BROOKHAVEN NATIONAL LABORATORY

NEWSLETTER

national synchrotron light source

December 2004

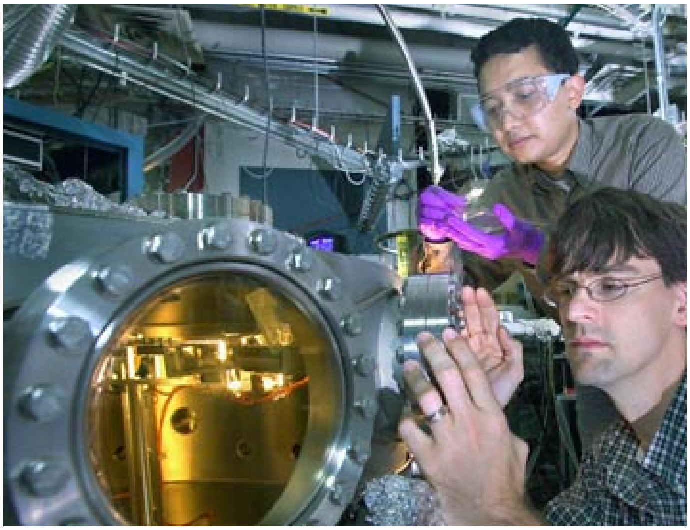
Research on "Holes" May Unearth Causes of Superconductivity

Laura Mgrdichian, NSLS Science Writer

Scientists at the NSLS have uncovered another possible clue to the causes of high-temperature superconductivity, a phenomenon in which the electrical resistance of a material disappears below a certain temperature. In a superconducting compound, they found evidence of a rarely seen arrangement of "holes" - locations where electrons are absent. The results appeared in the October 28, 2004, issue of *Nature*.

The researchers were studying a compound made of strontium, copper, and oxygen (which they've dubbed SCO) that is one of the "cuprates," a family of compounds that contain copper oxide. In SCO, the scientists found evidence of a "hole crystal" - a rigid, ordered arrangement of holes. Holes are positively charged and, like electrons, may interact with each other to produce a superconducting current.

"A hole crystal is a very unusual phenomenon," said NSLS physicist Peter Abbamonte, the study's lead researcher. "Its existence is a direct result of the correlations between holes, which are believed to produce superconductivity in other cuprates."



Peter Abbamonte (bottom) and student researcher Andrivo Rusydi

SCO consists of one layer of strontium atoms sandwiched by two sheets of different copper oxides. In one sheet, the copper-oxide molecules form long, parallel chains. The other copper oxide layer, which contains the hole crystal, has a ladder structure, resembling chains that are linked horizontally.

A hole crystal is just one type of arrangement of electric charge in a material. These arrangements are important because some researchers believe that superconductivity is the result of a particular arrangement, or occurs when a superconductor approaches a boundary between two arrangements. In other cuprates, for example, scientists are studying a charge arrangement in which ribbons of holes and magnetic regions form alternating "stripes."

"We believe the hole crystal and stripes may be linked," said Abbamonte. "Specifically, the hole crystal in SCO may be a 'low-dimensional' precursor to stripes, meaning it exists only along the copper-oxide ladders, rather than in an entire copper-oxide plane."

He and his collaborators studied SCO using x-rays at beamline X1B. They

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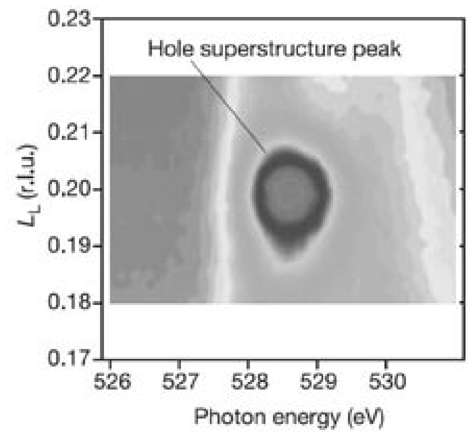
placed an SCO sample in the path of an x-ray beam, varied the wavelength of the beam, and watched how the x-rays reflected away from the sample.

At a particular energy, the sample reflected back the x-rays very intensely. The research group discovered that this reflection was caused by the holes, which led them to determine that the holes formed an ordered lattice since randomly placed holes could not have produced such a strong reflection.

Abbamonte and his collaborators plan to continue this research by varying the chemical composition of SCO to see if it changes the hole crystal. They will also examine another cuprate to see if its stripes are related to the crystal.



The peak intensity and ladder position (L_L) of the hole crystal reflection.

"Clearly, more research needs to be done to study these phases and their possible link to superconductivity," said Abbamonte.

The research was funded by the Office of Basic Energy Sciences within the U.S. Department of Energy's Office of Science, the National Science Foundation, Bell Laboratories, the Dutch Science Foundation, and the Netherlands Organization for Fundamental Research on Matter.

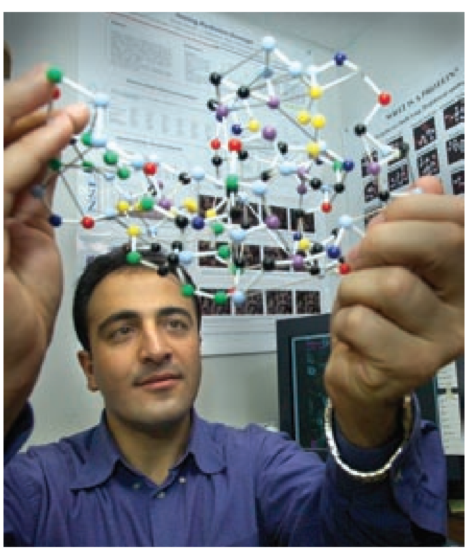
AWARDS

NSLS Visiting Scientist Mehmet Aslantas Wins Prestigious Lecturer Award

Laura Mgrdichian, NSLS Science Writer

National Synchrotron Light Source visiting scientist Mehmet Aslantas has won the prestigious Margaret C. Etter Student Lecturer Award for a talk on his recent work: how to reduce the effects of radiation damage to protein crystals during synchrotron x-ray studies.

He received the award at the American Crystallographic Association national meeting, held in Chicago, Illinois, on July 18-22, 2004. The Etter award, given out just once a year, recognizes achievement and future potential for scientists at an early stage in their independent careers.



Mehmet Aslantas holds a ball-and-stick model of the test protein he used in his research.

Aslantas, who initially came to the NSLS for six months through a U.S. Department of Energy Cooperative Research program, received an extension that allowed him to stay for over a year. "The NSLS is a great place to work, and I couldn't have completed my research or won this award without the research extension I received," said Aslantas. "I would like to thank the NSLS Chairman, Steve Dierker, the Associate Chair for User Science, Chi-Chang Kao, Vivian Stojanoff, and the User Administration office for their support."

Aslantas worked under Stojanoff's supervision at NSLS beamlines X6A and X17B1. In his talk, titled "Radiation Effects on Biological Samples," he described his work at the beamlines. At X6A, he studied the effect of low-energy x-rays on lyzozyme crystals, which are standard test protein crystals. At X17B1, the sample was subjected to high-energy x-rays.

"My experimental results show that, with lower-energy x-rays, the sample absorbs more radiation than at higher energies, in which it absorbs less energy and sustains no significant damage," he said. "This is because the low-energy x-ray beam interacts with the inner shell electrons in the atoms of the protein, causing an overall higher dose to the sample. This leads to structural damage and limits the structural information we can learn about the sample. However the high energy x-rays interact with the outer shell electrons in the atom of the protein. This interaction, known as Compton Scattering, plays a role in causing the overall dose deposited to the sample to be less significant. The sample will have a longer lifetime, too."

Aslantas' work is funded by a U.S. Department of Energy Cooperative Research program, which allows him to work at the NSLS as part of a scientific exchange program with another synchrotron, SESAME (Synchrotron light for Experimental Science and Applications in the Middle East). SESAME is under construction.

Currently, Aslantas is preparing three manuscripts describing his work at the NSLS. His experience will help him form a protein crystallography group at his home institution, Hacettepe University in Ankara, Turkey. In turn, this group will be working with SESAME to develop a protein crystallography beamline at the facility. After his return to Hacettepe University, Aslantas expects to keep in close contact with the NSLS and will continue his research.

Notes from the UEC

Larry Shapiro, Users' Executive Committee Chair
Columbia University

There are two issues of great importance to the NSLS user community that I'd like to discuss. The first is the need for a renewed commitment to safety. Recent incidents, including an electric shock received by an NSLS user, have resulted in major safety reviews and even work stoppages so that potential, similar hazards can be physically inspected. While these incidents involved users who were not full-time BNL employees, the NSLS is responsible for maintaining safe operating procedures for everyone who works here, and, from DOE's point of view, is accountable for all safety infractions. The same safety standards that apply to NSLS facility beamlines are equally applicable to PRT beamlines, and these high standards need to be maintained.

Since safety is paramount, the NSLS has begun to take actions to ensure that all PRTs have implemented adequate procedures. Over the last few months, an internal inquiry of PRT safety practices has been underway, and the results are now being analyzed. If the implementation of safe work practices is judged to be insufficient, the NSLS may need to provide more oversight. This would be an unfortunate outcome for everyone: NSLS staff, already stretched by their current workload, would have to take on additional responsibilities, creating an additional drain on limited resources. It's not only accidents that could lead to such an outcome, but poor practices, even those without bad results. We need to be mindful of this, and we must keep safety procedures high on our list of responsibilities.

The second issue is the difficulty faced by the NSLS administration in maintaining and operating the facility under extraordinary budget constraints. The current NSLS budget is simply insufficient to do all the things we'd like, including replacement of equipment near or past its life expectancy, hiring and training of more personnel for ring maintenance and upgrades, and bringing new capabilities to the machine. These budget limitations force the NSLS to make hard choices, sometimes leaving no option but to take from one area in order to give to another.

Our user community represents a large and remarkable group of scientists from some of the world's great universities and corporations. The NSLS has been an essential resource for us for two decades, and our community will have to find a way to address this funding problem so that the NSLS continues to be the extraordinary resource we've all come to depend on. If DOE does not hear from us or from leaders of our home institutions, they may assume that we're satisfied with the status quo. The NSLS is too important and too productive for us to allow that to happen. As UEC Chair, I will make every effort to communicate this message to DOE, and I hope that each of us will actively help to ensure the future of this great scientific resource.

SAVE THE DATE

2005 NSLS Users' Meeting
May 23-25, 2005

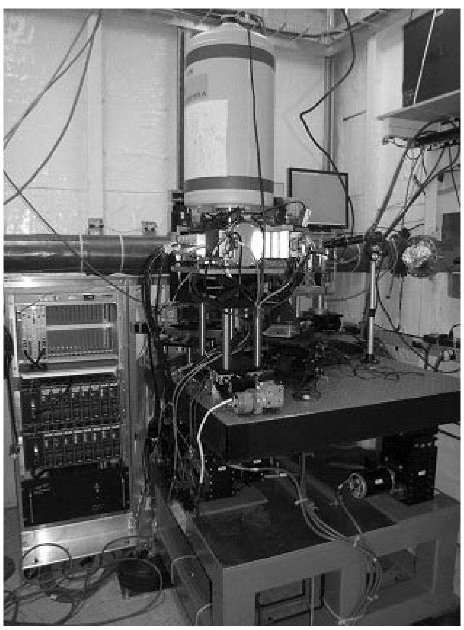
For meeting information see:
http://www.nsls.bnl.gov/users/meeting

UEC members and SpIG representatives: (Standing from left): Mary Anne Corwin (BNL-NSLS), Chi-Chang Kao (BNL-NSLS), Randy Smith (BNL-NSLS), Meghan Ruppel (Stony Brook U.), Dean Hesterberg (North Carolina State U.), Simon Bare (UOP LLC), Jeff Fitts (BNL-Environ. Sci.), Trevor Tyson (NJIT), John Sutherland (BNL-Biology), and Govindham Dhanaraj (standing in for Michael Dudley, Stony Brook U.). (Sitting from left): Hao Wu (Cornell U.), Elio Vescovo (BNL-NSLS), Mahbub Khandaker (Thomas Jefferson Nat. Lab.), Larry Shapiro (Columbia U.), Daniel Fischer (NIST), Peter Stephens (Stony Brook U.), Tom Hollis (Wake Forest U.). Missing from photo: Lisa Miller (BNL-NSLS), Laura Silvian (Biogen Inc.), and Valery Kiryukhin (Rutgers U.).

X27A: A New Hard X-Ray Microprobe Beamline for Environmental Research

James M. Ablett, BNL-NSLS

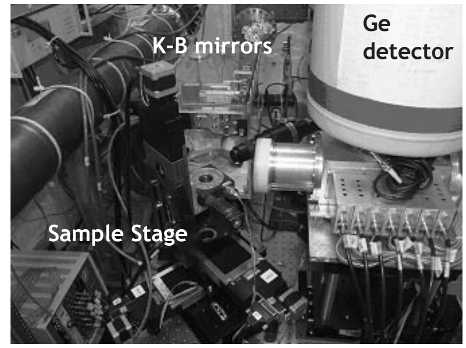
A new and advanced hard x-ray microprobe facility has been installed at NSLS bending-magnet beamline X27A. This beamline was constructed to meet the increasing demand of environmental molecular science users for state-of-the-art x-ray microprobe research, only previously served by the highly productive X26A beamline. Operated as a microprobe since 1986 by the University of Chicago's Consortium for Advanced Radiation Sources, the Savannah River Ecology Laboratory, and BNL's Environmental Sciences Department, X26A's research mission has been to provide a national facility for micro-spectroscopy to the environmental sciences and geosciences community. However, as the only dedicated hard x-ray microprobe at the NSLS, beamline X26A has been consistently oversubscribed. X27A will allow the NSLS to meet the demand of this ever increasing and vibrant user base.



The new X27A hard x-ray microprobe shown within the experimental hutch.

The new X27A microprobe facility consists of a newly designed monochromator and slit system, which is installed between the X27A & X27B hutches and enables both monochromatic and white-beam modes of operation. Si(111) and Si(311) channel-cut crystals are employed, enabling an energy accessible range from below 4 keV up to 32 keV. To micro-focus the incoming x-rays, a Kirkpatrick-Baez (K-B) bender system is used to form the required elliptical shapes from flat tapered rhodium-coated trapezoids. The x-ray beam is focused to a spot size of ~ 5 μm [vertical] x 15 μm [horizontal] at the sample location, which is ~ 9 cm from the end of the helium-filled mirror enclosure box. A 13-element, liquid-nitrogen cooled germanium detector is used to collect the fluorescence photons emitted from the sample. Transmission is collected with a photodiode. Spatially resolved information is obtained by raster-scanning the sample through the micro-focused x-ray beam with a high-resolution motorized sample stage.

Beamline control is VME-based EPICS through the SPEC and IDL (using X26A IDL routines) software programs.



Close-up of the microprobe setup: The K-B mirror system is located towards the top center, the high-resolution sample stage is towards the bottom center, and the 13-element fluorescence detector is on the right of the photograph.

The X27A microprobe facility involves a collaboration between the NSLS, EnviroSuite, and CEMS. EnviroSuite is a strategic initiative within BNL's Environmental Sciences Department that facilitates environmental molecular science research at the NSLS, and CEMS is the Center for Environmental Molecular Science, based at Stony Brook University. The funding for construction of the X27A facility, the detector system, and operation comes from the Department of Energy's Offices of Basic Energy Sciences and Biological & Environmental Research, and CEMS is supported by grants from the National Science Foundation and Department of Energy.

The January-April 2005 cycle is reserved for X27A commissioning, after which the beamline will be opened up for general user proposals, which should be submitted by January 31st 2005. For further information, please email James Ablett at jablett@bnl.gov.

High Resolution Powder Diffraction Data Collection and Analysis

January 25 - 27, 2005

An introductory practical course in powder diffraction based on synchrotron radiation

For course information see:
http://www.nsls.bnl.gov/newsroom/events/workshops/powderdiff/

X13A Magnetic Circular Dichroism Beamline Upgrade

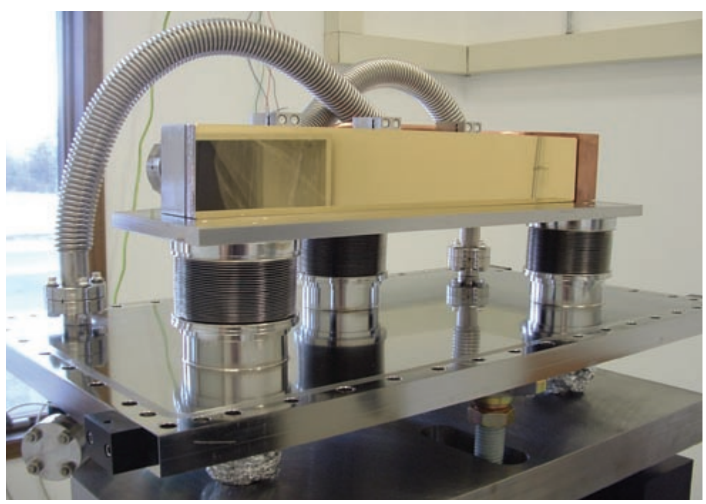
Cecilia Sanchez-Hanke, BNL-NSLS

Two insertion devices are installed in the X13 straight section: the mini gap undulator (MGU) and the fast-switching (22 Hz) elliptically polarizing wiggler (EPW). The X13A beamline, which utilizes the EPW source, is dedicated to the study of magnetic materials and their properties. The EPW provides alternately left- and right-handed elliptically polarized soft x-rays, which enables magnetic circular dichroism (MCD) measurements to be performed at a fixed magnetic field on the sample. The fast-switching capability simplifies the detection of small magnetic signals via the use of lock-in techniques.

The first optical element in the X13A beamline is a horizontally deflecting mirror (M0) that collects the central ~1 mrad of the EPW source, directs it to the X13A branch, and focuses it horizontally at the entrance slit of a horizontally dispersing spherical grating monochromator (SGM). The original (1980s) M0 mirror was too short, not well cooled, and suffered from mechanical stability problems and inadequate adjustment controls. We have replaced this mirror with a new one that remedies all of these problems. The new M0 mirror has twice the length of the old one, is integrally water-cooled, and is outfitted with a robust mounting and motor-driven mirror alignment system. These features have significantly improved the stability of the signal ratio between left and right elliptically polarized soft x-rays. Very often, the magnetic signals measured at X13A are quite small, such that an improvement in beam stability results in a significant improvement in data quality. In order to maximize beamline performance for demanding soft x-ray MCD measurements, the M0 mirror position for X13A operations has been centered on the EPW beam fan. This geometry necessarily blocks any output from the MGU, and results in a 50/50 scheduling split of X13 beamtime between X13A and X13B operations.

The new position of the X13A M0 mirror, both horizontally and along the beamline, required realigning the entire X13A beamline: the X13A SGM monochromator, I0 chamber, 22 Hz chopper, and diffractometer endstation. During initial commissioning of the newly rebuilt X13A beamline, it became clear that the EPW beam was not quite level, so we requested a vertical orbit correction for X13A. The new orbit bump was eventually made permanent, and contributed most of the factor-of-ten increase in intensity measured at the sample in the X13A endstation. (The doubled mirror length contributed only a factor of two.) The stability of the new mirror mounting system has also resulted in an improvement in stability of the left/right signal ratio. The flux and stability improvements combine to provide a significant increase in sensitivity, i.e. the ability to detect small magnetic signals. The newly renovated X13A beamline was tested by users during the fall 2004 scheduling cycle.

Principal thanks for the installation of this mirror, including the large amount of lead shielding required around the mirror chamber, go to the User Science Division technical group led by Tony Lenhard. In particular, Shu Cheung performed most of the mechanical assembly and installation work on this mirror chamber, once the vendor (Advanced Design Consulting, Lansing, NY) completed delivery. Thanks also go to the Operations and Engineering Division for mechanical survey work and control-room assistance during commissioning, as well as to the Accelerator Division for the X13 orbit bump work.



The new X13A M0 mirror before installation at the beamline. Only the bottom flange of the ultra-high vacuum chamber is shown in this photograph. The flexible bellows behind the mirror surrounds and vacuum-isolates the water-cooling plumbing. The mirror itself is gold-coated electroless nickel deposited on glidcop, which is explosion-bonded to a stainless steel substrate. The water-cooling channels are milled in the stainless steel/glidcop substrate, and then a stainless steel plate containing mechanical and plumbing fittings is welded to the mirror substrate. The three bellows underneath the mirror allow motor-driven adjustments of the mirror in the x and z translations and in rho and tilt rotations, while the surrounding chamber remains fixed.

X1A Monochromator and Laser Interferometer Upgrades

Chris Jacobsen, Stony Brook University

The X1A1 beamline received a new monochromator in May 2004. The purpose of this monochromator upgrade was to provide for exchangeable gratings with higher calculated diffraction efficiency, integrated water-cooling (such as will be required for NSLS-II), and improved vacuum performance to minimize carbon contamination. Due to constraints of the beamline length, the optical configuration could not be changed; it continues to be a spherical grating with a fixed exit arm and a resolving power of about 5000 at 290 eV. The monochromator was specified by Steve Hulbert of the NSLS, and manufactured by Physical Science Laboratories. It was installed by NSLS personnel during the May shutdown, and the electronic interfacing and alignment was done by the Stony Brook X1A group in late May and early June. The monochromator offers a significant improvement in ease of alignment, and the possibility of extending the operating energy range of X1A1. Two of the new gratings (Horiba Jobin-Yvon, Inc., Edison, NJ) are optimized for operation near the carbon K-edge (calculated diffraction efficiency 16% at 290 eV) and one is optimized for the oxygen K-edge (calculated diffraction efficiency 27% at 505 eV). At present it has been used primarily for carbon edge studies, and as the vacuum gradually improves we hope to see a reduction in the rate of carbon contamination. Thanks to Chi-Chang Kao, Steve Hulbert, Qing-Yi Dong, Gary Nintzel, and Dennis Carlson, along with many others from the NSLS, as well as Bjorg Larson, Mirna Lerotic, and Sue Wirick from Stony Brook, for their efforts with this system.

The new monochromator at beamline X1A1. It will provide for exchangeable gratings with higher diffraction efficiency, integrated water-cooling, and improved vacuum performance to minimize carbon contamination. It includes four selectable in-situ side-cooled grating holders, and provides for micro-radian angular precision and repeatability.

We are also in the middle of installing a laser interferometer upgrade to the scanning transmission x-ray microscope at X1A2, and then, at a later date, the one at X1A1. This will follow impressive developments at the Advanced Light Source by David Kilcoyne and others to use laser interferometer information on scanning stage position in a closed-loop feedback system to improve position stability in spectromicroscopy. The laser interferometer upgrade is also accompanied by a complete redesign of the control electronics and software, which will improve throughput of the microscope. This effort has included Holger Fleckenstein, Dan Flickinger, Benjamin Hornberger, and Mirna Lerotic from Stony Brook, and it is a key element to NASA-funded research performed by George Flynn of SUNY Plattsburgh in partnership with Stony Brook.

SBU/BNL Van Route Schedule

Monday - Friday (except holidays)

Pick Up Time	Pick Up Location	Drop Off Time	Drop Off Location
8:30 am	SBU-SAC Loop	9:15 am	BNL-Berkner Hall
9:30 am	BNL-Berkner Hall	10:15 am	SBU-SAC Loop
12:00 pm	SBU-SAC Loop	12:45 pm	BNL-Berkner Hall
1:00 pm	BNL-Berkner Hall	1:45 pm	SBU-SAC Loop
4:30 pm	SBU-SAC Loop	5:15 pm	BNL-Berkner Hall
5:30 pm	BNL-Berkner Hall	6:15 pm	SBU-SAC Loop

If you have any questions or concerns regarding the van, please contact Elyce Acierno at 631-632-4360 or Elyce.Acierno@stonybrook.edu. For the most up-to-date schedule, see: http://www.bnl.gov/staffservices/Transportation/transportation.asp.

Remembering Dale Sayers

Laura Mgrdichian, NSLS Science Writer

On November 25, 2004, Dale Sayers, a founder of the extended x-ray absorption fine structure (EXAFS) technique and a prominent NSLS user and advisor, passed away from complications due to a heart attack. He was 60 years old. He is remembered for his immense impact on NSLS science and operations, and his commitment to the field of synchrotron science.

Dale's part in developing EXAFS began in 1968 when he was a graduate student at the University of Washington. He was a student of Edward Stern, a UW faculty member and a consultant for the Boeing Scientific Research Laboratories (BSRL) in Seattle. Stern knew BSRL researcher Farrel Lytle and learned of his work on what would be the early theory of EXAFS. He decided that further work on the subject would be a good thesis project for Dale.

Dale began working with Lytle at his laboratory, measuring the EXAFS of various materials. By the end of the 1970 spring semester, the major parts of the theory were established, but one task was left: determining how to obtain structural information from the EXAFS equation they had formulated. The three decided that inverting the equation would be the way, and, in 1971, Dale tried applying the Fourier integral theorem to the equation. Success!

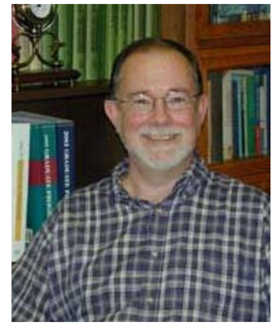
From left, Edward Stern, Dale Sayers, and Farrel Lytle accept the American Crystallographic Association's Bertram Warren Award in 1979, for their development of EXAFS.

In a 1999 Journal of Synchrotron Radiation paper, Lytle wrote, "In a defining moment, I can still visualize Dale's excitement as he ran down the hall to greet me with the first plot of the first Fourier transform of the EXAFS function of germanium!" The EXAFS technique is now used at every synchrotron across the globe.

During his time as a NSLS user, Dale was a physicist with the North Carolina State University (NCSU) but spent a great deal of time here. He was the chair of the NSLS Users Executive Committee (UEC) in the early 1980's when the NSLS was an "unrefined" scientific workplace, and often a difficult environment in which to perform research. Dale established trust between the NSLS and the user community, culminating in an excellent users' meeting in 1985 that included an especially memorable dinner event. He also chaired the UEC in 1987 and '88.

Dale's work at the NSLS led him to establish beamline X11A, which became one of the most scientifically productive beamlines at the NSLS. He also established a participating research team (PRT) at X11 (the longest-lived PRT beamline) and was its spokesperson from 1983 until 2001.

In the 1990's, Dale initiated a mammography project at the NSLS, working with former NSLS staff physicists Bill Thomlinson and Dean Chapman, and current NSLS physicist Zhong Zhong. The project led to the development of diffraction-enhanced imaging (DEI), a technique now used to image bone and soft tissue in a way not possible using conventional x-rays. Dale became the co-spokesperson for beamline X15A after a dedicated DEI system was established there in 1998. He was leading efforts to apply DEI to a clinical setting and was working to characterize bone and reconstruct DEI images using computerized tomography (CT).



While Dale was renowned internationally for his research, his influence extended far beyond raw science. Astute and determined, he was committed to the successful operation of synchrotrons and the success of synchrotron radiation research. He was a trusted advisor to many facilities, and sat on many scientific advisory committees.

Dale was known as a tough, yet fair, advisor, but his personal experiences were filled with laughter and frequent interactions with family, friends, and colleagues. He enjoyed traveling abroad with his wife, Anne, and did so often.

Dale earned his bachelor's degree from the University of California at Berkeley, his master's and Ph.D. degrees at the University of Washington, and joined the NCSU physics department in 1976. He received many awards, including the American Crystallographic Association's Bertram Warren Award, Case Western Reserve University's Centennial Scholar Award, and the Outstanding Achievement Award of the International XAFS Society.

Bill Thomlinson, Zhong Zhong, and Kumi Pandya contributed to this article.

X-Ray Ring Long Range Schedule

January 2005

Sun	Mon	Tue	Wed	Thu	Fri	Sat
						1 Lab Holiday 0000 Maint.
2 0000 Maint.	**3** 0000 Maint.	**4** 0000 Maint.	**5** 0000 Maint.	**6** 0000 Cond.	**7** 0000 Cond.	**8** 0000 Cond.
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30 0000 Ops.	**31** 0000 Ops. 1200 Studies					

February 2005

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27 0000 Ops.	**28** 0000 Ops. 1200 Studies					

March 2005

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27 0000 Ops.	**28** 0000 Ops. 1200 Studies	**29** 0000 Studies	**30** 0000 Studies 1200 Ops.	**31** 0000 Ops.		

April 2005

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					1 0000 Ops.	**2** 0000 Ops.
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17 0000 Ops. 1200 Studies	**18** 0000 Studies 0600 Interlock 1200 Studies	**19** 0000 Studies 1200 Ops.	**20** 0000 Ops.	**21** 0000 Ops.	**22** 0000 Ops.	**23** 0000 Ops.
24 0000 Ops.	**25** 0000 Ops. 1200 Studies	**26** 0000 Studies	**27** 0000 Studies 1200 Ops.	**28** 0000 Ops.	**29** 0000 Ops.	**30** 0000 Ops.

VUV Ring Long Range Schedule

January 2005

Sun	Mon	Tue	Wed	Thu	Fri	Sat
						1 Lab Holiday 0000 Maint.
2 0000 Maint.	**3** 0000 Maint.	**4** 0000 Cond.	**5** 0000 Cond.	**6** 0000 Cond.	**7** 0000 Cond.	**8** 0000 Cond./Ops.
9 0000 Cond./Ops.	**10** 0000 Ops.	**11** 0000 Ops.	**12** 0000 Ops.	**13** 0000 Ops.	**14** 0000 Ops.	**15** 0000 Ops.
16 0000 Ops.	**17 Lab Holiday** 0000 Ops.	**18** 0000 Ops.	**19** 0000 Ops.	**20** 0000 Ops.	**21** 0000 Ops. 1800 Studies	**22** 0000 Ops.
23 0000 Ops.	**24** 0000 Ops.	**25** 0800 Studies	**26** 0000 Studies	**27** 0000 Ops.	**28** 0000 Ops.	**29** 0000 Ops.
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February 2005

Sun	Mon	Tue	Wed	Thu	Fri	Sat
		1 0000 Ops.	**2** 0000 Ops.	**3** 0000 Ops.	**4** 0000 Ops. 1800 Studies	**5** 0000 Ops.
6 0000 Ops. 1200 Studies	**7** 0800 Maint.	**8** 0000 Maint.	**9** 0000 Ops.	**10** 0000 Ops.	**11** 0000 Ops. 1800 Timing	**12** 0000 Ops.
13 0000 Ops.	**14** 0000 Ops. 1800 Timing	**15** 0000 Ops.	**16** 0000 Ops.	**17** 0000 Ops.	**18** 0000 Ops. 1800 Studies	**19** 0000 Ops.
20 0000 Ops.	**21 Lab Holiday** 0000 Ops.	**22** 0000 Ops.	**23** 0000 Studies	**24** 0000 Studies	**25** 0000 Ops.	**26** 0000 Ops.
27 0000 Ops.	**28** 0000 Ops. 1800 Timing					

March 2005

Sun	Mon	Tue	Wed	Thu	Fri	Sat
		1 0000 Ops.	**2** 0000 Ops.	**3** 0000 Ops.	**4** 0000 Ops. 1800 Studies	**5** 0000 Ops.
6 0000 Ops. 1200 Studies	**7** 0800 Maint.	**8** 0000 Maint.	**9** 0000 Ops.	**10** 0000 Ops.	**11** 0000 Ops. 1800 Timing	**12** 0000 Ops.
13 0000 Ops.	**14** 0000 Ops. 1800 Timing	**15** 0000 Ops.	**16** 0000 Ops.	**17** 0000 Ops.	**18** 0000 Ops. 1800 Studies	**19** 0000 Ops.
20 0000 Ops.	**21** 0000 Ops.	**22** 0800 Studies	**23** 0000 Studies	**24** 0000 Ops.	**25** 0000 Ops.	**26** 0000 Ops.
27 0000 Ops.	**28** 0000 Ops. 1800 Timing	**29** 0000 Ops.	**30** 0000 Ops.	**31** 0000 Ops.		

April 2005

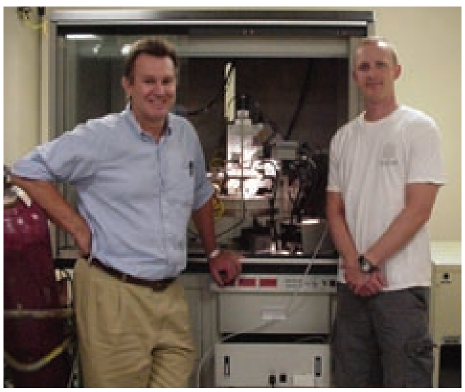
Sun	Mon	Tue	Wed	Thu	Fri	Sat
					1 0000 Ops. 1800 Studies	**2** 0000 Ops.
3 0000 Ops. 1200 Studies	**4** 0800 Maint.	**5** 0000 Maint.	**6** 0000 Ops.	**7** 0000 Ops.	**8** 0000 Ops. 1800 Timing	**9** 0000 Ops.
10 0000 Ops.	**11** 0000 Ops. 1800 Timing	**12** 0000 Ops.	**13** 0000 Ops.	**14** 0000 Ops.	**15** 0000 Ops. 1800 Studies	**16** 0000 Ops.
17 0000 Ops.	**18** 0000 Ops.	**19** 0800 Studies	**20** 0000 Studies	**21** 0000 Ops.	**22** 0000 Ops.	**23** 0000 Ops.
24 0000 Ops.	**25** 0000 Ops. 1800 Timing	**26** 0000 Ops.	**27** 0000 Ops.	**28** 0000 Ops.	**29** 0000 Ops. 1800 Studies	**30** 0000 Ops.

Time-Resolved Diffraction Studies of Ion Exchange: K^+ and Na^+ Exchange into Synthetic Aluminogermanate Molecular Sieve with the Gismondine Topology

Aaron J. Celestian[1], John B. Parise[1,2], Carmen Goodell[1], Akhilesh Tripathi[3], and Jonathan Hanson[4]

[1]Stony Brook University, Department of Geosciences; [2]Stony Brook University, Department of Chemistry; [3]Texas A&M, Department of Chemistry; [4]BNL, Department of Chemistry

Time-resolved in situ x-ray diffraction was used to determine how ions are exchanged in the potassium (K^+) and sodium (Na^+) forms of the aluminogermanate molecular "sieve" (AlGe-GIS) with the topology of the gismondine (GIS) family of zeolite minerals. The AlGe-GIS structure is of particular interest due to its highly flexible framework and its use in industrial processes. This study illustrates the ion site-selective exchange pathways that are created during the substitution process and also determines possible ion exchange mechanisms. Bond valence calculations indicated that the preferred charge-balancing cation in the GIS structure is K^+, due to its larger framework bonding coordination.



Authors (from left): John Parise and Aaron Celestian

Zeolites are nanoporous minerals built from a fully corner-shared framework of tetrahedra. In the gismondine (GIS) family of zeolites, the synthetic aluminogermanate (AlGe-GIS) framework is composed of aluminum (Al^{3+}) and germanium (Ge^{4+}) ions, resulting in a net negative (-1) charge for every Al^{3+} ion in the framework. Therefore, extra-framework cations must be incorporated to charge-balance the structure and maintain electro-neutrality (**Figures 1 and 2**). These extra-framework cations are found in the large channels of the zeolitic framework and can be substituted for other cations. Due to the size, shape, and composition of the zeolitic channels, these materials behave as molecular "sieves" that selectively absorb and desorb cations – a property often used in environmental and industrial applications.

The information obtained from time-resolved in situ x-ray diffraction measurements enables us to directly follow the ion exchange process. The exchange of potassium ions (K^+) into Na-AlGe-GIS proceeded to 90% (±1%) completion within the time frame of the experiment (**Figures 3 and 4**). During the first 10% of K^+ substitution, K^+ only entered the [-101] channel (**Figures 1 and 4**) of the Na-AlGe-GIS structure. After 10%, exchange site-specific substitution could no longer be followed. In the reverse exchange (Na^+ into K-AlGe-GIS; data not shown), a gradual growth of the Na-AlGe-GIS phase was observed and stopped after approximately 10% substitution (**Figure 4**) in the time frame of the experiment. Site-specific ion exchange was not observed during the substitution of Na^+ into K-AlGe-GIS.

The affinity of the GIS framework for the K^+ ion can be explained through bond valence analysis. In K-AlGe-GIS, K conducts most of its bond valence electrons to the O^{2-} framework (approximately 51% of its total valence), thus achieving direct framework charge balancing. In Na-AlGe-GIS, Na^+ conducts most of its bond valence electrons through interstitial water molecules (approximately 71% of

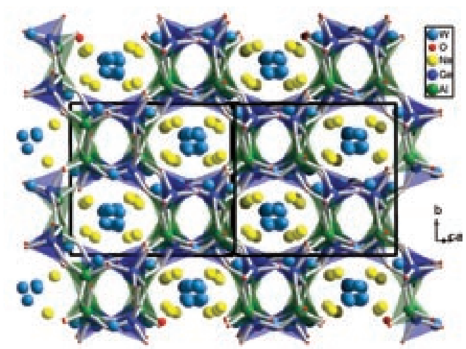


Figure 1. *Crystal structure of Na-AlGe-GIS $Na_{24}Al_{24}Ge_{24}O_{96}$•40 H_2O in the C2/c space group. The 8-member ring channel is filled with Na^+ and water molecules. Unit cell drawn in black. View is down the [-1 0 1] direction.*

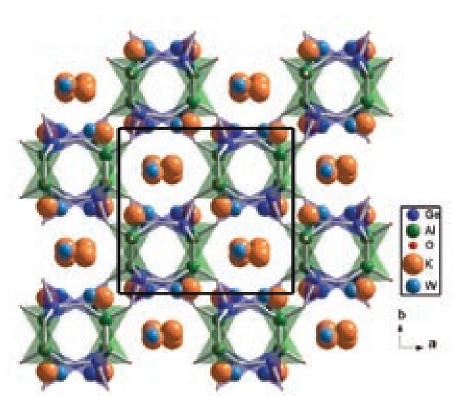


Figure 2. *Crystal structure of K-AlGe-GIS $K_8Al_8Ge_8O_{32}$•$8H_2O$ in the I 2/a space group. The 8-member ring channels are filled with K^+ and water molecules. The unit cell is drawn in black. View is down [0 0 1].*

its total valence). This effectively reduces the amount of direct charge balancing that Na^+ can accomplish and results in a less stable bonding configuration relative to the K^+ bonding environment.

For more details of this work see: A.J. Celestian, J.B. Parise, C. Goodell, A. Tripathi, and J. Hanson, "Time Resolved Diffraction Studies of Ion Exchange: K^+ and Na^+ Exchange into (Al, Ge) Gismondine (GIS) $Na_{24}Al_{24}Ge_{24}O_{96}\bullet 40H_2O$ and $K_8Al_8Ge_8O_{32}\bullet 8H_2O$," Chemistry of Materials, 16(11), 2244-2254 (2004). Experiments were conducted at beamline X7B.

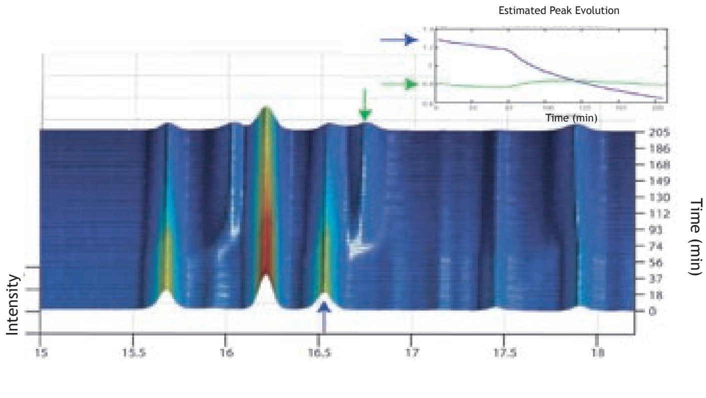


Figure 3. *In situ time resolved diffraction patterns (selected 2-theta range shown for clarity). Each diffraction pattern is collected for 60 sec with 2.5 min between each pattern. The onset of ion exchange is seen approximately 60 min from the start of the experiment. New peak growth at 2-theta 16° and 16.75° indicate the K-AlGe-GIS phase forming. Top right insert shows the Iterative Targeted Transformation Factor Analysis (ITTFA), which follows peak position and intensity over all the diffraction patterns. ITTFA serves as an indicator of when subtle changes in the diffraction patterns occur and identifies those patterns for subsequent structure refinements.*

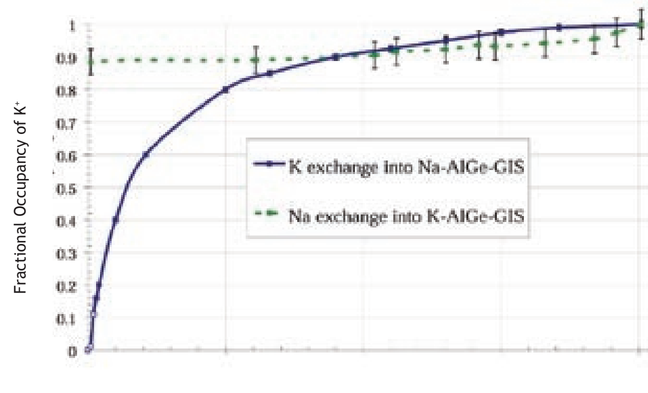


Figure 4. *Plot of K^+ occupancy as a function of time during forward and reverse ion exchanges in AlGe-GIS. Open circles represent structure refinements where site-specific occupancies were refined. Time is normalized due to different experimental time frames.*

Weekly NSLS Activities

TUESDAY

Bi-Monthly Symposia: 10:30 to 11:30 a.m., Seminar Room See URL below for Symposium calendar:
http://www.nsls.bnl.gov/newsroom/events/seminars.htm

WEDNESDAY

Joint VUV and X-Ray Users' Meeting: 11:30 a.m., Conference Room A. Experimenters and staff meet weekly to decide on any proposed short-term schedule changes, to make announcements, and to discuss issues of relevance to operations. To subscribe to the email list for meeting minutes and schedules, follow the instructions at the URL below:
http://www.nsls.bnl.gov/newsroom/events/weekly_meetings.htm

Coffee for Users and Staff: 3:30 p.m., NSLS Lobby. The NSLS hosts a coffee break as an opportunity for users to meet one another and NSLS staff.

THURSDAY

Student/Postdoc Pizza Get-Together: Every other Thursday (starting the first week of January), 1:30 p.m, Room 1-109 on the UV floor (corner kitchen). Funded by the Users' Executive Committee (UEC). All local and visiting students and postdocs are invited to attend. For more information, please contact Meghan Ruppel at (631) 344-2209 or ruppel@bnl.gov.

FRIDAY

Friday Lunch Seminars: 12:00 to 1:00 p.m., Seminar Room. Learn about the exciting research being done at the NSLS. Two unannounced, informal, half-hour presentations are made weekly by experimenters. Attendees can bring their own lunch or can place a sandwich order by contacting Lydia Rogers at (631) 344-4746 or lrogers@bnl.gov by 10:00 a.m. on Friday. Orders must be paid upon delivery.

NSLS Accelerator Complex Update

Erik Johnson, Associate Chair for Operations and Engineering

With fiscal year 2004 completed, it is appropriate to reflect on our goals and achievements. **Figure 1** gives an overall impression for the year, which shows reliability on the VUV ring remains high at 99%, and that x-ray performance is above 90% overall — better than last year, but still not to our own target of 95% reliability.

This global picture doesn't tell the full story. For a significant number of months, x-ray reliability was high, and it even exceeded 98% in February, March, and June. The unanticipated replacement of the x-ray injection ceramic in May was the single largest contributor of down time for the year. We also experienced a swarm of small system failures from late July into August that accrued over 45 hours of down-time, almost twice the average for a whole month. These two types of failures illustrate several important points.

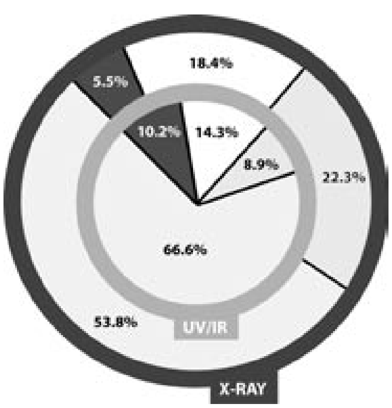
From the users perspective, the summer episode of unrelated equipment failures was more disruptive than the single large failure in May. In the case of the injection ceramic, we knew the magnitude of the problem and were able to provide the user community with advance notice. The series of problems we encountered this summer resulted in down-time scattered throughout a three week period of scheduled operations, impacting many more user experiments than the extension of the May shutdown.

While a few large events can dominate the reliability statistics for any given year, the impact of small-duration but more frequent failures can be devastating for a single user's experimental run. Recognizing this problem, the NSLS has for many years run a preventive maintenance program to minimize equipment failures. Down-time faults and system failures that do occur are carefully monitored to look for trends and address problems where possible. The observed trends can result in significant investment by the NSLS in machine improvement efforts.

This year, both the Accelerator Division and the Operations and Engineering Division devoted great effort to NSLS machine improvements. Digital Closed Orbit Feedback has now been implemented in both planes on the x-ray ring, the culmination of several years of work on orbit stabilization. New machine improvement activities have also been initiated. The injection system, including the linac, booster, and transport lines to the rings, has been the subject of an active study to characterize and improve their performance and reliability. Diagnostics are being added to the transport lines and booster ring to monitor and improve the injection efficiency into the storage rings. High-level accelerator modeling software, developed over the last five years at the ALS and SPEAR, was successfully ported to the NSLS for use in machine studies of the storage rings. These MATLAB-based tools are linked to the NSLS control system and were recently used to restore the eight-fold symmetry of the x-ray ring lattice.

The results of this work are evident in **Figure 2**, which shows a reduction in the photon beam spot size observed with the x-ray pinhole camera on beamline X28B, which is a consequence of a reduction of horizontal electron beam emittance. After several studies shifts with the corrected lattice to verify the robustness of the lattice modeling and the magnet power supplies, the corrected optics were implemented in routine operations before the winter shutdown. In the new year, the modeling tools will also be used to study the horizontal/vertical emittance coupling and its adjustment using the skew quadrupoles in the x-ray ring. The magnetic optics of the VUV ring will also be scrutinized for possible refinements. Beam quality improvement studies will continue through the next year with input from the user community.

The winter shutdown schedule is now underway and operations will resume in mid-January. A longer shutdown was originally planned with the goal of completing the radio frequency (RF) cavity upgrades on the x-ray ring. Although the



User Metrics	UV/IR	X-ray
Reliability	99.0%	91.7%
Availability	114.2%	101.1%

Activity/Hours	UV/IR	X-ray
Operations	5849.4	4725.4
Unscheduled Operations	894.0	483.5
Maintenance	1260.2	1612.1
Other	780.4	1963.0

Other Activities	UV/IR	X-ray
Studies	2.3%	8.4%
Com/Con	2.3%	3.5%
Holiday	2.4%	2.4%
Injection	1.2%	2.4%
Unscheduled Downtime	0.7%	4.9%
Interlock	0.0%	0.7%

YTD 8784 HRs 100 HRs = 1.1%

Figure 1*. Graphical summary of the operations activities for both machines for FY 2004.*

new cavity is ready and we are confident that the cavity can be installed successfully, the NSLS is currently operating with a very austere budget under a continuing resolution. History has shown that other systems are more prone to failure when significant work is undertaken in the ring, and correction of these kinds of problems draws on contingency funds that, at present, are in short supply. Under these circumstances, the decision was made to undertake only routine maintenance and compelling installation tasks as part of this shutdown.

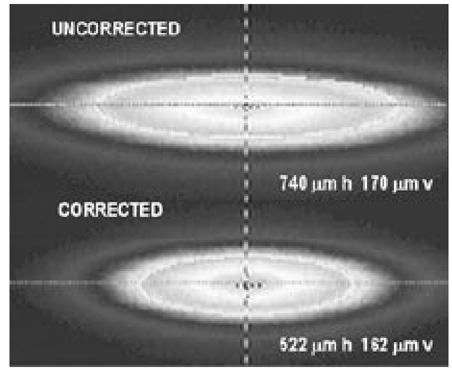


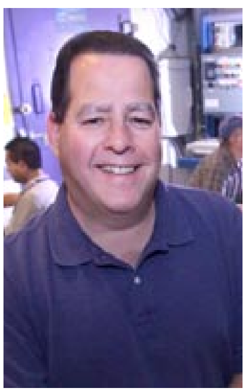
***Figure 2**. Images of the photon beam observed with the pinhole camera on beamline X28B taken in August of 2004 without, and with, the optics corrected. The reduced spot size indicates a reduction (improvement) in horizontal electron beam emittance.*

Finally, thanks again to all who provided input for the Winter 2005 schedule. Some adjustments were made to provide uninterrupted operations opportunities for the powder diffraction workshop and the RapiData 2005 course. It's not too late to provide input for the Summer 2005 schedule. If there are any special scheduling considerations, please let me know by April 2005.

SAFETY

PASS Safety Approval Forms

Andrew Ackerman, NSLS Safety Officer

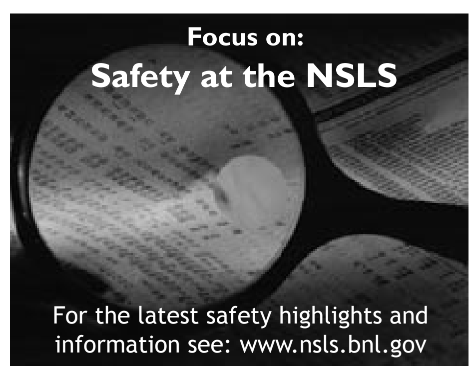


The PASS system is up and running, and our old electronic Safety Approval Form (SAF) system is gone. The switch to PASS has not been easy, as it has required submitting all new forms, but I, for one, will not miss the old system. PASS is a great improvement.

The new SAFs are similar to those we had before, but with some notable exceptions. We have replaced the "Task and Hazard Analysis" section with four new fields in an effort to clarify what information we are trying to gather. The intent is the same: We ask that you describe the mechanics of your experiment, analyze the potential risks, determine what controls are needed, and describe the required actions for responding to a mishap or emergency. In the past, trying to get all of that into a single field was confusing, and we often had to explain our intent and ask for more information. The new format provides better guidance and our submissions have been more complete.

The new system is more interactive and provides more information to users so that completing the forms is easier. Users will get more email messages from the system indicating their progress and status – a mixed blessing I know, but we expect that these emails will help. We have also added a way to designate the "lead experimenter" in the SAFs. We began this requirement some time ago, but did not have a good mechanism to implement it. We were asking you to designate this person when we enabled the beamlines by signing a form with the operations coordinator. That had obvious disadvantages, as the lead experimenter is expected to coordinate with the user group *prior* to their arrival at the NSLS. Now that designation happens early in the process and the lead experimenter has the opportunity to ensure that all the experimenters know the safety requirements before they come. Therefore, designating a lead experimenter is important. Past experience indicates that we need to assign a person to coordinate the safety review with the user group. The new system helps to ensure that happens and is making it easier to do.

For brevity, there are other changes in the new system that I will not list here. I hope that you are finding the PASS system easy to use and that you will speak up and let us know if you are having difficulties. The system is certain to have some problems, but we have the resources we need to make changes, and that process is ongoing. Above all, the purpose of this review program remains unchanged. We need to think about our experiments so that we can analyze and control the risks involved. We have been doing that since the NSLS started, and the new system is intended to make that process easier. Thank you for helping us keep the NSLS a safe place to work and for your patience as we work to improve the PASS system.



Summer Sunday Visitors Battle the Weather for a Great Day at NSLS

Laura Mgrdichian, NSLS Science Writer

Despite the rainy, humid weather, the NSLS Summer Sunday, held August 1, 2004 still pulled in over 450 members of the community and was one of the most enjoyable Sundays yet.

For eight consecutive Sundays each summer, the Brookhaven National Laboratory Summer Sundays program welcomes the public to see the popular Whiz-Bang Science Show and several hands-on science exhibits. Each Sunday also showcases a different BNL facility.

Visitors wishing to see the NSLS began the tour in Berkner Room B, where there were NSLS-specific exhibits and posters, manned by NSLS staff volunteers Steve Ehrlich, Nick Gmur, Payman Mortazavi, Eva Rothman, and Marty Woodle, and student volunteers, Meghan Ruppel and Jyoti Tibrewala. The visitors then saw a short "Introduction to the NSLS" overview film narrated by NSLS Chair, Steve Dierker, before boarding a bus for the facility.

Upon arrival, they were escorted upstairs to see a presentation by an NSLS scientist, who welcomed them and gave more detailed information on the facility and the research performed here. They also discussed how they use synchrotron light to perform their individual research. Many guests were very curious about the NSLS, and the speakers answered several questions after each talk. This year's speakers were Marc Allaire, Elaine DiMasi, Tony Lanzirotti, Lisa Miller, Peter Siddons, and Vivian Stojanoff.

Student volunteer Angela Padilla shows a group of young Summer Sunday visitors how to build a protein crystal model.

NSLS scientist Zhong Zhong shows several Summer Sunday guests how a monochromater divides visible light into a rainbow of colors.

After the talk, visitors filed down to the NSLS lobby and patio, where more activities awaited them, such as the "What am I looking at?" picture window that provides an impressive view of the VUV-IR experimental floor, a sight that is always fascinating for guests. NSLS staff members Steve Bennett, Mike Buckley, Susila Ramamoorthy, and Larry Fareria were on-hand to explain the view and answer questions, such as the common query, "What's the aluminum foil for?" This year, for the first time, large neon numbers were placed on beamline components, which made it easier for guests to see the features described to them.

The lobby also contained several exhibits, such as "See the Light," in which volunteers Randy Smith and Ted Feldman showed how a fiber optic cable siphoned actual NSLS light into the lobby, and "Flowing Lasers," in which Tom Dickinson and Raji Sundaramoorthy made a laser beam "flow" down a stream of water. The children enjoyed watching the laser light fill the water and seeing the light sparkle when they put their hands under the stream. Other displays were hosted by additional NSLS scientists, staff, and students: Peter Abbamonte, Alec Bernston, Brandon Chapman, Ed Haas, Amubhav Jain, Payman Mortazavi, Angela Padilla, Tejas Telivala, Adele Wang, and Zhong Zhong.

On the patio, the visitors saw how superconductivity can "levitate" a magnet and how boiling liquid nitrogen sends a sprinkler spinning. Scientists Wolfgang Caliebe and Cecilia Sanchez-Hanke kept watch over the outdoor activities.

A fun, new event this year was the quiz/raffle, which turned out to be quite successful. Each visitor received a yellow quiz card with questions, which could only be answered by visiting each exhibit. This encouraged them to stop at each one and also made the day more interactive. Every 20 minutes, the quiz cards were collected and Gerry Van Derlaske, the enthusiastic quiz/raffle MC, picked a winning name. Each winner received an NSLS flashlight.

Additionally, at several points during the day, Caliebe braved the rain to launch a giant water rocket in the parking lot across from the NSLS – a hit with all the guests.

The successful day was made possible by several additional volunteers, who served as tour guides, escorts, and support personnel: Melissa Abramowitz, Diane Hatton, Madeline Hughes, Laura Mgrdichian, Eileen Morello, Wendy Morrin, Gina Paveglio, Lydia Rogers, Nancye Wright, and Emil Zitvogel.

Awards and Good Times at the 2004 NSLS Barbeque

Laura Mgrdichian, NSLS Science Writer

On September 24, 2004 a crowd of National Synchrotron Light Source staff members joined the recipients of the 2004 Spotlight and Service awards to celebrate the winners' careers and accomplishments, and to enjoy food, drinks, and the early autumn weather. NSLS Chairman Steve Dierker led the ceremony.

NSLS Chairman, Steve Dierker, presented the Service and Spotlight Awards at the Annual Barbeque.

Service Awards

This year, the following staff members were honored with 25 years of service: Steve Bennett, Rich Biscardi, Conrad Foerster, Tony Lenhard, Bill Newburgh, Gary Ninztel, Stefan Palo, Sal Pjerov, Susila Ramamoorthy, Bob Scheuerer, and Jiunn-ming Wang.

Receiving the 20-year service awards were Bob Best, Pete Ratzke, Ray Raynis, and John Skaritka, and Qing-yi Dong received the 10-year award.

Spotlight Awards

The Spotlight awards, which commend deserving NSLS staff members for exceptional performance during the year, were presented to Laura Miller, recommended by Steve Dierker; Bob Best and Tony Santiago, both recommended by John Gallagher; and two groups (each group shared one award). The first group, nominated by Steve Hulbert, was Dennis Carlson, Michael Caruso, Shu Cheung, Rick Greene, Tony Lenhard, and Gary Nintzel. The second, nominated by Ed Haas, was Walter deBoer, Mike Radulescu, and Bob Scheuerer.

Bob Best: Bob received his award for building, testing, and debugging the laster interlock/controllers system at beamline X17B3. This required extensive planning and coordination between the other electricians at the NSLS. If not for Bob's hard work, one of two costly alternatives to controlling the inner cavity shutter at the beamline would have been explored, resulting in long delays to the program at X17B3.

Tony Santiago: Tony was honored for modifying the Source Development Laboratory's (SDL) laser interlock system, a task that required extensive electrical work and rearrangment. With direction from Scott Buda and John Gallagher, he worked through breaks, lunches, and put in overtime to complete the project, and managed to do so without impacting the operations of the SDL.

Laura Miller: Presented as a surprise, Laura received this award for organizing and planning many of the details of the NSLS-II Workshop. Her hard work, involving extended hours and even weekends, helped to make the workshop incredibly successful. In turn, this success was vital to helping ensure that NSLS-II becomes a reality.

Dennis Carlson, Michael Caruso, Shu Cheung, Rick Greene, Tony Lenhard, and Gary Nintzel: This group was recognized for their exceptional service to the NSLS during the May 2004 shutdown. During this time, three major beamline upgrades were performed *in addition* to the increased beamline maintenance during that period. At X21, the largest of the upgrades, where two nested wiggler beamlines had to be fabricated and installed, the group performed much of this work during the shutdown, and faced several problems that popped up during the process. At the same time, they worked on the upgrades at X13A and X1A1, which both required unexpected work.

Walter deBoer, Mike Radulescu, and Bob Scheuerer: Just before the NSLS May shutdown, a vacuum leak was found in the x-ray ring that worsened until x-ray operations were significantly affected. Walter, Mike, and Bob successful dealt with the problem and the intricate details surrounding it without impacting the x-ray schedule. Walter repeatedly came in after hours and on short notice to temporarily fix the leak. His repairs allowed operations to continue until he could properly fix the problem. From start to finish, Walter performed above and beyond the call of duty.

The leak forced the spring shutdown schedule to be changed, demanded that new work plans be reviewed and approved rapidly, required new hardware to be ordered, and necessitated the location, check, and approval of new fixtures. These details required coordinating many parties across varying time frames. Bob proved instrumental in making it happen.

Mike was the chief technician who performed the repair; he worked flawlessly and quickly, and put in long hours to complete it. His excellent, efficient work helped result in the quick-fix of a complex repair job – finished ahead of schedule with no significant errors.

A group of NSLS staff members enjoy a drink at the Annual Barbeque.

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NSLS Building 725B
P.O. Box 5000
Upton, NY 11973-5000

Call for NSLS General User Proposals

For Beam Time in Cycle	Deadline
May - August 2005	Monday, January 31, 2005

General User Proposal and Beam Time Request Forms with instructions can be found at:
http://www.nsls.bnl.gov/users/usersguide/experiments.htm
Proprietary Proposal Forms with instructions can be found at:
http://www.nsls.bnl.gov/users/usersguide/experiments_proprietary.htm

Safety Approval Forms

Safety Approval Forms (SAFs) are required for every experiment. Your SAF must be submitted online **at least one week before** your scheduled beam time. To submit, go to:

https://pass.nsls.bnl.gov/

NSLS User Administration Office

User Information, Registration, and Training:
Phone: (631) 344-USER   Fax: (631) 344-7206

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