BROOKHAVEN NATIONAL LABORATORY

NEWSLETTER

national synchrotron light source

April 2003

Magnets with Same-Size Nanoparticles Characterized at NSLS

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Scientists at the Naval Research Laboratory have synthesized nanoscale manganese zinc ferrite (MZFO) particles using colloidal aggregates of amphiphilic molecules (having a water-soluble and a water-insoluble component). By using a technique called extended x-ray absorption fine structure (EXAFS) spectroscopy at beamline X11A, the scientists have determined the distribution of the manganese, zinc and iron ions between the lattice sites of MZFO to a precision of eight percentage points.

Nanoscale magnets hold great promise for a wide range of future technologies: aside from improving the performance of microwave filters and power supplies, they could be used in targeted delivery of pharmaceuticals and as biological sensors. Although scientists have been synthesizing nanoscale magnets for many years, the magnetic particles have generally been produced with a wide range of sizes, whereas most applications require particles with a narrow size distribution, called monodisperse particles.

We created monodisperse nanoparticles made of manganese zinc ferrite (MZFO) by using micelles (**Figure 1**), which are colloidal aggregates of thousands of amphiphilic molecules (having a water-soluble and a water-insoluble component). The micelles were formed by adding a small amount of the surfactants nonylphenol poly(oxyethylene)$_5$ and nonylphenol poly(oxyethylene)$_9$ and water to cyclohexane. Micelle self-assembly sequesters the water into tiny droplets of a uniform size determined by the water-to-surfactant ratio, which limits the size of particles formed via aqueous reactions. In our case, the particles were approximately 11 nanometers in diameter. (One nanometer is a billionth of a meter.)

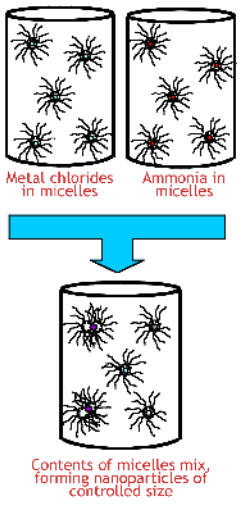


Figure 1. *Schematic of reverse micellar method of nanoparticle synthesis.*

In addition to the problem of monodispersion, the atomic-level structure of nanomagnets in their early development is not well known, so that the characteristics of devices made of nanomagnets are not well defined either. In the case of MZFOs, the manganese, zinc, and iron ions can each potentially reside in two different environments: tetrahedral sites surrounded by four oxygens, or octahedral sites surrounded by six oxygens. By knowing the distribution of the ions between these sites, scientists

INSIDE THIS EDITION

and engineers can better predict the performance of the materials made of MZFOs.

We studied the structure of MZFO by using extended x-ray absorption fine structure (EXAFS) spectroscopy at beamline X11A. In order to determine the distributions of the manganese, zinc, and iron ions, we first measured the ratio of absorbed photons versus the total incident photons. Then, we compared the experimental spectra to theoretical spectra, and developed a model of mixed ferrite materials for the purpose of extracting information from the absorption spectra.

Mark your Calendar

Hand-on Short Course in
EXAFS Data Collection and Analysis
July 14-17, 2003
National Synchrotron Light Source

This course will cover all aspects of EXAFS data collection and analysis: from sample preparation to first-shell fitting. The course is targeted towards new users and young scientists. This course will be similar to the one held last year. For full details, check the NSLS homepage.

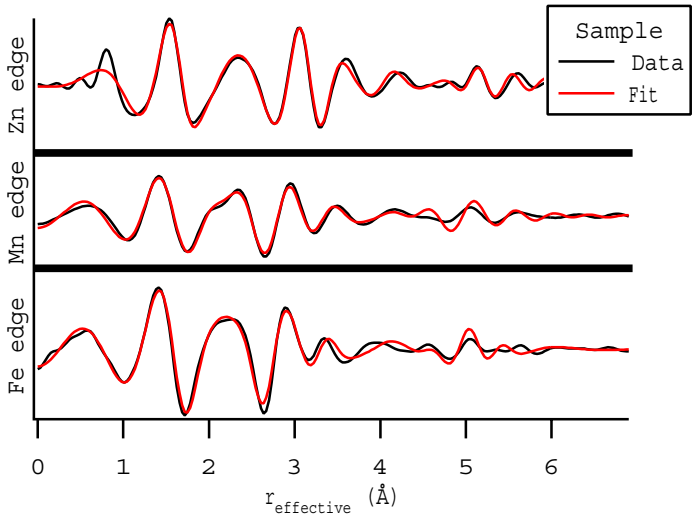
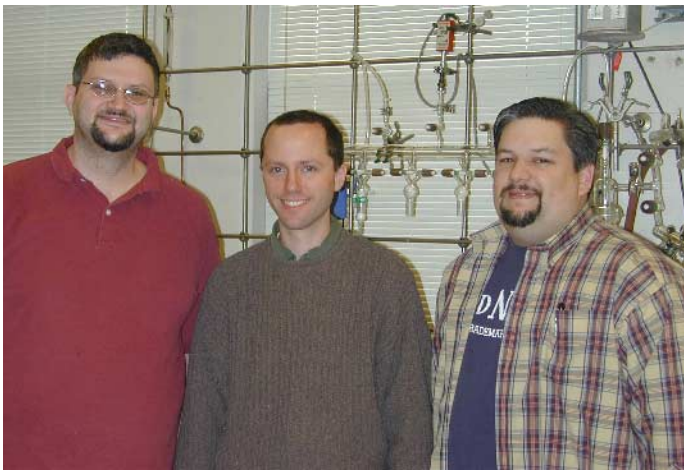


Figure 2. *Real part of the Fourier transform of the EXAFS data for one sample, along with the fitted theoretical model. Above 1 Å (the lower limit of validity for the fitting algorithm) the fitted models reproduce the data with high accuracy, confirming that the nanoparticles adopted the spinel ferrite structure.*

Previous EXAFS studies of magnetic nanoparticles have looked at each metal absorption spectrum separately, allowing scientists to identify, for example, that the zinc ions were in a tetrahedral environment and that the iron and manganese were distributed between tetrahedral and octahedral environments. But, in these studies, scientists could not easily untangle the tetrahedral and octahedral contributions, and determine precise quantitative distributions.

In this study, we fit the models to all three metal edges simultaneously, so that the result was constrained to agree with the stoichiometry of the material and lead to a precision of about eight percentage points for the distribution of manganese, zinc and iron ions (**Figure 2**). The technique outlined here promises to be an important tool in determining the structure of magnetic nanoparticle materials.

*For more details of this work see: S. Calvin, E. Carpenter, V. Harris, and S. Morrison, "Use of multiple-edge refinement of extended x-ray absorption fine structure to determine site occupancy in mixed ferrite nanoparticles," Applied Physics Letters, **81** (20): 3828-3830 (2003).*



Some of the authors of the study: (from left) Everett Carpenter, Scott Calvin, and Shannon Morrison

Notes from the UEC

Leemor Joshua-Tor, Users' Executive Committee Chair
Cold Spring Harbor Laboratory

We have been witnessing many changes at the NSLS in recent months with many more important ones to come. The UEC is actively engaged in giving NSLS management the users' perspective on many of these changes. In order to enhance our communication with the user community and inform you on our activities, we established a new UEC website at www.nslsuec.org. There you will find UEC meeting agendas, summaries from Town Meetings, nominations and voting for UEC and SpIG membership and awards and much much more. We hope that you will find this to be a useful resource.

First and foremost, we are very enthusiastic about the prospects of a major upgrade to the NSLS. We believe that this is critical to the continued vibrancy of the very productive user community of the NSLS and of vital importance to the rich scientific community of the Northeastern region of the United States.

A new user access policy statement was drafted by the directors of the four DOE synchrotron facilities in coordination with the Office of Basic Energy Sciences (BES) at the DOE, which will change the structure of some PRTs and beamline support. Please go to the UEC web site for the full text of the policy statement along with comments from the UEC. These comments are based on input we received from the user community. A much more detailed policy for the NSLS is currently under development. We will solicit comments from the users for this phase as well. In addition, a Proposal and Safety System (PASS), is under development by the Users Administration office to replace the current systems for general user proposals and safety reviews and would reduce the lead-time between proposal and scheduling cycles significantly. My colleagues on the UEC along with very conscientious members of the user community have been actively involved in these projects to make sure they all evolve with you, the user, as the main focal point. I'd like to acknowledge them, and especially Peter Stephens and Daniel Fischer who led these teams from the UEC, for their very hard work and enthusiasm. As always, we welcome your thoughts on any of these issues and we will convey them accordingly.

Most importantly, the UEC is reviewing together with NSLS management how to improve the overall safety record at the NSLS. Special thanks to Paul Stevens and Simon Bare for their efforts. The increase in the number of inexperienced users, who may only spend a few days at the facility, together with perceived lack of attention to safety guidelines by users, calls for a change in the overall culture and working habits at the NSLS. We, as users, have always appreciated the efforts of NSLS staff to place our experiments as the first priority and make the safety procedures as efficient as possible. However, this requires us, the users, to have respect for possible hazards to ourselves as well as to our fellow experimentalists on the floor and be less cynical towards these safety procedures.

Preparations for the Annual Users' Meeting on May 19-21 are well underway

The NSLS and the Users' Executive Committee is pleased to announce the 2003 NSLS Annual Users' Meeting
May 19-21, 2003

For meeting information and to register online, please visit our website at:
http://nslsweb.nsls.bnl.gov/nsls/users/meeting/

Workshops at the Meeting

- Frontiers in Powder Diffraction
- Spectroscopy in High Magnetic Fields: ESR, Infrared and Other Applications
- Applications of Synchrotron Radiation: A Pathway to Process Understanding in Environmental Systems
- Bio-Matters: From Infrared to X-rays
- High Pressure Mineral Physics using Synchrotron Radiation
- EXAFS Under Extreme Experimental Conditions: Small Spot Size, Low Energy, Low Sample Concentration, or Fast Time Resolution

Important Note

Meeting attendees who are foreign nationals planning to reserve housing onsite must register in BNL's Guest Information System no later than April 22, 2003. If you do not currently have a BNL appointment or your BNL ID Badge has expired, review and complete the User Registration requirements at:

http://nslsweb.nsls.bnl.gov/nsls/newuser/accesstothensls-1.htm

and the very capable hands of Tony Lanzirotti and the members of his Organizing Committee team. For details and to register please go to http://nslsweb.nsls.bnl.gov/nsls/users/meeting/ or through the UEC web site. We are looking forward to a very exciting meeting and ask that you mark the date on your calendar. This is an important year for the NSLS with the proposal for a major upgrade underway. An effective way for us as users to convey our enthusiasm for this plan and for the science at NSLS is by attending the meeting and the workshops in full force.

Last year, the UEC instituted a new award: **the NSLS User Community Service Award,** to acknowledge an individual from the NSLS user community in recognition of his/her service, innovation, and/or dedication to NSLS users. This is not an award for scientific achievement, but rather for contributions that have improved the quality of science at the NSLS. The award will be presented at the Annual NSLS Users' Meeting on May 20, 2003. Any member of the NSLS user community with an active appointment is eligible for receipt of this award, excluding current UEC/SpIG members. The award winner will receive a $250 cash award and his/her name engraved of the UEC award plaque in the NSLS lobby. Nominations are accepted through a web-based application form on the UEC website.

As this is my last Newsletter column, I would like to thank all the members of the UEC and SpIG representatives for all their hard work this year. The UEC has been involved in many projects this year and the dedication of the UEC members who stepped up to the plate in many subcommittees from safety issues to access policies to lobbying for funding is very much appreciated. It was a pleasure working with you all. Both the UEC and NSLS management have felt that facilitating the dialogue between us is critical to the success of the facility and the scientific community it serves. This year our communication with NSLS management has greatly improved and we look forward to continue communicating the interests of the users to them.

NSLS UEC website:

http://www.nslsuec.org

for information on all ongoing Users' Executive Committee activities

SAFETY

Are You Thoughtful in Your Approach to Safety?

Bob Casey, Associate Chair for ESH&Q

As has been mentioned on several occasions, last year's safety performance among the NSLS users was tarnished by a series of incidents brought about by noncompliance with NSLS and BNL safety requirements. These incidents resulted in a number of reviews, including an overall critique requested by DOE involving users and staff members. Several actions are being implemented involving improved definition of responsibilities, training and work planning. You will undoubtedly hear more about this as the year progresses.

All of these actions assume one thing – each of you is committed to working safely and in compliance with NSLS requirements. The NSLS management certainly expects that from you. Without your commitment to this issue, all other efforts to improve safety performance are almost meaningless.

As a measure of your commitment, how do you evaluate your own performance in these areas in the last year?

- Were your Safety Approval Forms submitted in a timely fashion and with sufficient detail to permit adequate evaluation of your experiment?
- Was the BLOSA training provided by your group sufficient to ensure that first time users know the important rules and requirements for working safely at your beamline?
- Are the beamline configuration checklists up-to-date and complete, and are they properly used before the beamline is authorized?
- Are your work place and labs maintained in an orderly fashion, and are all chemicals and wastes properly controlled and labeled?
- Have you kept your required training current?

Working safely involves far more than working without injury or incident. How many times have you seen a careless act conducted without harmful consequence? Working safely includes working with a respectful attitude to the requirements applicable to your task. It also means proper planning to ensure that hazards are addressed and that time or resource constraints do not create the temptation to take a risky short cut to complete the work.

Work at an operating facility like the NSLS creates many pressures – time is short, space is tight, rules are strict. Don't respond to these pressures with an attitude about safety that will create a problem for you and your experiment. Remember that expectations at every level of management are high.

So – I urge everyone to be thoughtful about these issues and apply the same attention to safety details that you bring to your experiment. You will find the ESH staff very willing to work closely with you to make your experiment successful.

I opened a fortune cookie recently which had the following saying:

"Attention to safety is never wasted."

Do you agree with that?

New Requirements for Foreign Visitors Approval

Mary Anne Corwin, NSLS User Administrator

As many of you know, the NSLS is now required to strictly adhere to DOE Notice 142.1 "Unclassified Foreign Visits and Assignments." In essence, the mandate requires that (1) all researchers coming to the NSLS to work at a beamline must have an active BNL appointment (for existing users, the expiration date of your appointment can be found on your ID badge), and (2) all foreign national users must have valid passports, visas and INS documentation.

Guests, visitors, and users who do not have approvals prior to arrival and foreign national users whose passport or visa has expired will not be permitted on Brookhaven National Laboratory property. The requirements and procedures to come into compliance were emailed to our users in December. Though we had hoped to see little disruption in our programs and use of the facility, many users have encountered problems accessing the site. Since January, several were required to leave BNL until valid visa and passport documentation was provided and/or appropriate approvals for site access were granted.

Provided below are some of the experiences our users have had, followed by the appropriate procedures to come into compliance. Times have changed and, as much as we wish to accommodate our users, it is extremely important that our users be cognizant of the new security policies and to act responsibly to ensure the process is as efficient as possible.

Tourist visas (i.e., B2 and WT) are not valid for conducting work or research at BNL. Upon entering the U.S. at JFK Airport, three different users were issued an I-94 for a B2 (tourist) visa rather than the appropriate B1. On arrival at BNL, registration could not be finalized until the I-94 was corrected. For two users, the process required a letter from BNL and that each guest return to the airport within 48 hours of entry accompanied by a BNL scientist familiar with their work. The third user was required to return to his country of citizenship since the 48 hours had elapsed.

Visit approval is required. For all new users and those with expired appointments, approval must be granted prior to arrival at BNL. Foreign nationals are required to submit the registration or extension form at least 30 days in advance. There were many instances where users submitted a registration form, providing less than 30 days notice of their intended visit. User Administration sent emails to advise these users not to make travel plans until approval was granted, yet several disregarded the instructions, arrived at BNL as planned, and were required to leave until approval was complete.

Renew your appointment when you receive a letter of termination. Approximately two months prior to the expiration of each user's appointment, User Administration emails users to advise of the upcoming termination and instructs them to extend their appointment if they plan to perform additional research at BNL. Several users have arrived with expired badges and without having submitted the form to request an extension. The badges were confiscated at the gate and the users were directed to User Administration. They were again provided instructions on requesting an extension and required to leave BNL until approval was granted. Their files indicated they were sent termination letters and instructions on extending their appointment. If you receive a termination letter, please take the opportunity at that time to request an extension. It will eliminate any possible delays to accessing the site, which may take up to 30 days.

Passports and Visas must be valid. All foreign national users must have valid passports, visas and INS documentation. User Administration enters this information into the laboratory's guest information system at the time an appointment is issued or renewed, and it must be updated if the documentation expires. As each badged user arrives at BNL, their badge is scanned at the gate. If their passport or visa has expired or the information is not currently in the lab's system, the scanner will indicate a "yellow" light. The user will be directed to User Administration (during normal working hours) or may be requested to leave BNL (evenings and weekends). In December, users were notified to carry valid passports and visa documentation with them at all times while onsite. In a few instances, users traveled considerable distances only to find they would not be granted site access because their documentation had been left at their home institution.

New requirements for Permanent Residents of Canada. Effective March 17, 2003, all Permanent Residents of Canada (often referred to as landed immigrants), must present a valid passport and visa when applying for admission to the U.S.

DIAL 344-USER FOR NSLS USER ADMINISTRATION

In our goal to facilitate user access to the National Synchrotron Light Source at Brookhaven National Laboratory, you may now dial (631) 344-USER to reach the NSLS User Administration Office, or simply Ext. USER while onsite. The old number (631) 344-7976 will remain in service as a rollover number.

COMPLIANCE OF DOE NOTICE 142.1

(1) Request and receive approval of the visit to BNL prior to arrival. **New users** use the BNL Guest Registration Form at: https://fsd84.bis.bnl.gov/guest/guest.asp. **Expired users** use the BNL Guest Extension Form at: https://fsd84.bis.bnl.gov/guest/bnlguest.asp. Note: Foreign nationals must submit the form at least 30 days prior to arrival. Citizens of Cuba, Iran, Iraq, Libya, North Korea, Sudan and Syria must submit the form at least 120 days prior to arrival (180 days is suggested).

(2) Bring identification. **U.S. citizens** must bring a driver's license or other official photo identification on the first visit. To avoid future delays at the gate, also bring your birth certificate or passport on your first visit so that your badge may be coded to eliminate the scanning requirement. **Foreign Nationals** must bring the following documentation and carry it with you at all times while at BNL: (1) Passport with I-94 attached, (2) Visa stamp in passport with INS or DOS documentation showing that visa status is valid, (3) Valid Employment Authorization Document (EAD) and an I-20AB approved by your university's international officer IF you have an F-1 Student status and are working on an Employment Authorization Document, (4) Academic institution identification card (if you are a student). **Permanent Resident Aliens** must bring a valid Green Card or passport (with valid I-551 stamp) and carry it with you at all times while at BNL.

(3) Proceed to User Administration on arrival. New users and users with expired appointments must arrive at NSLS User Administration between the hours of 8:00 a.m. and 3:00 p.m. Monday through Friday to finalize the registration process, verify or complete required training, and process an ID badge. Access will not be permitted until this process is complete.

(4) Check in/check out. Prior to arrival at BNL, all users must notify BNL of your arrival date. Use the Guest Check In/Out Form at https://fsd84.bis.bnl.gov/guest/guestlog.asp. Users arriving intermittently or infrequently (who do not work permanently onsite) must submit the dates as accurately as possible for each visit. Users who are at BNL on a permanent basis (working here every day) may use the start and end dates of their appointments. It is vitally important that this information be as accurate as possible. BNL has specific reporting requirements and is subject to periodic audits of this information by DOE.

If you have any questions concerning the requirements, please contact the NSLS User Administration Office at nslsuser@bnl.gov or (631) 344-USER.

Weekly NSLS Activities

TUESDAYS

Bi-Weekly Symposium: 10:30 to 11:30 a.m., Seminar Room

WEDNESDAYS

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://nsls.bnl.gov/nsls/announcements/listservers.htm#xray-minutes

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.

THURSDAYS

VUV Users' Meeting: 11:30am, 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://nslsweb.nsls.bnl.gov/nsls/announcements/listservers.htm#vuv-minutes

FRIDAYS

Student/Postdoc Pizza Get-Together: Every other Thursday, 4:00 p.m, NSLS x-ray ring kitchen (across from vending machines). Funded by the Users' Executive Committee (UEC). Organized by NSLS Postdoc, Udupi Ramagopal (acharya@bnl.gov). All local and visiting students and postdocs are invited to attend.

Friday Lunch Seminars: 12:00 to 1:00 p.m., Seminar Room. Anyone interested in learning about the exciting research being done at the NSLS is invited to the Friday lunch time seminar. 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 Joan Marshall at (631)344-3887 or jmarshall@bnl.gov by 10:00 a.m. on Friday. Orders must be paid upon delivery.

Journal Club: 3:00 to 4:00 p.m., Conference Room B. Students, postdocs, and staff present hot new research publications of their choice for group discussion. Everyone is invited to attend and volunteers are always welcome. For more information, contact Cecilia Sanchez-Hanke, (631)344-5699 or hanke@bnl.gov.

Brookhaven National Laboratory and Stony Brook University Open New Environmental Center

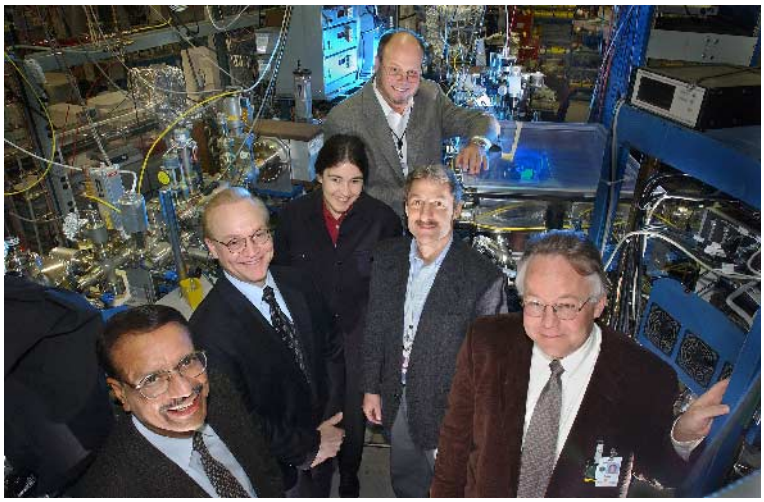
Patrice Pages, NSLS Science Writer

With funding from the U.S. Department of Energy and the National Science Foundation, Brookhaven National Laboratory and Stony Brook University have opened a new center for scientists investigating how contaminants affect the environment. Called the Center for Environmental Molecular Science, the new initiative has been established in collaboration with Penn State University and Temple University.

"Until now, most environmental research has been done by scientists working within their own disciplines, but there is a limit to what can be accomplished this way," said center director and Stony Brook professor Richard Reeder. "We created this center to bring together scientists from a variety of disciplines so that we can be better prepared to tackle major issues, such as cleanup efforts at nuclear waste sites and the behavior of contaminants in water."

The new center will bring together scientists working in areas as diverse as physics, chemistry, geosciences, microbiology, materials science, marine science, and waste technology. They will share the use of facilities at Brookhaven and Stony Brook.

For example, to study the chemical composition of soil contaminants, scientists use a device called an x-ray microprobe, set up at Brookhaven's National Synchrotron Light Source. The technique focuses x-ray beams to about one-millionth of a meter, which is the scale required to determine how contaminants are distributed among soil components. The technique has been so successful that the Light Source is adding a new microprobe, with funding from the Department of Energy's Office of Basic Energy Sciences and Office of Biological and Environmental Research.



Scientists and students at the new Center for Environmental Molecular Science will use Brookhaven's National Synchrotron Light Source. Pictured at the Light Source are (from left) A.J. Francis, Ralph James, Clare Grey, Creighton Wirick, Richard Reeder, and Doon Gibbs. Francis, James, Wirick, and Gibbs are Brookhaven scientists. Grey and Reeder are professors at Stony Brook.

An important aspect of the new center is student participation, according to Brookhaven scientist A.J. Francis, one of the center's two associate directors, along with Stony Brook professor Clare Grey. "We would like to involve students in environmental research," said Francis, whose own work has lead to a patented process for cleaning contaminated soils and incinerator ash with citric acid, naturally occurring soil bacteria, and sunlight. Adds Reeder, "It's a good way to get students excited about pursuing a career in science."

Faculty-Student Research Support Program

What is it? The Faculty Student Research Support Program is designed to encourage new faculty/student research groups to BNL's National Synchrotron Light Source. Faculty members that are new users to the NSLS and their research groups are eligible. In addition, newly appointed assistant professors (within 2 years of faculty appointment) and their students are also eligible, even if they are current or past NSLS users. The program covers expenses incurred during exploratory visits to the NSLS and while performing initial experiments. Expenses covered include travel, housing, per diem, and some incidental costs.

Who is it for? Members of U.S. academic institutions of higher education.

How do you apply? To find out more information and apply for the program online, visit:

http://nslsweb.nsls.bnl.gov/nsls/users/funding/fsrsp/

X-Ray Ring Long Range Schedule

May 2003

Sun	Mon	Tue	Wed	Thu	Fri	Sat
				1 00-0800 Ops. 08-2400 Maint.	**2** 00-2400 Maint.	**3** 00-2400 Maint.
4 00-2400 Maint.	**5** 00-2400 Maint.	**6** 00-2400 Maint.	**7** 00-2400 Maint.	**8** 00-2400 Maint.	**9** 00-2400 Maint.	**10** 00-2400 Maint.
11 00-2400 Maint.	**12** 00-2400 Maint.	**13** 00-2400 Maint.	**14** 00-2400 Maint.	**15** 00-2400 Cond.	**16** 00-2400 Cond.	**17** 00-2400 Cond.
18 00-2400 Cond.	**19** 00-2400 Cond.	**20** 00-2400 Cond. and/or Ops.	**21** 00-2400 Ops.	**22** 00-2400 Ops.	**23** 00-2400 Ops.	**24** 00-2400 Ops.
25 00-2400 Ops.	**26 Holiday** 00-2400 Ops.	**27** 01-0800 template 08-2400 Ops.	**28** 00-2400 Ops.	**29** 00-2400 Ops.	**30** 00-2400 Ops.	**31** 00-2400 Ops.

June 2003

Sun	Mon	Tue	Wed	Thu	Fri	Sat
1 00-1200 Ops. 12-2400 Studies	**2** 00-0600 Studies 06-1200 Intlk. 12-2400 Studies	**3** 00-1200 Studies 12-2400 Ops.	**4** 00-2400 Ops.	**5** 00-2400 Ops.	**6** 00-2400 Ops.	**7** 00-2400 Ops.
8 00-2400 Ops.	**9** 00-1200 Ops. 12-2400 Studies	**10** 10-2400 Studies	**11** 00-1200 Studies 12-2400 Ops.	**12** 00-2400 Ops.	**13** 00-2400 Ops.	**14** 00-2400 Ops.
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29 00-2400 Ops.	**30** 00-2400 Ops.					

July 2003

Sun	Mon	Tue	Wed	Thu	Fri	Sat
		1 00-2400 Ops.	**2 Holiday** 00-2000 Ops.	**3 Holiday** No beam	**4 Holiday** No beam	**5 Holiday** No beam
6 Holiday No beam	**7** 00-0600 Studies 06-1200 Intlk. 12-2400 Studies	**8** 00-2400 Studies	**9** 00-2400 Ops.	**10** 00-2400 Ops.	**11** 00-2400 Ops.	**12** 00-2400 Ops.
13 00-2400 Ops.	**14** 00-2400 Ops.	**15** 00-2400 Ops.	**16** 00-2400 Ops.	**17** 00-2400 Ops.	**18** 00-2400 Ops.	**19** 00-2400 Ops.
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August 2003

Sun	Mon	Tue	Wed	Thu	Fri	Sat
					1 00-2400 Ops.	**2** 00-2400 Ops.
3 00-1200 Ops. 12-2400 Studies	**4** 00-0600 Studies 06-1200 Intlk. 12-2400 Studies	**5** 00-1200 Studies 12-2400 Ops.	**6** 00-2400 Ops.	**7** 00-2400 Ops.	**8** 00-2400 Ops.	**9** 00-2400 Ops.
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31 00-1200 Ops. 12-2400 Studies						

VUV Ring Long Range Schedule

May 2003

Sun	Mon	Tue	Wed	Thu	Fri	Sat
				1 00-2400 Ops.	**2** 00-2400 Ops.	**3** 00-1800 Ops. 18-2400 Studies
4 00-2400 Ops.	**5** 00-2400 Maint.	**6** 00-2400 Maint.	**7** 00-2400 Maint.	**8** 00-2400 Maint.	**9** 00-2400 Maint.	**10** 00-2400 Maint.
11 00-2400 Maint.	**12** 00-2400 Maint.	**13** 00-2400 Maint.	**14** 00-2400 Maint.	**15** 00-2400 Maint.	**16** 00-2400 Maint.	**17** 00-2400 Cond.
18 00-2400 Cond.	**19** 00-2400 Cond.	**20** 00-2400 Cond.	**21** 00-2400 Ops.	**22** 00-2400 Ops.	**23** 00-1800 Ops. 18-2400 Studies	**24** 00-2400 Ops.
25 00-2400 Ops.	**26 Holiday** 00-2400 Ops.	**27** 00-2400 Ops.	**28** 00-2400 Ops.	**29** 00-2400 Ops.	**30** 00-1800 Ops. 18-2400 Studies	**31** 00-2400 Ops.

June 2003

Sun	Mon	Tue	Wed	Thu	Fri	Sat
1 00-2400 Ops.	**2** 00-2400 Ops.	**3** 00-2400 Studies	**4** 00-2400 Studies	**5** 00-2400 Ops.	**6** 00-2400 Ops.	**7** 00-2400 Ops.
8 00-2400 Ops.	**9** 00-2400 Ops.	**10** 00-2400 Ops.	**11** 00-2400 Ops.	**12** 00-2400 Ops.	**13** 00-1800 Ops. 18-2400 Studies	**14** 00-2400 Ops.
15 00-2400 Ops.	**16** 00-2400 Ops.	**17** 00-1800 Ops. 18-2400 Studies	**18** 00-2400 Maint.	**19** 00-2400 Maint.	**20** 00-1800 Ops. 18-2400 Timing	**21** 00-2400 Ops.
22 00-2400 Ops.	**23** 00-1800 Ops. 18-2400 Timing	**24** 00-2400 Ops.	**25** 00-2400 Ops.	**26** 00-2400 Ops.	**27** 00-1800 Ops. 18-2400 Studies	**28** 00-2400 Ops.
29 00-2400 Ops.	**30** 00-2400 Ops.					

July 2003

Sun	Mon	Tue	Wed	Thu	Fri	Sat
		1 00-2400 Ops.	**2 Holiday** 00-2000 Ops.	**3 Holiday** No beam	**4 Holiday** No beam	**5 Holiday** No beam
6 Holiday No beam	**7** 00-2400 Cond.	**8** 00-2400 Studies	**9** 00-0800 Studies 08-2400 Ops.	**10** 00-2400 Ops.	**11** 00-1800 Ops. 18-2400 Studies	**12** 00-2400 Ops.
13 00-2400 Ops.	**14** 00-2400 Ops.	**15** 00-2400 Ops.	**16** 00-2400 Ops.	**17** 00-2400 Ops.	**18** 00-1800 Ops. 18-2400 Studies	**19** 00-2400 Ops.
20 00-2400 Ops.	**21** 00-2400 Ops.	**22** 00-1800 Ops. 18-2400 Studies	**23** 00-2400 Maint.	**24** 00-2400 Maint.	**25** 00-2400 Ops.	**26** 00-2400 Ops.
27 00-2400 Ops.	**28** 00-1800 Ops. 18-2400 Timing	**29** 00-2400 Ops.	**30** 00-2400 Ops.	**31** 00-2400 Ops.		

August 2003

Sun	Mon	Tue	Wed	Thu	Fri	Sat
					1 00-1800 Ops. 18-2400 Studies	**2** 00-2400 Ops.
3 00-2400 Ops.	**4** 00-2400 Ops.	**5** 00-2400 Studies	**6** 00-2400 Studies	**7** 00-2400 Ops.	**8** 00-2400 Ops.	**9** 00-2400 Ops.
10 00-2400 Ops.	**11** 00-2400 Ops.	**12** 00-2400 Ops.	**13** 00-2400 Ops.	**14** 00-2400 Ops.	**15** 00-1800 Ops. 18-2400 Studies	**16** 00-2400 Ops.
17 00-2400 Ops.	**18** 00-2400 Ops.	**19** 00-1800 Ops. 18-2400 Studies	**20** 00-2400 Maint.	**21** 00-2400 Maint.	**22** 00-1800 Ops. 18-2400 Timing	**23** 00-2400 Ops.
24 00-2400 Ops.	**25** 00-1800 Ops. 18-2400 Timing	**26** 00-2400 Ops.	**27** 00-2400 Ops.	**28** 00-2400 Ops.	**29** 00-1800 Ops. 18-2400 Studies	**30** 00-2400 Ops.
31 00-2400 Ops.						

Superbug's Resistance to Antibiotics Revealed

Daniel Lim and Natalie C. J. Strynadka

University of British Columbia, Vancouver, Canada

Some strains of the bacterium Staphylococcus aureus *have developed resistance to multiple antibiotics and have emerged as major pathogens in hospitals worldwide. Resistance of these "superbugs" to the clinically important β-lactam class of antibiotics is mediated by a bacterial enzyme called penicillin-binding protein 2a (PBP2a). This enzyme catalyzes the formation of the bacterial cell wall, a process inhibited by β-lactam, thus weakening the bacterium, and ultimately killing it. The three-dimensional structure of PBP2a, determined on beamline X8C by researchers from the University of British Columbia in Vancouver, Canada, reveals the structural basis of the resistance of* S. aureus *to β-lactam, and provides insights for the design of more effective inhibitors of the bacterium.*

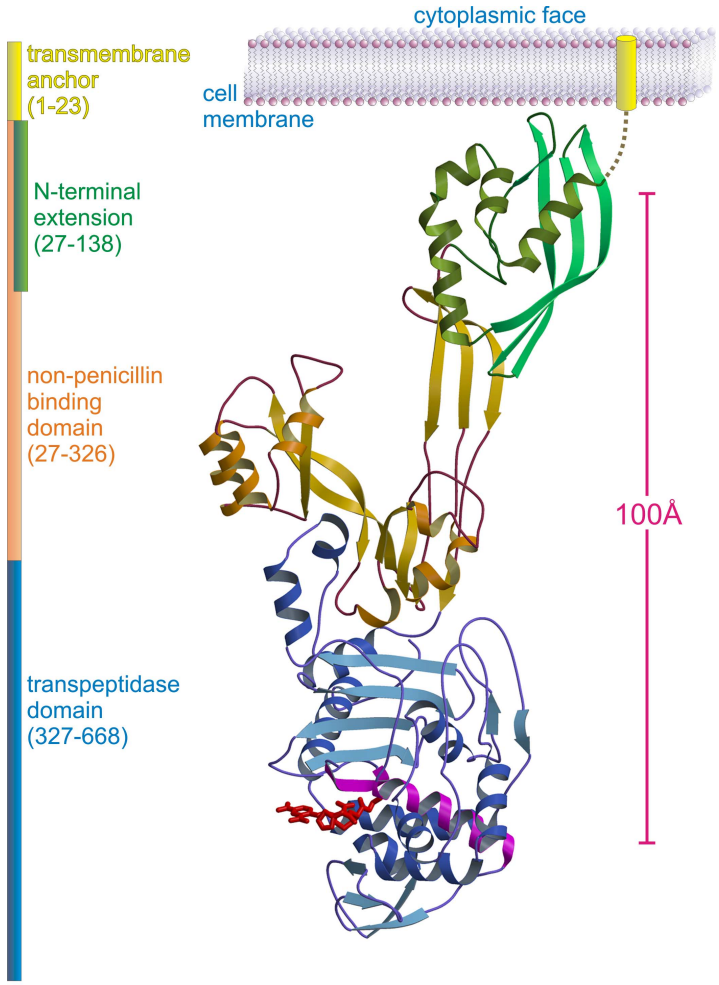


Figure 1. *Structure of penicillin-binding protein of the bacterium* Staphylococcus aureus *(SauPBP2a*). The bilobed N-terminal (nPB) domain is colored orange with the N-terminal lobe (N-terminal extension) colored green. The transpeptidase domain is colored blue with the position of the active site indicated by the red nitrocefin adduct (shown in stick rendering). The secondary structure elements of the transpeptidase domain were labeled in accordance with the labeling scheme used for R6 PBP2x. The N- and C-termini are labeled N and C, respectively. Shown to the left of the ribbon representation is a linear representation of the domain structure of SauPBP2a* with residue numbers shown in parentheses.*

The introduction of penicillin in the 1940s quickly selected for resistant strains of the bacterium *Staphylococcus aureus* that produced penicillinase, an enzyme that hydrolyzes β-lactam antibiotics, the most commonly used line of defense against bacterial infections. To counter these resistant bacterial strains, methicillin, a semisynthetic penicillinase-resistant penicillin derivative, was subsequently introduced.

Resistance to methicillin began to appear just one year after its introduction and has since spread to hospitals world-wide with alarmingly high prevalence of these strains, called methicillin-resistant strains of *Staphylococcus aureus* (MRSA), among clinical isolates in the United States and in a number of Asian and European countries. As MRSA strains are resistant to other classes of antibiotics, vancomycin has often been the treatment of choice against MRSA infections. But the appearance of vancomycin resistance in MRSA clinical isolates – first in Japan, and then in other countries, including the United States in recent months – underlines an urgent need for novel antibiotics.

β-lactams act as substrate analogs of bacterial enzymes called penicillin-binding proteins (PBPs) that catalyze the formation of peptide cross-links in the bacterial cell wall. By binding to PBPs, β-lactams irreversibly inhibit PBPs, resulting in a weakened cell wall and eventual cell death. Methicillin resistance in MRSA

strains is due to the horizontal acquisition – from an unidentified species – of the *mecA* gene, which encodes PBP2a, a novel PBP distinct from the PBPs normally found in *S. aureus*. PBP2a is highly resistant to inhibition by all clinically used β-lactams and remains active to maintain cell wall synthesis at normally lethal β-lactam concentrations.

To identify the structural features of PBP2a that are responsible for *S. aureus* resistance, we determined the protein's crystal structure. To obtain crystals of PBP2a, a soluble derivative was constructed by removing the N-terminal transmembrane anchor – which does not affect its interaction with β-lactams. The excellent facilities at beamline X8C at the NSLS, allowed us to collect data to 1.8 angstrom resolution for crystals of the apoenzyme (the enzyme with no inhibitor bound), and to 2.0 angstrom resolution for crystals of PBP2a bound to nitrocefin (a type of β-lactam). By comparing these structures, we noticed novel conformational changes at the active site that have not been observed in structures of β-lactam sensitive PBPs. Thus the active site of apoenzyme part of PBP2a is distorted relative to those of non-resistant PBPs.

Previous kinetic studies have shown that while the initial binding affinities of PBP2a for β-lactams are comparable to those of non-resistant PBPs, the subsequent acylation step, during which the PBP and β-lactam bind with an RCO- group (R being an organic group), is 1000 fold slower in PBP2a than in non-resistant PBPs. Acylation is key to the inhibition of PBPs by β-lactams, so reduction of acylation rate confers broad-spectrum resistance of *S. aureus* to antibiotics. But acylation is also key to the normal function of PBPs, so that the distorted active site of PBP2a provides a means of modulating acylation rate to balance resistance with retention of activity.

Given that slow acylation is an intrinsic property of PBP2a, more effective inhibitors could be designed by improving their initial binding affinity to PBP2a. For example, novel forms of widely used antibiotics called cephalosporins provide a larger number of stabilizing interactions with and better shape complementarity to the narrow PBP2a active site groove, and thus show improved affinities for PBP2a. Optimization of cephalosporins and other inhibitors will be greatly facilitated by the structural information on the active site from our studies.

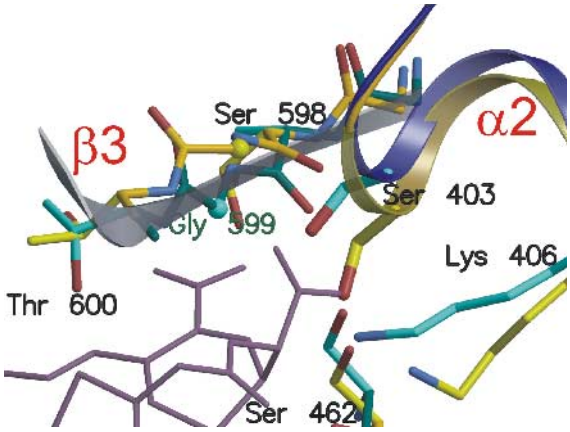


Figure 2. *Superposition of the active site region from the native penicillin-binding protein of the bacterium* Staphylococcus aureus *(SauPBP2a*) and SauPBP2a* acylated with nitrocefin. Nitrocefin is shown in thin stick rendering. Covalent binding of nitrocefin to SauPBP2a* requires conformational changes at strand β3 and at the N-terminus of helix α2.*

For more details of this work see: D. Lim and N.C.J. Strynadka, "Structural basis for the β-lactam resistance of PBP2a from methicillin-resistant Staphylococcus aureus," Nature Structural Biology ***9****, 870 (2002).*

RING STATUS

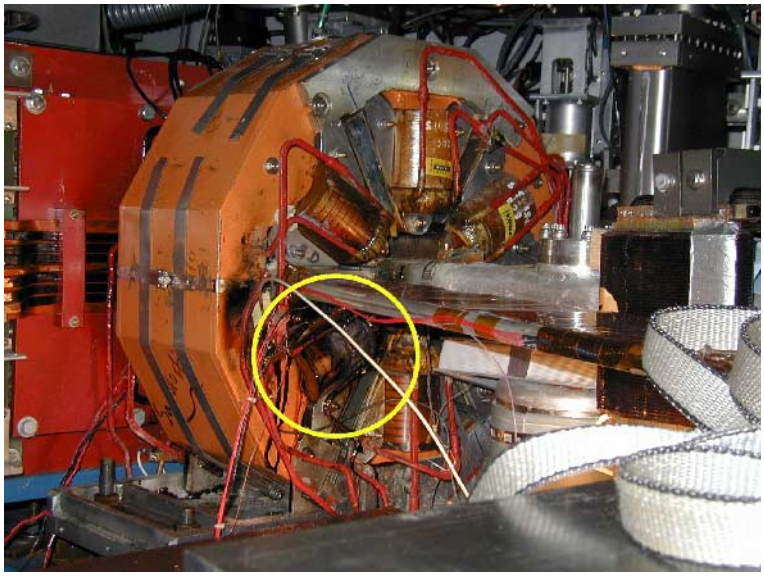
NSLS Accelerator Complex Update

Erik Johnson, Associate Chair for Operations and Engineering

During the winter shutdown just passed, the central planned activity was the installation of the third of our new x-ray cavities. This work, combined with the shield wall modifications at X29, continues to pave the way for a new Mini-Gap Undulator (MGU) beamline to add to the complement of NSLS insertion device instruments. As the shutdown was winding down to a successful conclusion in January, our staff was confronted by a major component failure that set us back considerably.

On January 10th, as the magnets were being ramped to full power for the first time since the shutdown started, one of the sextupoles experienced a loss of cooling water sufficient to lead to a catastrophic failure of one of the coils, in what turned out to be just a few minutes. Even determining the exact nature of the failure when the smoke cleared was difficult, because as luck would have it the failed magnet was located down stream of the X5 (LEGS) straight section in one of the most inaccessible areas in the ring.

An operation, which was in its own right a major shutdown, was quickly organized to extract, rebuild, and reinstall the failed magnet. Staff from the LEGS



Shown at left is the failed sextupole and, even with some of the LEGS equipment already removed, it is very difficult to see, much less work on. In the photo above, the LEGS spectrometer magnet has been removed, exposing the downstream end of the sextupole where the failed coil comes clearly into view (circled in yellow).

experiment came in and disassembled their equipment to provide access for the removal of the sextupole, taking their own experiment off line for an extended period of time. The recovery program was managed by Don Lynch, with an extraordinary effort from many members of staff. Bill Bambina, Walter deBoer, Mike Fulkerson, Jim Garrison, Rodger Hubbard, Pat Moylan, Jim Newburgh, Jorge Oliva, Sorin Pop, Mike Radulescu, Lenny Santangelo, Bob Scheurer, Mike Schwarz, Tom Seda and Gerry van Derlaske were especially heavily involved, although staff from every section of the division pitched in as needed to speed the process along.

The actual failure was due to overheating of one of the coils, which under normal operation carries more than 800 Amperes current. The coils are water cooled, and loss or reduction of water flow will result in a runaway heating. A partial temporary blockage in the failed coil is thought to be the cause of the failure in this case based on analysis and circumstantial evidence, since testing of the magnet when it was removed did not show any significant blockage. Under these circumstances, the most probable scenario is thought to be excess braze material in a joint, which caught some foreign matter during operation. This partial blockage caused a reduction of cooling sufficient for the coil to overheat, and that overheating was sufficient to open the braze joint, clearing the blockage.

The failed coil was replaced, and additional heat sensors were attached to the magnet to allow more rapid fault detection as protection against a repeat failure. The magnet was reinstalled, and commissioning resumed. The LEGS equipment is being reinstalled during studies and maintenance periods to bring their experiment back on line. Overall, the return to operations was delayed by 9 days, making this the most significant down time event for NSLS in recent memory.

On a personal note, not that I wish for events like these, it did my heart good to see everyone pull together on this effort so well. I'm privileged to have the opportunity to work with people who take such pride in their work, and who share the common goal of keeping the NSLS running for our user community. I'd like to extend my thanks to them, and to the LEGS team for helping us return to operations as quickly as possible.

Operations on both rings during February returned to levels of reliability more typical for the NSLS with 3 hours of down time on VUV and 17 hours on X-ray, occurring mostly in interruptions of an hour or less.

With the winter shutdown now behind us, work is already well underway for the spring shutdown. The major activity planned involves the installation of the MGU for X29. The U14 water cooled mask will be replaced, and significant booster maintenance time is scheduled. Other work is under consideration as time and staffing levels allow. The return to operations on both rings is planned to coincide with the conclusion of the NSLS users meeting.

NSLS Facility Report

Gerry Van Derlaske, NSLS Building Manager

The annual winter maintenance shutdown is now just a memory, but what a memory it is. Many notable projects were completed, including the installation of a new radio frequency (RF) cavity in the X-ray ring, the X29 beamline front-end components, and the reworking of the X29 sawtooth entrance and shield wall. Unfortunately, these projects were temporarily overshadowed by the failure of a magnet coil located near the LEGS dipole magnet. This coil overheated during the start-up/commissioning phase. Quick responses by the appropriate Control Room and Emergency Services personnel likely averted a much bigger catastrophe. Upon evaluation of the scene, a determination was rendered to remove and repair the coil and resume commissioning as soon as possible. Many crews, ranging from the Scientific/Technical Sections to Plant Engineering and other Lab Support Services, worked long and hard to keep the downtime to a minimum. Dedication and sweat was rewarded as the payoff resulted in a delay in the commissioning of just over a week.

The long awaited construction of the new X17B2/B3 hutches has been completed; users will be in full occupancy of the hutches as of this printing. Feel free to stop by and take a look at these most unique steel/lead/steel prefabricated panel hutches. A few of the special design features incorporated into the hutches are: integral runs of uni-strut channel mounting surfaces — used to prevent drilling into and through the hutch walls, and lockable hinged-operated labyrinths — installed for ease of passing cables and utilities into and out of the hutches. No exposed lead surfaces are found in the construction of these units, a plus for all involved who work within the area.

The NSLS stockroom overhead crane underwent a major overhaul, which included the installation of a five-speed hoisting controller. This upgrade has tremendously improved the resolution of the cable payout and has eliminated any "jerky" motions that were incurred in the past. Users have been reluctant to utilize the crane when positioning certain delicate pieces of equipment due to the lack of sensitivity of the pendant controller. Give this new unit a test drive and experience the difference.

While you are touring the facility, one can't help but notice the new carpet installed on the second floor in the directorate wing, including the Seminar Room and Conference Room "A". These rugs were installed via BNL Special Maintenance Funding, which supports such projects, keeping the NSLS up to its standards as a world-class research center. To compliment the new carpet, replacement desktops have also been installed on the entire set of chairs in the Seminar Room. Finally, many interior areas of Bldg. 725 received a fresh coat of paint and occupants of Bldgs. 726/727 also benefited from a visit by the BNL Team Maintenance Crews.

Snow events of the winter reached near record-breaking levels. While beautiful to observe, snow can wreck havoc and create conditions that have enduring effects. Slippery conditions, lost parking spaces, snow mounds in parking lots, ice melt compounds being tracked into the buildings, and sporadic roof leaks are all concerns encounter each day. My thanks are extended to all of you who, like me, have worked around these conditions- and done so safely.

Lastly, a public note of thanks to all of the groups who work together behind the scenes on a daily basis to keep the NSLS facility at the forefront of science and research. The teamwork exhibited during the winter shutdown periods, and when emergency situations arise, never cease to amaze me. Considering all the activities and interactions involved between the varied trades crews, contractors, engineers, technicians, and scientific and administrative personnel, it is not hard to see that each person is committed to excellence in their field. It is truly my pleasure to work with such dedicated and talented people.

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Workshop on Frontiers in Synchrotron X-Ray Microbeam Diffraction

Jean Jordan-Sweet, IBM Research Division

A workshop on Frontiers in Synchrotron X-Ray Microbeam Diffraction was held on January 10, 2003 in the Hamilton seminar room in the Chemistry Department at BNL. The purpose of the workshop was to discuss a proposal to design and install a state-of-the-art microdiffraction instrument at NSLS minigap undulator beamline X13B. The workshop's participants explored the scientific opportunities that could be accomplished with this instrument and solicited user input.

Among the many workshop presentations was a survey of synchrotron microdiffraction capabilities around the world, given by Cev Noyan of IBM. He pointed out that several synchrotrons, in particular the European Synchrotron Radiation Facility in Grenoble, France, and the Advanced Light Source in Berkeley, California, have put great emphasis and resources into microbeam diffraction. Ken Evans-Lutterodt of Agere and Jean Jordan-Sweet of IBM also described in detail the microdiffraction capabilities currently available at the NSLS, at beamlines X16C and X20A, respectively.

The proposed microdiffraction instrument to be built at X13B was described by NSLS scientists James Ablett and Ken Evans-Lutterodt. The microdiffraction instrument is designed to be robust, easy to align and use, and modular, to serve a variety of users, from students to busy experts, Evans-Lutterodt explained.

Doon Gibbs, BNL's Associate Laboratory Director for Basics Energy Sciences (BES), described two projects that are expected to have a significant impact on microbeam diffraction science at BNL: The proposed upgrade of the NSLS and the Center for Functional Nanomaterials (CFN). One of five new DOE Nanoscale Science Research Centers (NSRCs), the CFN will focus on six scientific themes involving interdisciplinary research on atomic-level tailoring of nanomaterials to achieve desired properties and functions, as described on the CFN website: http://www.cfn.bnl.gov/. The instrumentation and capabilities of the CFN will be organized into "lab clusters," such as materials synthesis, proximal probes, and nanopatterning. Two of the NSLS beamlines, a SAXS beamline on X21 and the X13B microdiffraction beamline, will be optimized to serve the needs of CFN general users.

Two presentations emphasized the need for a microdiffraction instrument. Valery Kiryukhin, of Rutgers University, described several correlated electronic systems that exhibit large changes in electrical or magnetic properties under relatively weak external perturbations. To study these systems, a microdiffraction instrument with temperature control, precise sample positioning, optical access, and tunable energy is needed, Kiryukhin said. Jeffrey Kysar, of Columbia University, discussed the difficulty in determining the relationship between stress and strain in materials and explained that a microbeam diffraction beamline would allow for the measurement of residual stresses and dislocation density in these materials.

At the end of the workshop, committee members encouraged researchers to try currently available microbeam experiments in order to provide advice on how to improve and adapt them to users' needs. More information is available on the web at http://nslsweb.nsls.bnl.gov/nsls/. Click on "User Information> Requesting Beamtime" on the menu in the blue field on the left-hand side of the page.

More information about the workshop is available at:

http://nslsweb.nsls.bnl.gov/nsls/org/workshops/fsxmd/summary.htm

Workshop Attendees

Congressman Tim Bishop and DOE's Ray Orbach visit NSLS

Liz Seubert, Community, Education, Government and Public Affairs

On December 30, 2002, Raymond Orbach, the Director of DOE's Office of Science, journeyed to BNL to meet with U.S. Representative Timothy Bishop, the newly elected First District Congressman, who was visiting the Lab for the first time. The visitors, who included Office of Science advisor Todd Harding and Congressional staffer Lee Leshen, were welcomed by Peter Paul, BNL Interim Director, and Michael Holland, Manager of DOE's Brookhaven Area Office (BAO).

Highlights of Bishop's brief tour of the Lab included a stop at the NSLS. Doon Gibbs, Interim Associate Laboratory Director for Basic Energy Sciences, and NSLS Chair Steven Dierker explained a proposed NSLS upgrade which will dramatically improve the capabilities available to the approximately 2,500 researchers from scientific institutions and industry who use the NSLS for their research each year.

At BNL on December 30, 2002 are: (from left) Peter Paul, BNL Interim Director, Timothy Bishop, then U.S. Representative-elect; Raymond Orbach, Director of DOE's Office of Science; and Michael Holland, Manager of DOE Brookhaven Area Office.

They also discussed plans for the new BNL Center for Functional Nanomaterials (CFN), for which Secretary of Energy Spencer Abraham announced DOE approval when he visited the Lab on June 14, 2002.

Bishop, who was sworn in on Tuesday, January 7, 2003, and Orbach then visited the staff on the NSLS experimental floor and saw research results on osteoporosis and the makeup of newly formed bone. They also met with facility users whose findings about human papillomavirus may lead to drugs to prevent cervical cancer.

News and Notable

Dr. Praveen Chaudhari Named Director of BNL

On January 30, 2003, Brookhaven Science Associates announced the selection of Dr. Praveen Chaudhari as the new director of Brookhaven National Laboratory. Dr. Chaudhari, who began his new duties on April 1, joins Brookhaven Lab after 36 years of distinguished service at IBM as a scientist and senior manager of research. More details can be found at: http://www.bnl.gov/bnlweb/pubaf/pr/2003/bnlpr013003.htm

DOE Nanoscience Workshop Draws a Crowd

More than 400 attendees of the first DOE Nanoscale Science Research Centers workshop, held February 27-28 in Washington, DC, were treated to a blue-ribbon lineup of political and scientific speakers, including BNL's Bob Hwang, who spoke about the Lab's Center for Functional Nanomaterials. The message the participants heard was loud and clear: Nanotechnology research may involve the study of very small things, but it represents potentially very big things in terms of federal funding for the physical sciences. For details, see: http://nslsweb.nsls.bnl.gov/nsls/sci&tech/news/2003/03-nanoworkshop.htm

Visit Brookhaven's Center for Functional Nanomaterials New Website

BNL's Center for Functional Nanomaterials has an updated website to highlight all of the recent news and activities. Visit the website to learn about the facilities, research projects, and job opportunities. The CFN is also now accepting new user proposals. For this information and more, the website can be found at: http://www.cfn.bnl.gov/

BNL Summer Student Becomes a Finalist in the Siemen's Westinghouse Science Competition

Congratulations to Alec Berntson a summer student at BNL for becoming a Finalist in the Siemen's Westinghouse Science Competition. During the summer of 2002, Alec worked with scientists, Helio Takai (Physics) and Vivian Stojanoff (NSLS), to write computer software that is used to accurately determine if a protein crystal is good for crystallography data collection or has gone bad during x-ray exposure. As one of eight regional finalists, Alec receives a $1,000 award. For more on his project, see: http://intranet.bnl.gov/newsclips/TT_022703.htmscience.

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Brookhaven National Laboratory
NSLS Building 725B
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Call for NSLS General User Proposals

For Beam Time in Cycle	Deadline
September - December 2003	Monday, June 2, 2003

General User Proposal and Beam Time Request Forms including instructions can be found at:
http://.nsls.bnl.gov/nsls/users/procedures/proposals/general_user.htm
Proprietary Proposal Forms including instructions can be found at:
http://nslsweb.nsls.bnl.gov/nsls/users/procedures/proposals/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:

http://130.199.76.84/safety/default.asp

NSLS User Administration Office

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