purity is kept to a level of a few parts in 10^7. Top-up at a 2-min interval is needed for this pattern due to the relatively short beam lifetime (about 7 h).

- 324 uniformly spaced bunches in non-top-up mode, used 22% of the time. Non-top-up operation, whereby the storage ring is refilled to 100 mA twice every 24 h, is mainly used to allow for injector maintenance and improvement, operator training, and injector beam time for parasitic injector study. The beam lifetime in the 324-bunch mode is about 65 h, such that the beam decays to about 85 mA after 12 h. With smaller bunch currents compared with 24 singlets, the bunch length in the 324-bunch mode is 25 ps rms.

- 1 + 8 × 7 hybrid pattern in top-up mode with 16 mA in the isolated bunch, used 15% of the time. In this pattern, a single 16-mA bunch is injected on one side of the ring. The remaining 84 mA of stored beam current resides in eight groups of seven bunches on the other side of the ring. This arrangement results in symmetrical, beam-free regions with a duration of 1.59 μsec on either side of the intense bunch. The bunch length of the 16-mA bunch is 65 ps rms and that of the remaining bunches is 32 ps rms. Top-up is essential for the hybrid pattern. Because of the shorter lifetime of the intense bunch, the top-up interval is 1 min when using this pattern. Roughly three out of four top-up injections go toward maintaining the current in the intense bunch.

THE RHB LATTICE

The standard symmetric low-emittance lattice introduced in CY 2003 was utilized for almost all user operations during CY 2008. In 2006, for the first time, the APS delivered beam to users in the RHB (non-symmetric) lattice where the rms horizontal beam size at beamline 32-ID is reduced from 280 μm to 120 μm. In 2008, the APS had one- or two-week periods using this lattice in each run, amounting to 15% of the total time. The same amount of operation with this lattice is planned for CY 2008.

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APS Storage Ring Monopulse Beam Position Monitor System Upgrade

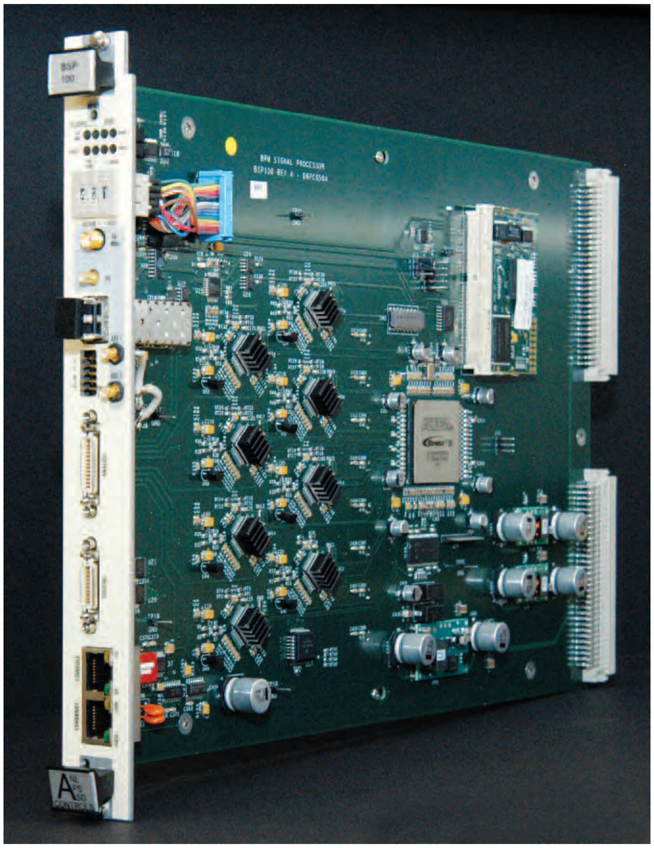

Fig. 1. The new BPM signal processor (BSP100) data acquisition board.

The APS storage ring employs two different types of electron beam position monitor (BPM) systems to measure and control beam motion. A broadband (10-MHz) monopulse radio frequency (rf) BPM system and a narrowband BPM (300-Hz) system. The two electron BPM systems complement each other, providing AC and DC data to correct the beam orbit around the storage ring.

The broadband system was designed in the early 1990s and as such is limited to 12-bit data acquisition collected at the 271-kHz storage ring revolution frequency. In addition, spare parts for some of the old system components are in short supply.

The broadband rf BPM system upgrade completely streamlines the data flow though the data acquisition system. The raw data from four receivers are sent directly into a new data acquisition VXI card. This change involved completely rethinking the system architecture to process BPM data more efficiently and accurately, resulting in a dramatic reduction in the noise floor for AC orbit correction.

The upgrade repartitions the existing system hardware such that the rf front end connected to the in-tunnel, button-style pickup electrodes remains unaltered, while the data acquisition system is replaced. This approach repackages the high-frequency monopulse receiver into its own designated chassis. For this purpose, a customized 8-slot EMI chassis houses the monopulse receivers, preserving much of this very expensive rf hardware. Within this chassis, the monopulse receivers are mounted on individual aluminum carriers that act as a heat sink as well as a guide for sliding the module into the chassis. On the reverse side of each aluminum carrier is an interface circuit board that provides power-supply filtering and regulation for the receiver. In addition, it provides drive circuitry for buffering the video bandwidth signals to be sent from the receivers to the data acquisition block; buffers digital control signals to the receiver; and provides a self-test capability to enhance reliability.

The data acquisition block, otherwise known as the BSP100 BPM Signal Processor and shown in Fig. 1, contains eight 14-bit analog-to-digital converters, an embedded Experimental Physics and Industrial Control System input/output controller (IOC), and a single Altera Stratix® II field-programmable gate array. A single VXI board performs data acquisition for up to four BPMs. The slow 12-bit data digitizers have been replaced by analog-to-digital converters (ADCs) running at a beam-synchronized frequency of 88 MS/sec, one quarter of the rf frequency.

Prototype testing conducted in storage ring Sector 38 has demonstrated the upgrade's performance. With the 24-bunch fill pattern, measurements indicate ~150 nm of rms instrumentation noise in the 1-Hz to 200-Hz band. This result shows the significant noise reduction provided by averaging additional data samples and using higher resolution ADCs. The noise floor is expected to drop further when applied to the more sensitive pickup electrodes mounted on the small-aperture insertion device vacuum chambers. The upgrade also allows users to observe small beam motions over a large range of time scales with the ability to trigger on injection, on beam dump, or on demand. This provides a very powerful diagnostic tool for post-mortem analysis and accelerator physics research.

The upgrade was divided into a three-phase program. During the first phase, two channels of the data acquisition system were prototyped by using development kits proving the design concept. The second phase involved instrumenting Sector 38 with first-article VXI boards, which were installed in December 2008 and commissioned in run 2009-01. The last phase of this project will be full deployment, thus instrumenting the remaining sectors as funding becomes available.

Coupled with other efforts to improve beam stability in the areas of photon beam position monitoring and real-time feedback system infrastructure enhancement, the APS is well on its way to achieving 100-nrad-scale pointing stability.

Contact Robert Lill (blill@aps.anl.gov)

UPGRADING APS STORAGE RING MAGNET POWER SUPPLIES

NOTE: This is an expanded version of the article "Upgrading APS Storage Ring Magnet Power Supplies" that appears in the printed version of APS Science 2008.

A storage ring DC-to-DC converter.

The power supplies for the magnets in the APS accelerators were designed and constructed or procured in the early 1990's. In the last 7 years the power supplies have performed remarkably well, consistently achieving availability better than 99.2% and mean-time-between-failure, or MTBF, greater than 240 h (Fig. 1). Recently, however, there have been signs of aging. Some components are obsolete and some are approaching the end of their lifetime. To maintain a high level of reliability and availability, the power supplies need to be upgraded or replaced. An upgrade or replacement also provides an opportunity to utilize the latest technology to further improve performance.

The majority of the more than 1400 power supplies in the storage ring are switching-mode dc-to-dc converters. The key component in the converter's power section is a semiconductor switching device called an insulated-gate-bipolar transistor, or IGBT. While there have been improvements in IGBTs in the last decade, the technology used in the storage ring dc-to-dc converters is still up to date. The components are widely used in industry and will continue to be available in the foreseeable future. Therefore, the power section, including the chassis and mechanical hardware, will stay unchanged, saving an estimated $6.7M for materials.

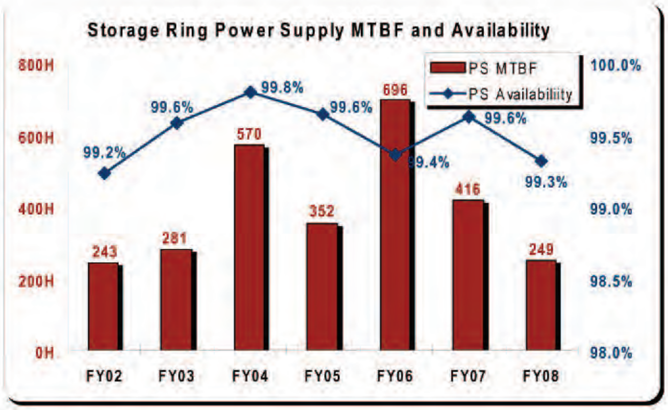

Fig. 1. Storage ring power supply operation reliability.

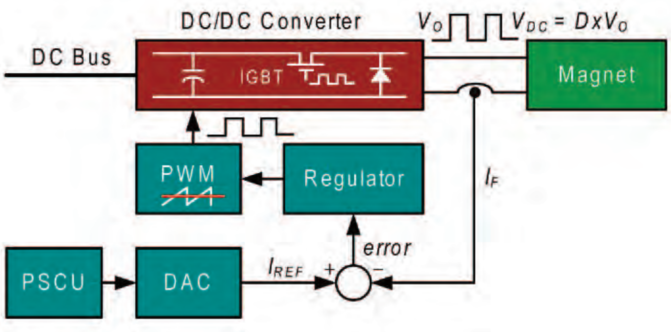

Fig. 2. Function diagram of a dc-to-dc converter.

The situation is different, however for the converters' control and communication electronics. Several major components are obsolete and the spare parts will be exhausted in the next few years. The power supply control and communications hardware has a very small capacity, prohibiting performance improvements. The upgrade proposes to use digital control technology to replace the converters' electronics. Digital converters have the advantage of fewer parts and, therefore, better reliability. They have great flexibility for optimal control and future firmware upgrade. They can also provide more functions for diagnostics and post mortem analysis. The new digital converters will have embedded high speed communication modules and thus eliminate the need for external power supply control units.

In a switching-mode power supply, a power transistor is switched between "on" and "off" with a duty cycle proportional to the desired output voltage. This control method is called pulse width modulation (PWM). Figure 2 shows the function diagram of a typical unipolar dc-to-dc converter with traditional analog control circuits. The upgrade will implement the control loop and the PWM generation with a field-programmable gate array or FPGA. Figure 3 shows the function diagram of the digital dc-to-dc converter

Figure 4 shows the present communication configuration for power supplies in a double sector. The power supply control unit, or PSCU, receives set points and commands for eight

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ESAFs for Safety's Sake

NOTE: This is an expanded version of the article "ESAFs for Safety's Sake" that appears in the printed version of APS Science 2008*.*

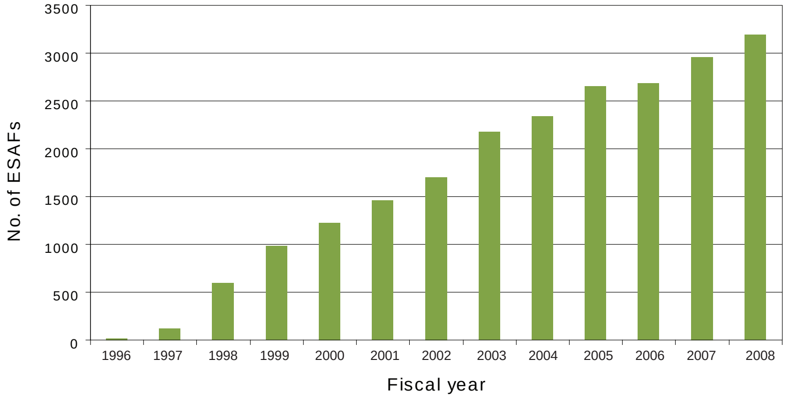
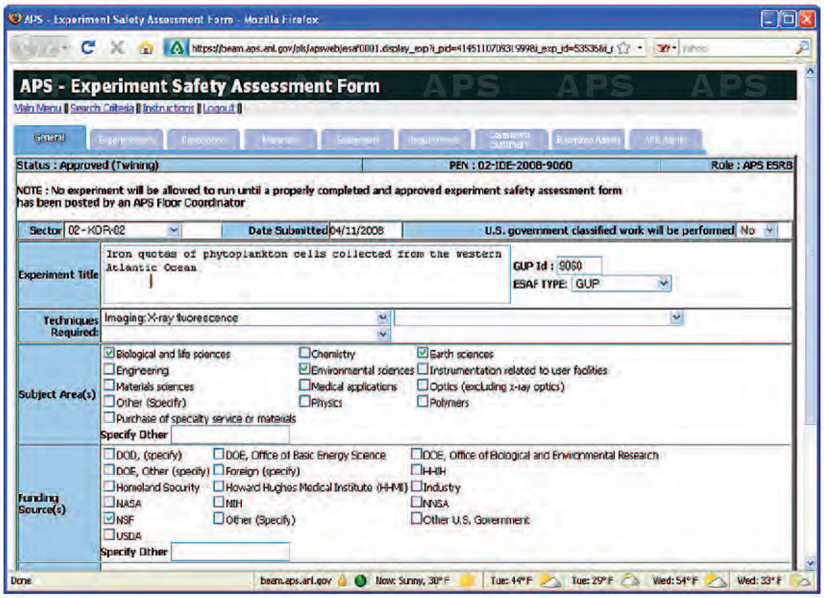


Fig. 1. Increase of ESAFs at the APS over time.



Status : Approved (Twining)

PEN : 02-IDE-2008-9060

Role : APS ESRB

NOTE : No experiment will be allowed to run until a properly completed and approved experiment safety assessment form has been posted by an APS Floor Coordinator

Sector: 02-XOR-02

Date Submitted: 04/11/2008

U.S. government classified work will be performed: No

Experiment Title: Iron quotas of phytoplankton cells collected from the western Atlantic Ocean

GUP Id : 9060

ESAF TYPE: GUP

Techniques Required: Imaging:X-ray fluorescence

Subject Area(s):
☑ Biological and life sciences
☐ Engineering
☐ Materials sciences
☐ Other (Specify)
☐ Purchase of specialty service or materials
☐ Chemistry
☑ Environmental sciences
☐ Medical applications
☐ Physics
☑ Earth sciences
☐ Instrumentation related to user facilities
☐ Optics (excluding x-ray optics)
☐ Polymers
Specify Other

Funding Source(s):
☐ DOD, (specify)
☐ DOE, Other (specify)
☐ Homeland Security
☐ NASA
☑ NSF
☐ USDA
☐ DOE, Office of Basic Energy Science
☐ Foreign (specify)
☐ Howard Hughes Medical Institute (HHMI)
☐ NIH
☐ Other (Specify)
☐ DOE, Office of Biological and Environmental Research
☐ HHIH
☐ Industry
☐ NNSA
☐ Other U.S. Government
Specify Other

Fig. 2. A typical ESAF data-entry screen.

The APS has had user experiment operations since 1996 when 17 experiments were completed, followed by 120 in 1997 (Fig. 1). Since before the start of user operations, APS management recognized that proper safety reviews of experiments were a necessity and a requirement. Chapter 21.2 of the Argonne Environment, Safety, and Health (ES&H) manual spelled out the requirements for experiment safety reviews. The APS adopted the policy that individual experiments would be reviewed as there would be different groups of experimenters from a multitude of institutions present at various times and blanket reviews could not be used. In compliance with ES&H chapter 21.2 and the principles of Integrated Safety Management, the APS implemented an experiment safety approval form (ESAF) for gathering information about the location of each experiment, a description of the work to be done, the users that would be present, the materials and equipment to be used, the hazards associated with them (toxic, biohazard, flammable, radioactive, other and equipment hazards) and the processes of the experiment, and waste disposal.

The early ESAF was a paper form that was submitted to beamline personnel for approval. This form included sections for beamline review comments and approval; verification of controls, training, and safeguards; and authorization to begin the work. The ESAF implemented the idea of safety envelopes to assist the users and beamline personnel in classifying experiments according to the type of hazards that would be encountered.

The ESAF system has been evolving since this beginning and was converted to a Web-based form in 1998, using Oracle as the engine behind the form. The form duplicated the paper version that was in use but allowed easier accessibility to the information by users, beamline personnel, and the APS. This required setting up an administration level for the ESAF. Access to a particular ESAF was based on the sector where the experiment would take place. Beamline personnel were only required to review ESAFs that would run at their secto,r and users could only access ESAFs that contained their badge number. The Web ESAF also generated a report on the experiment that looked like the original paper ESAF and could be used for posting at the end of the beamline. The material hazards and equipment lists were expanded to cover the types of experiments that were being proposed to aid the CATs in their reviews.

By 2003 the number of user experiments being performed at the APS was over 2000 per year. The number of updates to the system was exceeding the capability of the coding. The ESAF was rewritten using updated programming technology that would allow an easier application of a graded approach to identifying the hazards of an experiment. The single page was replaced with a series of tabs for gathering information and allowed the displaying of the pages to be completed based on hazard triggers built in to the system (Fig. 2). This was the beginning of the Experiment Safety Assessment System. The tab system allowed for not only increased efficiency in han-

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dling hazard inputs but greatly increased the ease with which the system could be modified and expanded to handle new requirements. The system continued to be an Oracle-based Web application. The implementation team received a Pacesetter Award and the Argonne Director’s Award for the update.

One of the key upgrades in the new system was the direct incorporation of the hazard classes into the ESAF form. The APS safety envelopes were updated and became the APS Experiment Hazard Classes (EHC). The EHCs contain requirements for Engineered and Procedural Controls; Design Reviews and Equipment Inspections; Personal Protective Equipment (PPE); Signs and Labeling; Dosimetry and Monitoring; and Safety Training. These requirements are drawn from the Argonne ES&H manual and other Federal requirements. The incorporation of the EHCs into the ESAF allows for a series of triggers based on user input to control the flow and content of the finished ESAF.

The information in the original ESAF is divided among a series of tabs—General, Experimenters, Description, Materials, Equipment, Requirements, Comment Summary, Beamline Administration, and APS Administration—as the basis for an ESAF. Additional tabs that may be triggered during the completion of the ESAF cover Human Materials, Radioactive Samples, Lab Use, and Electrical Inspection. Most of the administrative information is on the General tab. Information about the experimenters has its own page and includes contact and training information. A link is provided to gather user contact information for each user on the ESAF directly from the APS User Database. The training completion status for the APS core training of each user is loaded directly from TMS records and displayed on the page. In addition to core training, the status of Laser Safety, Radiation Worker 1, and Nanomaterials Awareness training is displayed via triggers from other pages of the ESAF. This allows the customization of training requirements for a given experiment. In order to make the completion of an ESAF easier the system is linked to the APS general user proposal (GUP) system for the creation of ESAFs. If a user has an active beam-time request (BTR) for a GUP, when an ESAF is created for that BTR the administrative information and list of users is copied from the GUP and inserted into the ESAF.

The Description, Materials, and Equipment pages allow the user to input information about the proposed experiment. This includes a description of the proposed work, materials/chemicals to be used and the hazards associated with them, and the equipment that will be used. The equipment page also allows the user to designate which equipment will be brought to the APS and which is existing APS beamline equipment. Files can be attached to the Description page for more detailed information about the experiment including standard operating procedures that will be used, MSDS information, pictures of equipment, proposed hazard mitigation plans, etc. The Description page is also used to define the location and starting/ending dates of the experiment.

The Materials page is used to gather hazard information about all samples/materials that are brought to and used at the APS for the experiment. The hazard categories for the materials include: toxic, biohazard, flammable, radioactive, carcinogen, corrosive, oxidizer, explosive, nanomaterials, and other along with columns for Disposal at ANL, Lab Use, and declaration of confidential samples. The Name column for the material contains a link to the APS policy for identifying samples, and the hazard column labels are links to definitions of the hazard types. This Materials tab is also used to ask if any of the following will be used or required at the APS: radioactive sealed sources; human tissue/materials/cell lines (Institutional Review Board process, triggers Human Material tab); regulated foreign or domestic soil (USDA permit requirements); live animals; or if beamline laboratory facilities will be used for experiment preparation (triggers Lab Use tab). The equipment choices cover low- and high-temperature work, pressure systems, lasers, electrical equipment, magnets, radio frequency and microwaves, and x-ray generators. There is an “Other” option for equipment not listed in the table. Several categories are subdivided to allow easier identification of equipment (e.g., lasers by class). The equipment choices on this tab are directly tied to the EHCs.

The user input to the form ends with these tabs. The remaining tabs are used for administrative function and review documentation. The Requirements tab is a summation of all of the EHCs activated from the information supplied by the user. It contains excerpts from the Argonne ES&H Manual for hazard control requirements tied to a particular EHC. The Beamline and APS Administration tabs are used for safety review comments and approval by either designated beamline ESAF approvers or an APS ESRB member. The approver’s name is captured from the badge number that is logged into the system.

The ESAF system is also used to generate an Experiment Hazard Control Plan (EHCP) and an Experiment Authorization Form (EA). The EHCP contains a summary of the on-line ESAF including Materials and Equipment Hazards, the Experiment Description, Lab Use Description, summary of the EHCs and Requirements tab, Beamline and APS review comments and hazard controls, a list of files attached to the ESAF, and the APS core training status of each of the on-site users. The EHCP is posted on the door of the x-ray station where the experiment is taking place in a safety pouch. It is available to all participants in the experiment.

The EA form constitutes the authorization to do work. The user designated as the on-site spokesperson signs the form affirming that the ESAF is complete and correct, that all materials/samples to be used are listed and the hazards have been identified, and that all users are listed on the ESAF. The form contains the approval date and approver name for both beamline personnel and the APS.

“ESAFs” continued on page 141

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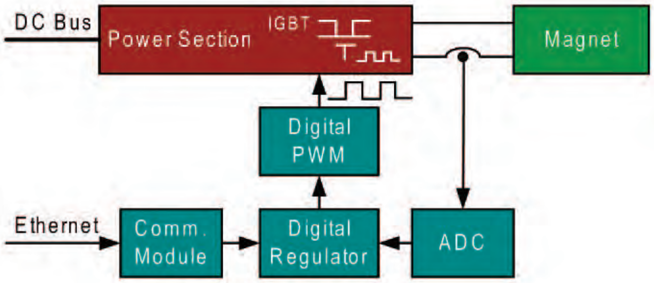

Fig. 3. Function diagram of a digital dc-to-dc converter.

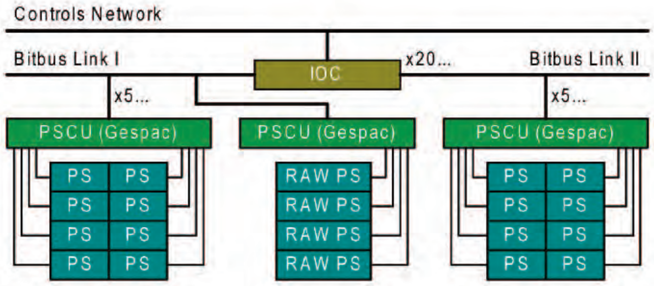

Fig. 4. Present communication configurations.

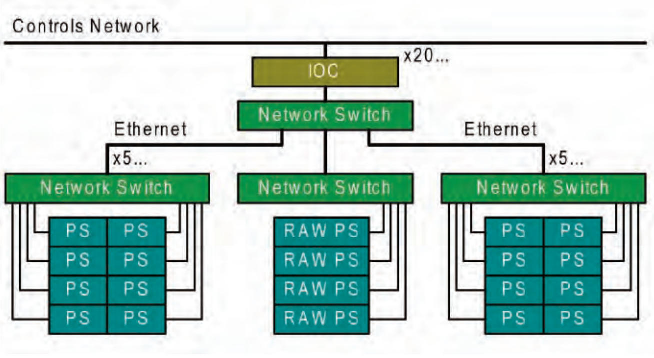

Fig. 5. Proposed communication configurations.

converters from an input-output controller (IOC). Monitored data also communicate back to the IOC through the PSCU. Because of the small processing capacity of the PSCU and the limited bandwidth (375 kBit/s) of the Bitbus link, the monitored points are limited to the basic conditions of the converters; remote or detailed diagnostics cannot be achieved.

The upgrade proposes to replace the PSCU and the Bitbus link with high-speed Ethernet and embedded communication modules. The elimination of the PSCUs and associated interface boards and ribbon connections increases the system’s reliability. The new design will implement diagnostics for detailed analysis such as waveform capture or post-mortem analysis. The new design will also provide an interface to accommodate the requirements from the real-time-feedback (RTFB) system for fast correctors. Figure 5 shows the proposed communication configuration (the interface to the RTFB system is not shown).

There are several challenges in designing digital converters. The proposed upgrade of the current resolution to 18-bit may require a PWM resolution of more than 18 bit. Combined with an IGBT switching frequency of 20 kHz, this resolution may result in a PWM generator clock frequency of more than 5.24 GHz. Alternative methods such as dither have to be used to reduce the clock frequency. Another challenge is to design an analog-to-digital converter with true 18-bit ac and dc performance. High-performance digital dc-to-dc converters have been in use in other synchrotron accelerator facilities such as Swiss Light Source and Diamond Light Source. However, the high power rating and the hard switching circuits in the APS storage ring converters present a big challenge in mitigating the strong electromagnetic interference. Presently, R&D and engineering of a prototype digital converter are under way. It may take up to two years to complete the prototyping and produce the production units. Deployment time in the storage ring, distributed over machine shutdowns, is estimated to be two years.

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A member of the beamline staff signs the form verifying that all required controls, training, and safeguards are in place to begin the experiment and all users are listed. In the case of a high-risk category experiment (e.g., radioactive sample, elevated Biosafety level, etc.) the APS will also have a member of the ESRB or other ESAF safety committee sign the safeguards verification.

When the ESAF is completed, has been reviewed and the safety plan has been approved, and all signatures are received, the on-duty APS floor coordinator posts the Experiment Authorization Form and Hazard Control Plan on the station door, the EA form in the beamline end cabinet, and enters the start date time in their shift log. The action of posting an ESAF causes the transfer of a copy of the record from the ESAF system to an Experiments database that is used to track which experiments were actually run at the APS.

The ESAF has been reviewed many times since its inception and has received very positive reports and feedback. In reviews by Argonne ESQ, The University of Chicago, and DOE ISM Reverification, the ESAF system was found to be a best-in-class experimental review and work approval process that clearly meets the requirements of 48 CFR 970.5223-1 and the intent of DOE P450.4.

The Web-based experiment process was found to be an efficient method for handling experiment safety reviews at a large user facility and is considered a particularly noteworthy practice.

The ESAF system will continue to evolve to meet the needs of user experiments and safety requirements. The system is currently handling over 3300 experiments per year.

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SAVING ENERGY FOR SCIENCE

The existing APS cooling towers on a winter's night.

NOTE: This is an expanded version of the article "Saving Energy for Science" that appears in the printed version of APS Science 2008.

The Advance Photon Source (APS) is a state of the art laboratory facility that continues to develop and grow to serve the scientific user community. Unique to the vision for design of the facility's infrastructure was the flexibility to accommodate multiple expansion and growth scenarios and the ability to easily undergo modifications and upgrades as building technology evolved. As with all ongoing facility expansion and development, costs are incurred that require funding for planning, engineering, and construction. The AES Site Operations group has been extremely active in identifying technological advancements in energy efficiency that would yield operating cost savings that could be used to finance these necessary infrastructure upgrades and enhancements. The goal is twofold; reduce energy usage and apply operating cost savings to finance infrastructure upgrades critical to the facility's scientific mission.

The first round of infrastructure enhancements occurred at the end of 2006 when the APS storage ring air handling system was upgraded and space temperature stability was dramatically improved. These performance enhancements were achieved by using waste heat extracted from the APS DI water cooling system to control tunnel air temperature. This work was performed under a DOE sanctioned "Energy Savings Performance Contract (ESPC)," where design and construction funding was provided from a third party contractor and repaid through energy savings resulting from the modifications. In 2007 the DOE launched the Transformational Energy Action Management (TEAM) Initiative, a Department-wide effort aimed at reducing energy usage across the nation-wide DOE complex by 30 percent. This program provided additional incentive and support from the DOE in the Laboratory's pursuit to reduce energy usage and apply the resulting cost savings to fund infrastructure upgrades necessary to further mission critical functions. Under the new performance contract (ESPC III), scheduled to begin implementation in February 2009, the APS has committed to multiple initiatives targeting system performance, waste heat utilization, and space lighting improvement. The resulting energy savings from these changes will achieve an estimated annual reduction in operation costs of $460,000 with a simple payback of approximately 7 years.

The APS generates large quantities of waste heat in the production of x rays. The majority of this heat, approximately 7.5 Mw, is removed via a deionized cooling (DI) water system. Heat rejection is primarily accomplished with mechanical refrigeration except during mild weather when evaporative cooling becomes effective. During winter months when outdoor air temperatures are extreme the existing cooling towers providing evaporative cooling experience excessive freezing making this process inoperative. This forces the APS to fall back on mechanical refrigeration which consumes over 6 times more energy than evaporative cooling. Under the ESPC III contract the APS will supplement the existing cooling tower with new tower cells specifically constructed to be easily defrosted, permitting winter evaporative cooling of the entire 7.5 Mw load. It is estimated that this will result in a reduction of approximately $180,000 per year in energy cost. These new tower cells will at the same time add to the APS summer peak cooling capacity thereby accommodating the increased summer cooling demands that have resulted from recent growth in the ANL 400 area.

New inroads will be made in utilizing both air and water borne waste heat for conditioning of outdoor make up air for the APS LOM and Experiment Hall buildings. The experiment hall requires a continuous flow of large quantities of outdoor air for both ventilation and beam line exhaust systems. The LOM's also have high outdoor air demands set by the need to ventilate their chemistry laboratories. The total inflow of outdoor air into these buildings exceeds 47,000 liters per sec (100,000 cu ft per min) and imposes a peak heating load of 2.5 Mw (8.64 x 106 Btu/hr). During extreme cold weather conditions a substantial portion of this heat is being supplied by the Argonne site wide heating plant. By implementing minor modifications to

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the existing air handling equipment waste heat from the APS can be more effectively utilized to provide nearly all this heating.

In the category of space lighting; new energy efficient fixtures will replace existing fixtures in buildings 411 and 412 and in the Experiment Hall service areas. In total, nearly 1600 fixtures will be replaced and upgraded. The new fixtures in buildings 411 and 412 will have integral presence sensors to automatically activate lighting when personnel enter defined areas within the buildings. This will allow all non emergency lighting in these buildings to remain off during a substantial portion of time. The light quality itself will be improved as the existing HID lighting will be replaced with high efficiency fluorescent fixtures using electronic ballasts. In the experiment hall, existing lighting in the service aisles (the areas underneath the mechanical mezzanine and behind the storage ring on infield side of the building) will be replaced with higher efficiency fixtures with electronic ballasts and will be controlled by time clocks to reduce illumination levels during night time hours.

The cost savings generated from the reduction in facility energy usage, will be leveraged to maintain and insure the integrity and of the APS infrastructure. Of main concern is the APS site wide computerized temperature control network that monitors and data logs all system status and performance parameters, and reports all systems alarms including those related to laboratory and fume life containment. This system has reached obsolescence and requires replacement. Operating cost savings realized under this project will make that possible.

Implementation of this project would not have been possible without the close cooperation and coordination between the Laboratory's FMS and AES divisions. With the implementation of this project Argonne will be able to reduce overall facility energy consumption while simultaneously providing essential infrastructure upgrades and improvements at no "direct" cost to the Laboratory.

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THE APS WATER SYSTEMS

Noble laureate Albert Szent-Gyorgyi said "water is life's matter and matrix, mother and medium. There is no life without water" and the same can be said of X rays at the Advanced Photon Source (APS). Water is the medium which transport's all the heat generated in the production of X Rays, it cools and heats the spaces we work in and maintains the stable temperatures demanded by our experiments. One can even say without water the electricity that powers the APS would not exist. Water at APS is utilized in all states, as a vapor steam is used to heat our facility, as a liquid it is used for both heating and cooling and as a solid it is used as an ice heat sink for cooling. The water at APS also comes in multiple flavors; in a de-mineralized state it is used for cooling magnets, power supplies, and vacuum chambers. In its raw form water from the regions sanitary and ship canal is filtered and used as make up for evaporative cooling. In its treated form, water from Lake Michigan fills our heating and cooling systems. Potable water makes our coffee and tea, washes our hands and non-potable water is supplied to our laboratories for our experiments. Water fills the pipes above our heads to protect us in the event of fire.

Given the diverse needs and varying levels of water quality required, the APS operates 4 individual water systems all originating at the APS central plant distributed throughout the facility. These include tower water used for evaporative cooling, chilled water used for air conditioning and primary heat transfer from secondary sources, low temperature heating water used to heat the buildings, and deionized water used to cool accelerator equipment, storage ring components, and user beam line equipment. Within these categories are a number of sub systems dedicated to specific equipment such as the vacuum chamber cooling systems. Steam, potable, and non potable waters originate outside the APS and are supplied by the Laboratory. The operation and maintenance of these systems is a complex affair and is the result of a close cooperation between the AES Site Operations and Mechanical Operations and Maintenance groups and FMS building maintenance.

There is an interrelationship between all of the APS water systems involved in temperature control. Deionized water is used to remove heat from accelerator components and power supplies, from user beam line equipment, and from vacuum chambers. During warm weather this heat is transferred to the chilled water system where a refrigeration process is used to reject the heat to the out of door through evaporative cooling provided by the cooling towers. The low temperature heating water not only provides heat to the facility in the winter but operates in conjunction with the cooling systems to control space temperatures via air reheating during the entire year. Each system while controlled and operating independently is integrated into processes that maintain space and equipment temperature stability within the stringent limits set at the APS.

Since the APS generates waste heat continuously cooling systems operate at all times, making cooling the primary function of the water systems. Direct water cooling of accelerator equipment and beam line components is supplied by a network of interconnected deionized water cooling loops that represents one of the world's largest DI water distribution systems. With a primary flow rate of 30,000 liters/min (8000 gpm) it supplies one central distribution piping loop with nearly 3100 meters (10,000 feet) of piping that feeds numerous secondary distribution loops. These secondary loops consist of 36 temperature control magnet and power supply pumping stations, 20 vacuum chamber cooling skids, 5 Linac cooling skids, and 6 small gravity feed systems. Careful attention is paid to water temperature stability which has a direct impact on beam orbital stability and the alignment of critical accelerator and beam line components. Temperature stability of

"Water" continued on page 144

"Water" from page 143

the primary water loop is on the order of + 0.28 deg C (± 0.5 deg F). The secondary water subsystems provide either pressure boost or water isolation and trims the temperature control to maintain the required precise point of use temperature tolerance ranging from + 0.11 deg C (± 0.2 deg F) down to + 0.06 deg C (± 0.1 deg F).

All DI water system processes occur in the APS central plant where the heat is rejected, the water polished to remove ions, particulate, and biological contaminants. The water is also degasified to remove dissolved gases before being sent back to the secondary water systems.

The chilled water refrigeration plant carries the burden of all primary cooling at the APS including those spaces that require tight temperature control and the direct cooling of the DI water system during hot summer weather. This system consists of a network of primary, secondary, and tertiary distribution loops with miles of piping running to each building on site. The system at APS is supplemented with a 750,000 liter (200,000 gallon) ice water heat sink that is used to shift load from the refrigeration system during peak electric demand periods and to supplement system cooling for temperature stability and additional dehumidification on exceptionally humid days. Working in conjunction with the chilled and tower water system the DI water heat rejection can be shifted between mechanical refrigeration and evaporative cooling depending upon outdoor weather conditions. This allows the APS to minimize the energy expended in the heat rejection process. The APS heating plant distributes 220 deg F water throughout the APS site for both heating and reheating of air. This water is heated by steam delivered to the APS central plant from the Argonne steam system. This water is operated with an expanded supply to return water temperature differential to reduce the peak demand flow rates and as in the case of the chilled and DI water systems uses primary and secondary loops to vary temperature and pressure at the point of use.

Recent and ongoing adaptations to the DI water system include efforts to extract and reclaim the relatively "low grade" waste heat for general heating purposes and for temperature control reheat. This work began in with a successful prototype designed and constructed by the AES Site Operations group for the APS Linac tunnel. Once proven, the concept was adapted to the APS storage ring and most recently to Building 440 the new Center for Nanoscale Materials (CNM). These heat recovery processes demonstrate the efficacy of heat recovery for direct heat exchange without the need to utilize mechanical refrigeration heat pumps. It has been demonstrated that 35 percent or more of the heating demands can be met by this application.

The inherent interconnectivity of the individual water systems at APS was designed specifically to enable transfer of heat between systems. The APS Site Operations group has been successful at extending the envelope of system capabilities to convert the process from a simple heat extraction to a heat reclaim system. This has resulted in reduced operating costs that have been leveraged for the continuing upgrade and expansion of the APS facility infrastructure without additional cost burden. The ongoing expansion of our heat recovery capability will continue to be utilized not only to enhance the facility's energy efficiency but to provide a resource for maintaining its state of the art infrastructure capability into the foreseeable future.

Contact Marvin Kirshenbaum
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THE APS USER COMMUNITY IN 2008

During FY2008, the APS user community continued to grow, despite budget-induced limitations on facility operating hours. Four new beamlines (13-BM-C, 21-ID-F, 21-ID-G, and 26-ID) became operational during the year and began hosting general users. As a result, the overall number of hours available to APS users actually increased (from 261,294 h to 264,249 h). The number of unique on-site users dropped slightly (from 3412 in FY2007 to 3229 in FY2008). However, the increase in the number of off-site general users who sent samples for analysis and/or operated beamlines remotely, as well as the number of off-site general user co-proposers, caused the total number of users for the year to increase from 3552 in FY 2007 to 3608 in FY2008 (Fig. 1), as did total user visits (Fig. 2)—the 13th straight year that APS user numbers have increased. Although we have a core cadre of repeat users, Fig. 3 shows clearly that new users constitute a healthy percentage of our annual user numbers. Other user information is shown in figures 4-6.

Demand also continued to increase. During 2008, the total number of beam-time requests (BTRs) for general-user time increased to 2899 (from 2252 in 2007), with the oversubscription rate (number of BTRs submitted divided by the number allocated) rising to 189% in 2008 vs. 176% in 2007.

Beginning mid-year, users were given an opportunity to use their time on-site more efficiently by completing required core training courses prior to coming to the APS. A new Web-based application (www.aps.anl.gov/Safety_and_Training/Training/) now allows a registered user to review training materials, complete each core course, and/or take a stand-alone challenge exam from anywhere off site. Since this capability was instituted, more than 8562 core courses have been completed via this route.

Contact Susan Strasser
(strasser@aps.anl.gov)

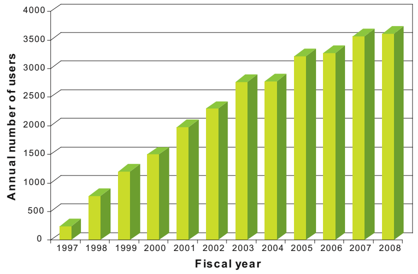


Fig. 1. User visits (unique) to the APS*.

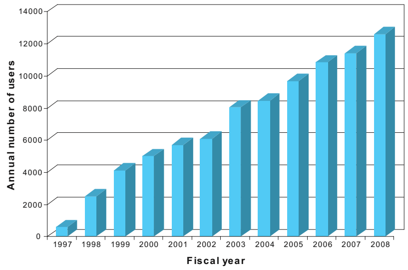


Fig. 2. Total APS user visits*.

*Includes users never at the APS but listed as co-proposers, mail-in, badged co-proposers, and remote/off-site

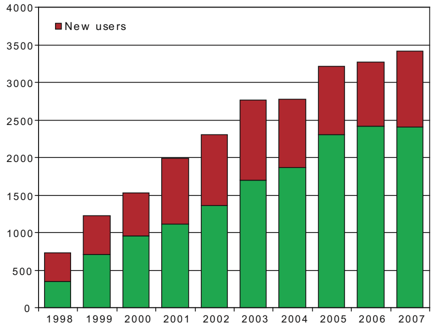
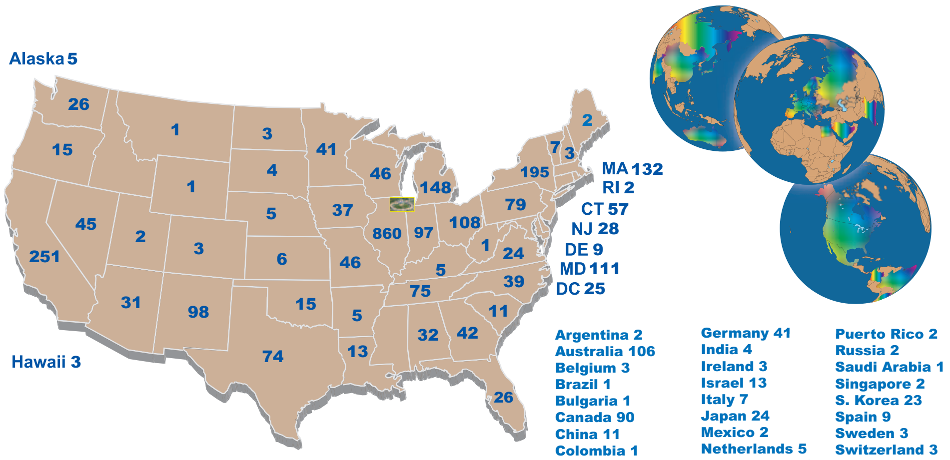


Fig. 3. New APS users by year.



Argentina	2
Australia	106
Belgium	3
Brazil	1
Bulgaria	1
Canada	90
China	11
Colombia	1
Czech Republic	1
Denmark	20
France	17
Germany	41
India	4
Ireland	3
Israel	13
Italy	7
Japan	24
Mexico	2
Netherlands	5
New Zealand	6
Portugal	1
Puerto Rico	2
Russia	2
Saudi Arabia	1
Singapore	2
S. Korea	23
Spain	9
Sweden	3
Switzerland	3
Taiwan	15
UK	35

Fig. 4. FY08 APS users by geographic distribution.

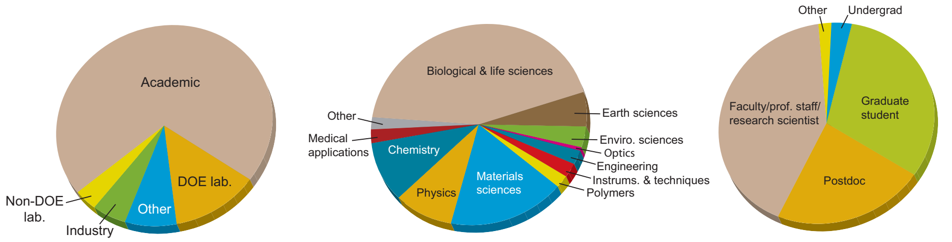


Fig. 5. FY08 APS user demographics.

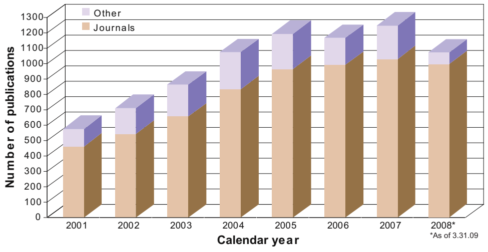


Fig. 6. APS publications

USER WEEK 2008

Left to right: Murray Gibson, Oleg Shpyrko, then-APSUO Chair Tim Graber, and incoming APSUO Chair Larry Lurio.

Outstanding science characterized all aspects of User Week 2008 (May 4-9) at Argonne National Laboratory. More than 650 individuals spent one or more days during the week attending plenary science sessions, workshops, poster sessions, vendor exhibits, and short courses all targeted to users of the Argonne APS, Center for Nanoscale Materials (CNM), and Electron Microscopy Center (EMC). Kicking off the week was the premier performance (a staged reading) of a new play, “Bernal's Picasso,” written by Celerino Abad-Zapatero, noted crystallographer and APS user. This play, which explores the relationship between science and art through imagined conversations with a variety of scientists and Pablo Picasso, was followed by a reception, during which users could interact with the actors, visit vendor exhibits, and relax before the scientifically invigorating week.

The early part of the week focused primarily on the APS. The opening session included reports from Pat Dehmer, then Deputy Director for Science Programs, U.S. Department of Energy (DOE), Office of Science, as well as updates from Argonne Associate Laboratory Director for Photon Sciences and APS Director Murray Gibson; Stephen Streiffer, newly appointed interim Director of the CNM; and EMC Director Dean Miller. Kicking off the APS portion of the day was a talk given by Dennis Mills (Photon Sciences Deputy Associate Director for X-ray Science) on the process to be used in formulating the APS Renewal (http://www.aps.anl.gov/Renewal/) strategy and plan. The afternoon session included excellent science presentations, which were followed by the presentation of the 2008 APS Users Organization Rosalind Franklin Young Investigator award to Oleg Shpryko (see sidebar). A lively poster session in one of the APS laboratory/office modules rounded out the day.

On Wednesday, the focus shifted to the CNM and EMC, highlighted by a talk on “Single Molecule Studies: From Quantum Dots to Proteins” from Nobel laureate Rudolph Marcus (California Institute of Technology). Science sessions for both the CNM and EMC, as well as a preview of the proposed Argonne Scattering, Imaging, and Spectroscopy Institute, were followed by a well-attended poster session in the lobby of the CNM building.

Workshops on Tuesday and Thursday, a meeting banquet at the Shedd Aquarium in Chicago, and short hands-on courses for CNM users completed the week. A full program and additional information can be found at www.aps.anl.gov/Users/Meeting/2008/.

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THE 2008 ROSALIND FRANKLIN YOUNG INVESTIGATOR AWARD TO OLEG G. SHPYRKO

The APS Users Organization (APSUO) named Oleg G. Shpyrko (University of California, San Diego) as the recipient of the 2008 Rosalind Franklin Young Investigator Award. The award recognizes an important technical or scientific accomplishment by a young investigator that depended on, or is beneficial to, the APS. Shpyrko received the award on May 5 at the 2008 Users Week at Argonne National Laboratory, where he also presented a talk on his work.

Shpyrko was cited for reaching a remarkably high level of achievement very early in his career. In particular, he was recognized for applying challenging surface and coherent x-ray scattering techniques to understanding the structure and dynamics of liquid-metal surfaces and quantum states in condensed matter systems. He was also recognized as a dedicated and enthusiastic teacher.

As a postdoctoral fellow at Argonne, Shpyrko studied domain wall fluctuations in antiferromagnets, technologically important materials used to tailor the properties of magnetic sensors used in hard-drive read heads. Shpyrko applied the newly developed x-ray photon correlation spectroscopy technique to observe fluctuations of domain walls for the first time. An important finding was a crossover from classical to quantum behavior at low temperatures, indicating that magnetic noise cannot be eliminated. The ability to observe domain wall fluctuation is important both for engineering tailored materials and for fundamental studies in condensed matter physics.

For his thesis work, Shpyrko resolved a long-standing controversy on whether or not atomic layering is unique to liquid metals.

Scenes from the User Week 2008 poster sessions.

< Jim Vicarro (left), ChemMatCARS Principal Investigator and Executive Director, The University of Chicago's Center for Advanced Radiation Sources; and Pedro Montano, Director, Scientific User Facilities Division, DOE Office of Basic Energy Sciences.

^ Murray Gibson (left); Ron Lutha, DOE Argonne Site Office Manager; and Pat Dehmer, DOE Deputy Director for Science Programs, Office of Science, confer prior to the start of the first user meeting session, where Gibson presented an update on the APS and Dehmer delivered the "DOE Perspective."

> Steven Richardson, Argonne Deputy Director for Operations/Chief Operating Officer, at Users Week 2008.

> Stephen Streiffer, Acting Director of the Argonne Center for Nanoscale Materials, gave a status report on the CNM.

> Dean Miller, Director of the Argonne Electron Microscopy Center, brought attendees up-to-date on the EMC.

> Eric Rohlfing, DOE Associate Director of Science for Basic Energy Sciences (Acting), and Director of the Chemical Sciences, Geosciences, and Biosciences Division, gave an "Update from Washington."

MEETINGS, WORKSHOPS, SEMINARS, ETC.

Short-Pulse X-rays at the APS • May 9, 2008 • The goal of this workshop was to identify the many untapped areas for research and novel applications that would be enabled by the realization of an Argonne short-pulse x-ray source. Attendees brainstormed on future science that will become possible with the unique capabilities afforded by the APS short-pulse CW source, enabling leading-edge research in AMO, chemistry, condensed matter physics, materials science, and engineering. They formulated a comprehensive path leading to a proposal requesting funds to implement a short-pulse x-ray source at the APS, to instrument facilities for short-pulse experiments that may include both hard and soft x-rays, and build and continue to grow the ultrafast-science user community for cutting-edge time-resolved science at the APS.

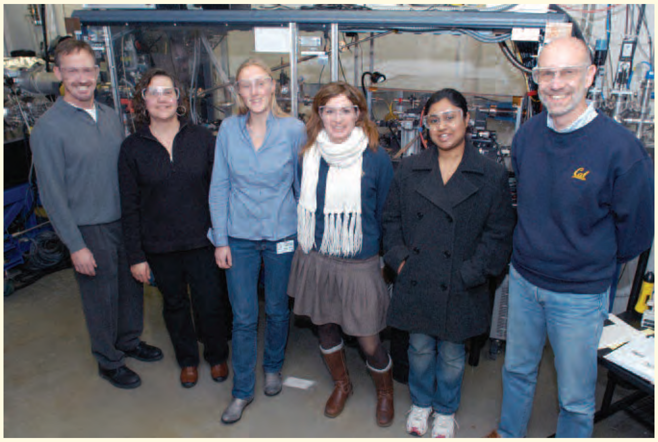
Workshop to Introduce High-Resolution Inelastic X-ray Scattering on Earth Materials Using Synchrotron Radiation • May 31-June 1, 2008 • This workshop was organized within the COMPRES infrastructure development initiative, which is aimed at creating state-of-the-art, high-resolution inelastic x-ray scattering (IXS) techniques for characterizing the properties of materials under the high-P-T conditions of planetary interiors. The intent was to provide a basic introduction of high-resolution IXS to the Earth-science community; define the state of the art of high-resolution IXS, especially at high pressure; discuss IXS experiments and theory and their applications to important geophysical problems; develop productive collaborations; and address experimental issues confronting users. The program was specifically designed for scientists and graduate students with no prior experience in IXS or synchrotron radiation.

Workshop on Understanding Condensed Matter Dynamics at the Microscopic Level • June 23-24, 2008 • The goal of the workshop was to see how national facilities like the APS can be utilized to examine and understand the real-time response of dynamically compressed materials at the microscopic level. Presentations focused on scientific challenges and opportunities in understanding the dynamic response of materials subjected to large compressions, high temperatures, and large deformations on short time scales (picosecond to microsecond).

Small-Angle Scattering Short Course 2008: "Beyond RG" • June 28-July 2, 2008 • The objective of the course is to raise the capabilities of the small-angle scattering (SAS) community by providing an intermediate-level course for those in need of a better understanding of SAS theory and techniques utilized at the APS. The SAS short course offers an overview of SAS theory, capabilities, and data reduction and analysis tools to enable the community to submit highly effective beam time proposals and to facilitate better utilization of the resources at the APS. The course includes hands-on experiments at a selected APS small-angle x-ray scattering facility, and data reduction and evaluation. *Contact ilavsky@aps.anl.gov*

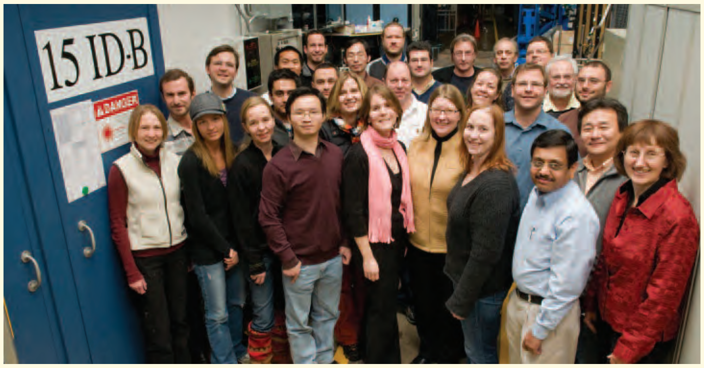
2008 APS XAFS School • August 5-8, 2008 • The fourth annual X-ray Absorption Fine Structure (XAFS) School instructed students about XAFS and how to incorporate it into their own research programs. The curriculum was aimed at the novice- to intermediate-level XAFS practitioner. Lectures for the 2008 school focused on basic theory, and the processing and analysis of XAFS data. Significant time was spent on hands-on instruction in data processing and data analysis using FEFF, IFEFFIT, and ATHENA and ARTEMIS. The 2008 program did not include hands-on experiments at APS spectroscopy beamlines, but experimental practice will be included in the 2009 APS XAFS School. *Contact jox@aps.anl.gov*

National School on Neutron and X-ray Scattering • September 24-October 11, 2008 • The main purpose of the school is to educate graduate students on the utilization of major neutron and x-ray facilities. Lectures, presented by researchers from academia, industry, and national laboratories, include basic tutorials on the principles of scattering theory and the characteristics of the sources, as well as seminars on the application of scattering methods to a variety of scientific subjects. Students conducted five short experiments at the APS and at the Oak Ridge National Laboratory Spallation Neutron Source and High Flux Isotope Reactor facilities to provide hands-on experience for using neutron and synchrotron sources. *Contact nxschool@dep.anl.gov*



School for Environmental Sciences and Synchrotron Radiation • November 17-26, 2008 • The two-week school, which marked its second year in 2008, introduces graduate students and postdoctoral fellows to the capabilities of the APS, under the tutelage of established environmental scientists to encourage the next generation of environmental scientists to begin their own research projects at the APS and other synchrotron facilities. Workshop attendees are given training on the scanning x-ray microscope at XOR beamline 2-ID-B by environmental researchers with synchrotron radiation science experience and carry out hands-on work on their own samples, assuring that the experiments are relevant to their work. The teams each give seminars on their research to the APS community. *Contact jthieme@gwdg.de, mcnulty@aps.anl.gov*

BioCARS Workshop on Time-Resolved Macromolecular Crystallography 2008 • November 20-22, 2008 • This workshop provides hands-on training in designing and conducting time-resolved experiments, and in Laue data processing and analysis. In 2008, new and returning BioCARS users also learned about the exciting new capabilities at beamline 14-ID (see page 89). The workshop featured lectures, data collection on samples provided by BioCARS and participants, and data processing of both new and previously collected datasets. Participants also had opportunities to discuss with experts in the field application of the technique to their own scientific projects. *Contact v-srajer@uchicago.edu*



ChemMatCARS Advanced Crystallography Workshop • December 3-5, 2008 • In this workshop, participants conducted experiments on the upgraded ChemMatCARS crystallography beamline and learned to use various software packages for advanced data analysis of modulation structures and microcrystals. Most participants collected and analyzed data on their own samples and received on-the-spot advice from experts on solving difficult structures.

Typical APS Machine Parameters

Linac

Output energy	325 MeV
Maximum energy	450 MeV
Output beam charge	1–3 nC
Normalized emittance	10–20 mm-mrad
Frequency	2.856 GHz
Modulator pulse rep rate	30 Hz
Gun rep rate (1–6 pulses, 33.3 ms apart every 0.5 s)	2–12 Hz
Beam pulse length	8–15 ns
Bunch length	1–10 ps FWHM

Particle Accumulator Ring

Nominal energy	325 MeV
Maximum energy	450 MeV
Circumference	30.66 m
Cycle time	500 ms
Fundamental radio frequency (RF1)	9.77 MHz
12th harmonic rf frequency (RF12)	117.3 MHz
RMS bunch length (after compression)	0.34 ns

Injector Synchrotron (Booster)

Nominal extraction energy	7.0 GeV
Injection energy	325 MeV
Circumference	368.0 m
Lattice structure	10 FODO cells/ quadrant
Ramping rep rate	2 Hz
Natural emittance	65 nm-rad-92 nm-rad
Radio frequency	351.930 MHz

Storage Ring System

Nominal energy	7.0 GeV
Circumference	1104 m
Number of sectors	40
Length available for insertion device	5.0 m
Nominal circulating current, multibunch	100 mA
Natural emittance	2.5 nm-rad
RMS momentum spread	0.096%
Effective emittance	3.1 nm-rad
Vertical emittance	0.040 nm-rad
Coupling	1.5%
Revolution frequency	271.554 kHz
Radio frequency	351.930 MHz
Number of bunches	24 to 1296
Time between bunches	153 to 2.8 ns
RMS bunch length	25 ps to 40 ps
RMS bunch length of 16 mA in hybrid mode	65 ps

APS Source Parameters

Undulator A

Period: 3.30 cm
Length: 2.4 m
K_{max}: 2.74 (effective; at minimum gap)
Minimum gap: 10.5 mm
Tuning range: 3.0–13.0 keV (1st harmonic)
3.0–45.0 keV (1st-5th harmonic)
On-axis brightness:
5.0 × 10^{19} ph/s/mrad^2/mm^2/0.1%bw at 7 keV
Source size and divergence at 8.0 keV:
Σ_x: 275 μm Σ_y: 9 μm
$\Sigma_{x'}$: 12.6 μrad $\Sigma_{y'}$: 6.4 μrad

2.30-cm Undulator (sectors 1, 11, 14)

Period: 2.30 cm
Length: 2.4 m
K_{max}: 1.19 (effective; at minimum gap)
Minimum gap: 10.5 mm
Tuning range: 11.8–20.0 keV (1st harmonic)
11.8–70.0 keV (1st-5th harmonic, non-contiguous)
On-axis brightness:
8.7 × 10^{19} ph/s/mrad^2/mm^2/0.1%bw at 12 keV
Source size and divergence at 12.0 keV:
Σ_x: 275 μm Σ_y: 9 μm
$\Sigma_{x'}$: 12.2 μrad $\Sigma_{y'}$: 5.5 μrad

2.70-cm Undulator (sectors 3 & 14)

Period: 2.70 cm
Length: 2.4 m
K_{max}: 1.78 (effective; at minimum gap)
Minimum gap: 10.5 mm
Tuning range: 6.7–16.0 keV (1st harmonic)
6.7–60.0 keV (1st-5th harmonic, non-contiguous)
On-axis brightness:
7.0 × 10^{19} ph/s/mrad^2/mm^2/0.1%bw at 8.5 keV
Source size and divergence at 8.0 keV:
Σ_x: 275 μm Σ_y: 9 μm
$\Sigma_{x'}$: 12.6 μrad $\Sigma_{y'}$: 6.4 μrad

APS Source Parameters

3.00-cm Undulator (sectors 12, 21, 23, 30)

Period: 3.00 cm
Length: 2.1 m in sectors 21 and 23, 2.4 m in Sector 30
K_{max}: 2.20 (effective; at minimum gap)
Minimum gap: 10.5 mm
Tuning range: 4.6–14.5 keV (1st harmonic)
4.6–50.0 keV (1st-5th harmonic)
On-axis brightness:
5.9×10^{19} ph/s/mrad^2/mm^2/0.1%bw at 8 keV
Source size and divergence at 8.0 keV:
Σ_x: 275 μm Σ_y: 9 μm
$\Sigma_{x'}$: 12.6 μrad $\Sigma_{y'}$: 6.4 μrad

3.50-cm SmCo Undulator (Sector 4)

Period: 3.50 cm
Length: 2.4 m
K_{max}: 3.08 (effective; at minimum gap)
Minimum gap: 9.5 mm
Tuning range: 2.3–12.5 keV (1st harmonic)
2.3–42.0 keV (1st-5th harmonic)
On-axis brightness:
4.5×10^{19} ph/s/mrad^2/mm^2/0.1%bw at 7 keV
Source size and divergence at 8.0 keV:
Σ_x: 275 μm Σ_y: 9 μm
$\Sigma_{x'}$: 12.6 μrad $\Sigma_{y'}$: 6.4 μrad

5.50-cm Undulator (Sector 2)

Period: 5.50 cm
Length: 2.4 m
K_{max}: 4.97 (effective; at minimum gap)
Minimum gap: 14.0 mm
Tuning range: 0.6–7.0 keV (1st harmonic)
0.6–25.0 keV (1st-5th harmonic)
On-axis brightness:
2.0×10^{19} ph/s/mrad^2/mm^2/0.1%bw at 4 keV
Source size and divergence at 4.0 keV:
Σ_x: 275 μm Σ_y: 9 μm
$\Sigma_{x'}$: 13.9 μrad $\Sigma_{y'}$: 8.6 μrad

APS Source Parameters

Circularly Polarized Undulator (Sector 4)

Period: 12.8 cm
Length: 2.1 m
Circular mode:
K_{max}: 2.65 (effective; for both horizontal and vertical fields at maximum currents of 1.2 kA horizontal and 0.34 kA vertical)
B_{max}: 0.26 T (peak fields)
Tuning range: 0.5–3.0 keV (1st harmonic)
On-axis circular brightness:
3.6×10^{18} ph/s/mrad^2/mm^2/0.1%bw at 1.8 keV
Linear mode:
K_{max}: 2.80 (effective; for both horizontal and vertical fields at maximum currents 1.4 kA horizontal and 0.40 kA vertical)
B_{max}: 0.29 T (peak fields)
Tuning range: 0.8–3.0 keV (1st harmonic)
0.8–10.0 keV (1st–5th harmonic)
On-axis linear brightness:
2.7×10^{18} ph/s/mrad^2/mm^2/0.1%bw at 2.1 keV
Switching frequency: 0-5 Hz
Switching rise time: 20 ms
Source size and divergence at 1.5 keV:
Σ_x: 275 μm Σ_y: 9 μm
$\Sigma_{x'}$: 18.0 μrad $\Sigma_{y'}$: 14.3 μrad

APS Bending Magnet

Critical energy: 19.51 keV
Energy range: 1–100 keV
On-axis brightness:
6.5×10^{15} ph/s/mrad^2/mm^2/0.1%bw at 16 keV
On-axis angular flux density:
9.6×10^{13} ph/s/mrad^2/0.1%bw at 16 keV
On-axis horizontal angular flux density:
1.6×10^{13} ph/s/mradh/0.1%bw at 6 keV
Source size and divergence at the critical energy:
Σ_x: 92 μm Σ_y: 26 μm
$\Sigma_{x'}$: 6 mrad $\Sigma_{y'}$: 47 μrad

APS BEAMLINE DIRECTORY*

KEY: CPU: Circularly polarized undulator; (CU): Canted undulator; GU: accepting general users

Beamline	Operator	Disciplines	Techniques	Source	Status
1-BM-B,C	XOR	Physics, materials science, chemistry	Powder diffraction	Bending magnet	Operational/GU
1-ID-C	XOR	Materials science, physics, chemistry	High-energy x-ray diffraction	3.3-cm Undulator A	Operational/GU
2-BM-B	XOR	Physics, life science	Phase-contrast imaging, tomography, microdiffraction, general diffraction	Bending magnet	Operational/GU
2-ID-B	XOR	Materials science, environmental science, physics	Coherent x-ray scattering (soft x-ray), microfluorescence (soft x-ray)	5.5-cm undulator	Operational/GU
2-ID-D	XOR	Life science, materials science, environmental science	Microfluorescence (hard x-ray), microdiffraction, micro x-ray absorption fine structure (XAFS)	3.3-cm Undulator A	Operational/GU
2-ID-E	XOR	Life science, environmental science, materials science	Microfluorescence (hard x-ray)	3.3-cm Undulator A	Operational/GU
3-ID-B,C,D	XOR	Physics, geoscience, life science, chemistry, materials science	Nuclear resonant scattering, high-pressure diamond anvil cell, inelastic x-ray scattering	2.7-cm undulator	Operational/GU
4-ID-C	XOR	Physics, materials science	X-ray photoemission electron microscopy, x-ray photoemission spectroscopy, magnetic circular dichroism (soft x-ray), x-ray magnetic linear dichroism, magnetic x-ray scattering, anomalous and resonant scattering (soft x-ray)	CPU; 3.5-cm undulator (CU)	Operational/GU
4-ID-D	XOR	Physics, materials science	Anomalous and resonant scattering (hard x-ray), magnetic x-ray scattering, magnetic circular dichroism (hard x-ray)	3.5-cm undulator	Operational/GU
5-BM-C	DND-CAT	Materials science, polymer science	Tomography, powder diffraction	Bending magnet	Operational/GU
5-BM-D	DND-CAT	Materials science, polymer science	XAFS, high-energy x-ray diffraction	Bending magnet	Operational/GU
5-ID-B,C,D	DND-CAT	Materials science, polymer science	Powder diffraction, x-ray reflectivity, small-angle x-ray scattering, surface diffraction, wide-angle x-ray scattering, x-ray standing waves, x-ray optics development/techniques	3.3-cm Undulator A	Operational/GU
6-ID-B,C	MU/XOR	Physics, materials science	Anomalous and resonant scattering (hard x-ray), liquid scattering, magnetic x-ray scattering, general diffraction, grazing-incidence diffraction, surface diffraction (UHV)	3.3-cm Undulator A	Operational/GU
6-ID-D	MU/XOR	Physics, materials science	High-energy x-ray diffraction, magnetic x-ray scattering, powder diffraction, pair distribution function	3.3-cm Undulator A	Operational/GU
7-ID-B,C,D	XOR	Materials science, atomic physics, chemistry	Time-resolved x-ray scattering, radiography, time-resolved XAFS	3.3-cm Undulator A	Operational/GU

*Source: https://beam.aps.anl.gov/pls/apsweb/beamline_display_pkg.beamline_dir as of 3.23.09

Beamline	Operator	Disciplines	Techniques	Source	Status
8-ID-E	XOR	Materials science, polymer science, physics	Intensity fluctuation spectroscopy, x-ray reflectivity, x-ray photon correlation spectroscopy, grazing-incidence small-angle scattering	3.3-cm Undulator A	Operational/Gu
8-ID-I	XOR	Polymer science, materials science, physics	Intensity fluctuation spectroscopy, coherent x-ray scattering, small-angle x-ray scattering, x-ray photon correlation spectroscopy	3.3-cm Undulator A	Operational/GU
9-BM-B,C	XOR/CMC	Materials science, chemistry	X-ray absorption fine structure	Bending magnet	Operational/GU
9-ID-B,C	XOR/CMC	Physics, materials science	Liquid scattering, inelastic x-ray scattering, resonant inelastic x-ray scattering	3.3-cm Undulator A	Operational/GU
10-ID-B	MR-CAT	Materials science, environmental science, chemistry	Microfluorescence (hard x-ray), XAFS, diffraction anomalous fine structure, micro-XAFS	3.3-cm Undulator A	Operational/GU
11-BM-B	XOR/BESSRC	Chemistry, materials science, physics, geoscience, life science	Powder diffraction	Bending magnet	Operational
11-ID-B	XOR/BESSRC	Chemistry, environmental science, materials science	High-energy x-ray diffraction, pair distribution function	2.3-cm Undulator A	Operational/GU
11-ID-C	XOR/BESSRC	Materials science, geoscience, physics, chemistry	Diffuse x-ray scattering, high-energy x-ray diffraction, pair distribution function	2.3-cm undulator	Operational/GU
11-ID-D	XOR/BESSRC	Chemistry, geoscience, materials science	XAFS, general diffraction, time-resolved XAFS	3.3-cm Undulator A	Operational/GU
12-BM-B	XOR/BESSRC	Materials science, geoscience, chemistry, polymer science, physics, environmental science	XAFS, fluorescence spectroscopy, powder diffraction, x-ray reflectivity, general diffraction	Bending Magnet	Operational/GU
12-ID-B,C,D	XOR/BESSRC	Chemistry, physics, materials science	Small-angle x-ray scattering, wide-angle x-ray scattering, grazing-incidence small-angle scattering, surface scattering	3.3-cm Undulator A	Operational/GU
13-BM-C	GSECARS	Geoscience, environmental science	Single-crystal diffraction, surface diffraction, high-pressure diamond anvil cell	Bending magnet	Operational/GU
13-BM-D	GSECARS	Geoscience, environmental science	Tomography, XAFS, high-pressure diamond anvil cell, high-pressure multianvil press	Bending magnet	Operational/GU
13-ID-C,D	GSECARS	Geoscience, environmental science	Microfluorescence (hard x-ray), XAFS, microdiffraction, micro-XAFS, high-pressure diamond anvil cell, high-pressure multianvil press, inelastic x-ray scattering	3.3-cm Undulator A	Operational/GU
14-BM-C	BioCARS	Life science	Macromolecular crystallography, fiber diffraction, biohazards at the BSL2/3 level, subatomic (<0.85-Å) resolution	Bending magnet	Operational/GU

Continued on page 148

KEY: CPU = Circularly Polarized Undulator; CU: Canted undulator; GU: General Users

Beamline	Operator	Disciplines	Techniques	Source	Status
14-ID-B	BioCARS	Life science	Macromolecular crystallography, time-resolved x-ray scattering, Laue crystallography, anomalous diffraction (multiwavelength anomalous dispersion [MAD]/single-wavelength anomalous dispersion [SAD]), biohazards at the BSL2/3 level	2.7-cm undulator	Operational/GU
15-ID-B,C,D	ChemMatCARS	Materials science, chemistry	Anomalous and resonant scattering (hard x-ray), liquid scattering, microdiffraction, single-crystal diffraction, small-angle x-ray scattering, surface diffraction, wide-angle x-ray scattering	3.3-cm Undulator A	Operational/GU
16-BM-B	HP-CAT	Materials science, geoscience	Powder EDXD diffraction, single-crystal diffraction	Bending magnet	Operational/GU
16-BM-D	HP-CAT	Materials science, geoscience	Powder ADXD diffraction, single-crystal diffraction	Bending magnet	Operational/GU
16-ID-B	HP-CAT	Materials science, geoscience	Microdiffraction, powder diffraction, single-crystal diffraction, high-pressure diamond anvil cell	3.3-cm Undulator A	Operational/GU
16-ID-D	HP-CAT	Materials science, geoscience, physics	Nuclear resonant scattering, inelastic x-ray scattering, x-ray Raman scattering, x-ray emission spectroscopy	3.3-cm Undulator A	Operational/GU
17-BM-B	IMCA-CAT	Life science	Macromolecular crystallography, anomalous diffraction (MAD/SAD)	Bending magnet	Operational/GU
17-ID-B	IMCA-CAT	Life science	Macromolecular crystallography, anomalous diffraction (MAD/SAD)	3.3-cm Undulator A	Operational/GU
18-ID-D	Bio-CAT	Life science	Microfluorescence (hard x-ray), microdiffraction, small-angle x-ray scattering, time-resolved x-ray scattering, micro-XAFS, fiber diffraction	3.3-cm Undulator A	Operational/GU
19-BM-D	SBC-CAT	Life science	Anomalous diffraction (MAD/SAD), ultra-low-temperature (15K)	Bending magnet	Operational/GU
19-ID-D	SBC-CAT	Life science	Anomalous diffraction (MAD/SAD), subatomic (<0.85-Å) resolution, ultra-low-temperature (15K)	3.3-cm Undulator A	Operational/GU
20-BM-B	XOR/PNC	Materials science, environmental science, chemistry, geoscience	Microfluorescence (hard x-ray), XAFS, micro-XAFS	Bending magnet	Operational/GU
20-ID-B,C	XOR/PNC	Materials science, environmental science, chemistry, geoscience	Microfluorescence (hard x-ray), XAFS, surface diffraction, micro-XAFS, x-ray Raman scattering, time-resolved XAFS	3.3-cm Undulator A	Operational/GU
21-ID-D	LS-CAT	Life science	Macromolecular crystallography, anomalous diffraction (MAD/SAD)	U33S undulator	Operational

Beamline	Operator	Disciplines	Techniques	Source	Status
21-ID-F	LS-CAT	Life science	Macromolecular crystallography, anomalous diffraction (MAD/SAD)	3.0-cm undulator	Operational/GU
21-ID-G	LS-CAT	Life science	Macromolecular crystallography, anomalous diffraction (MAD/SAD)	3.0-cm undulator	Operational
22-BM-D	SER-CAT	Life science	Macromolecular crystallography	Bending magnet	Operational/GU
22-ID-D	SER-CAT	Life science	Macromolecular crystallography, MAD	3.3-cm Undulator A	Operational/GU
23-BM-B	GM/CA-CAT	Life science	Macromolecular crystallography, MAD	Bending magnet	Operational
23-ID-B	GM/CA-CAT	Life science	Macromolecular crystallography, microdiffraction, anomalous diffraction (MAD/SAD), microbeam, subatomic (<0.85-Å) resolution	3.3-cm Undulator A	Operational/GU
23-ID-D	GM/CA-CAT	Life science	Macromolecular crystallography, microdiffraction, anomalous diffraction (MAD/SAD), microbeam, subatomic (<0.85-Å) resolution	3.0-cm undulator	Operational/GU
24-ID-C	NE-CAT	Life science	Macromolecular crystallography, anomalous diffraction (MAD/SAD)	3.3-cm Undulator A (CU)	Operational/GU
24-ID-E	NE-CAT	Life science	Macromolecular crystallography, microbeam	3.3-cm Undulator A (CU)	Operational/GU
26-ID-C	CNM/XOR	Physics, materials science	Microfluorescence (hard x-ray), tomography, microdiffraction	3.3-cm Undulator A	Operational/GU
30-ID-B,C	XOR/IXS	Physics, materials science, geoscience, life science	Inelastic x-ray scattering	3.0-cm undulator	Operational/GU
31-ID-D	SGX-CAT	Life science	Macromolecular crystallography, single-crystal diffraction, fiber diffraction, SAD	3.3-cm Undulator A	Operational/GU
32-ID-B,C	XOR	Materials science, life science	Phase-contrast imaging, ultra-small-angle x-ray scattering, radiography	3.3-cm Undulator A	Operational/GU
33-BM-C	XOR/UNI	Materials science, physics, chemistry	Anomalous and resonant scattering (hard x-ray), diffuse x-ray scattering, powder diffraction, x-ray reflectivity, general diffraction, grazing incidence diffraction	Bending magnet	Operational/GU
33-ID-D,E	XOR/UNI	Materials science, physics, chemistry	Anomalous and resonant scattering (hard x-ray), diffuse x-ray scattering, x-ray reflectivity, surface diffraction, x-ray standing waves, general diffraction	3.3-cm Undulator A	Operational/GU
34-ID-C,E	XOR/UNI	Materials science, physics	Coherent x-ray scattering, microdiffraction	3.3-cm Undulator A	Operational/GU

FY08 Completed or Active Approved Partner User Proposals*

Investigators	Partner User Proposal Title (PUP number)	Beamline	Beam Time Award
R. Garrett	Australian Synchrotron Research Program-XOR Partnership Proposal (PUP-15)	1,3,4	Negotiated each run
L. Soderholm, P. Burns, J. Neuefeind, M. Beno, S. Skanthakumar	Short-Range Order in Solution: Development of a Dedicated Beamline for Pair Distribution Functions (PDF) studies at the APS (PUP-52)	11-ID-B	20% beginning 2005-3 through 2008-2
J. Miao, M. Glimcher, S. Risbud, J. Amonette, I. McNulty, D. Paterson	Three-dimensional Imaging of Nanoscale Systems By Using Coherent X-rays (PUP-53)	2-ID-B	15%/beginning 2005-3 through 2008-2 (completed)
E. Stern, E.D. Crozier, S. Heald, G. Seidler, D. Brewe, J. Cross	Novel X-ray Spectroscopies and Microscopies for the Determination of Structure with Atomic Resolution (extension of PUP-24) (PUP-55)	20-ID	Various allocations for different programs
L. Chen, K. Attenkofer, G. Jennings, D. Tiede	Developing a Laser-Initiated, Time-Resolved X-ray Facility at 11-ID-D for Photochemical Research By Using XAS and WAXS (PUP-56)	11-ID-D	20% beginning 2006-2 through 2007-3 (completed)
A. Allen, L.E. Levine	Advanced USAXS Studies for Solution-Mediated Nanoscale Processing, Nanostructural Materials Imaging, and High-Spatial-Resolved Gradient Microstructure Characterization (PUP-59)	32-ID	10% beginning 2007-1 through 2008-3
E.D. Crozier, T.-K. Sham	Pacific Northwest Consortium Synchrotron Radiation Facility XOR Bending Magnet Partnership Proposal (PUP-60)	20-BM	10% beginning 2007-1 through 2009-3
B. Ocko, K. Blasie, T. Gog, I. Kuzmenko	Partner User Proposal: Liquid Surface Scattering (LSS) at Sector 9 (PUP-61)	9-ID	15% beginning 2007-1 through 2009-3
J. Hill, Y.-J. Kim, T. Gog, D. Casa	Partner User Proposal: Inelastic X-ray Scattering (IXS) at Sector 9 (PUP-62)	9-ID	15% beginning 2007-1 through 2009-3
E. Landahl et al.	Picosecond Science at the Advanced Photon Source, Partner User Proposal: Sector 7-ID (PUP-63)	7-ID	15% beginning 2007-1 through 2007-3 (completed)
Y. Hwu, T.-K. Lee, J.H. Je, G. Margaritondo, K.S. Liang	Short Proposal for Limited Scope Partnership User at the Advanced Photon Source: Phase-Contrast Hard X-ray Microscopy for Biological and *In Situ* Materials Science Applications at Sub-6-nm Spatial Resolution (PUP-64)	32-ID	20% of the beam time on 32-ID for 2007-2 through 2010-1
E.D. Crozier, T.-K. Sham	Renewal Proposal for PUP-21, Pacific Northwest Consortium Synchrotron Radiation Facility-XOR Insertion Device Partnership User Proposal (PUP-65)	20-ID	10% for 2007-1, 20% for 2007-2, and 15% for 2007-3 through 2009-3
A. Sandy, S. Narayanan, M. Sprung, K. Evans-Lutterodt, S. Mochrie, L. Lurio	Vertical Focusing Applied to X-ray Photon Correlation Spectroscopy (PUP-66)	8-ID-I	8% for six cycles (two years) beginning with 2007-3 through 2009-2
Z. Islam, J. Lang, D. Haskel, Y. Matsuda, H. Nojiri, B. Gaulin, Z. Mao, I. Fisher, P. Canfield	A Portable High-Field (30-45 Tesla) Pulsed-Magnet Setup for Novel Scattering and Spectroscopic Studies of Materials in Extreme Conditions (PUP-67)	4-ID-D	18 shifts/cycles for two years (108 shifts total) beginning with 2007-3 through 2009-2
L. Young, S. Southworth, E. Kanter, B. Kraessig, R. Dunford, R. Santra, D. Arms, E. Dufresne, E. Lindahl, J. Ye, D. Yost	High-Repetition-Rate Ultrafast Laser/X-ray Techniques (PUP-71)	7-ID	~15% of the time on 7-ID/cycle for three years beginning with 2007-3 through 2010-2
K. Nugent, A. Peele, L. Tilley, G. Williams, M. Pfeifer, M.-T. Tang, T.-K. Lee, I. McNulty, Q. Shen	Short Proposal for Limited-Scope Partnership User at the Advanced Photon Source; Dedicated Fresnel Coherent Diffractive Imaging Facility at 2-ID-B (PUP-74)	2-ID-B	Thirty-six shifts/cycle for three years begining with 2008-2 through 2011-1

* As of 3.10.09 Source: http://www.aps.anl.gov/Users/Scientific_Access/Partner_User_Information/Results/index.html

Abstracts for these proposals are at the URL above.

Collaborative access teams are the most comprehensive type of partner users.

Another type is a collaborative development team, an external partner group that drives the development of a beamline that will be ultimately operated by the APS.

Typically, a partner user requires access to more than 10% of the beam time on a beamline or sector for two years or more.

(Source: www.aps.anl.gov/Users/Scientific_Access/Partner_User_Information/index.html)

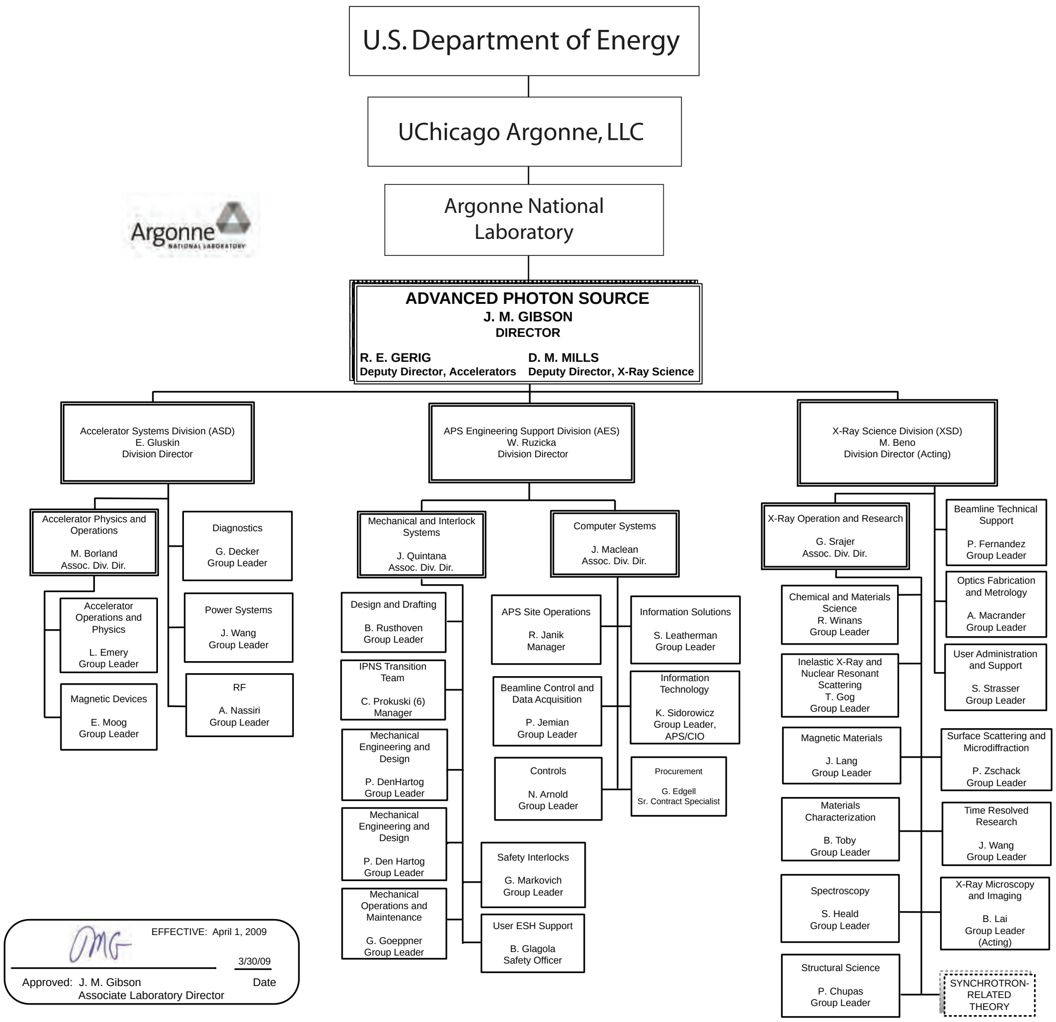
Completed partner user proposals: http://www.aps.anl.gov/Users/Scientific_Access/Partner_User_Information/Results/completed.html

Partner user call for proposals: www.aps.anl.gov/Users/Scientific_Access/Partner_User_Information/Call_For_Proposals/index.html

Partner user policy: http://centraldocs.aps.anl.gov/policy_procedures/user/docs/APS_1258423.htm

Partner users are individuals or groups whose work involves a greater degree of collaboration with the APS than is generally expected of general users.

APS ORGANIZATION CHART

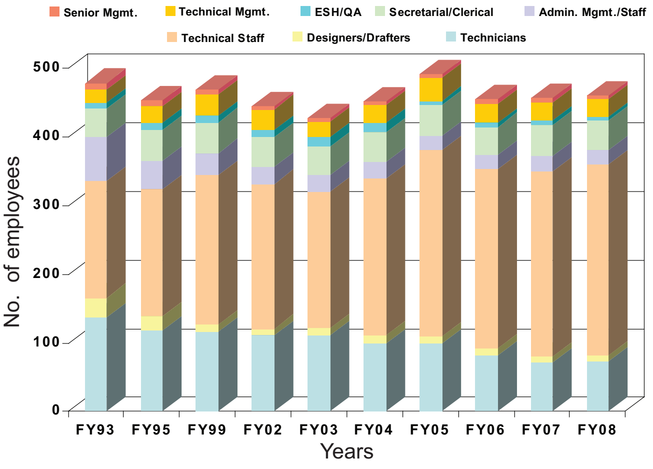


EFFECTIVE: April 1, 2009

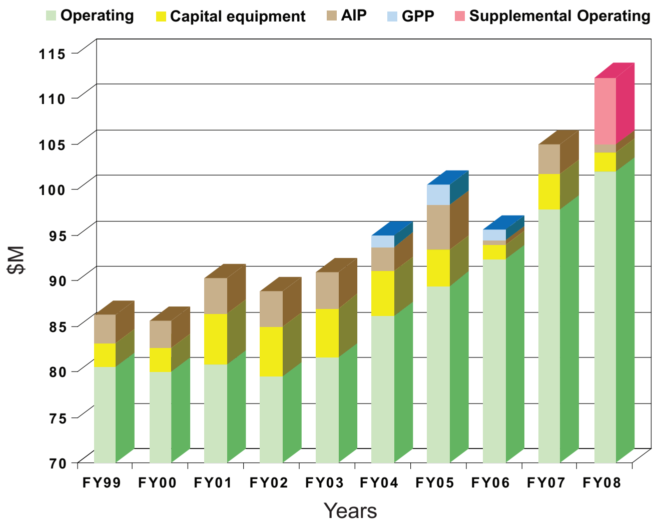
JMG 3/30/09

Approved: J. M. Gibson Date
Associate Laboratory Director

APS STAFFING AND FUNDING



APS staffing levels, FY93-FY08.



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