



nsls

National Synchrotron Light Source ♦ Brookhaven National Laboratory

Newsletter

March 2002

Fab-mediated Crystallization of a Potassium Channel

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In order to study structures of integral membrane proteins by x-ray crystallography, one has to overcome multiple obstacles including low expression levels and poor protein stability in detergents. After achieving sufficient quantities of membrane protein, there comes the most difficult part of the journey: crystallization. If integral membrane proteins crystallize at all, they rarely form high quality crystals, presumably because the interference of detergent micelles hinders the specific protein-protein contacts that are required to produce well-ordered crystals. A few novel approaches have been developed to overcome these difficulties [1,2], each of which has yielded only a handful of high quality structures. One of these approaches, developed by Michel, H. et. al.[1], is to co-crystallize membrane proteins with antibody Fv fragments. After inspecting the small database of existing membrane protein structures, they observed that most crystal contacts are formed between the polar groups of proteins, whereas hydrophobic interactions appear to be exceptional. Based on this observation, they produced the Fv fragment of a monoclonal antibody to the bacterial cytochrome c oxidase, and co-crystallized the Fv fragment bound to its protein epitope. (This specific cytochrome c oxidase can be crystallized alone but no structure determination has been reported.) The crystal structure of the complex was solved at 2.8Å resolution. The result showed that the Fv fragment indeed mediated the important crystal lattice contacts through polar interactions: each Fv fragment binds to one oxidase molecule through antibody-antigen recognition; at the same time it contacts another oxidase molecule as well as another Fv frag-

ment through crystal packing. Years after the first publication, however, cytochrome c oxidase remains the lone example of a membrane protein co-crystallized with an antibody fragment. Recently, we employed a similar method to obtain a high-resolution structure of the potassium channel KcsA, implying that this method can serve as a general approach to aid membrane protein crystallization.

Potassium channels are integral membrane proteins that control the electric potential across cell membranes by catalyzing the rapid, selective diffusion of potassium ions

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[3]. The basic ion permeation pathway within this class of proteins was outlined in the 3.2Å resolution structure of a bacterial potassium channel KcsA [4]. The ion conduction pore has a water-filled cavity roughly in the middle of the membrane and a narrow selectivity filter near the extracellular side. The cavity is apparently designed to overcome the dielectric barrier by keeping a K⁺ ion in a fully hydrated state, and the selectivity filter is designed to catalyze the dehydration, transfer and re-hydration of K⁺ ions. Due to the limited resolution, K⁺ ions within the selectivity filter were not clearly resolved, nor could the hydration shell of the K⁺ ion in the cavity be directly observed. To elucidate the mechanism of ion translocation in potassium channels, it was necessary to solve the K⁺ channel structure at a resolution that would reveal detailed protein chemistry and ordered water molecules with high accuracy.

loop region connecting them is in general flexible, therefore it was necessary to use the constant domain and variable domain as separate search models for molecular replacement.

Our structure shows that nearly all of the crystal contacts are formed between neighboring Fab fragments, which constructed a cage-like frame into which the K⁺ channel is conveniently anchored (Fig. 1). This packing effectively avoided detergent micelle in crystal contacts and undoubtedly accounts for the high resolution. Compared with the original KcsA structure [4], the presence of Fab has little effect on the conformation of the channel, except for a small change in the extracellular loop (the turret) region where the Fab binds (Fig. 2). Binding of Fab to the turret also leaves the ion pathway wide open; therefore, ion binding should not be affected

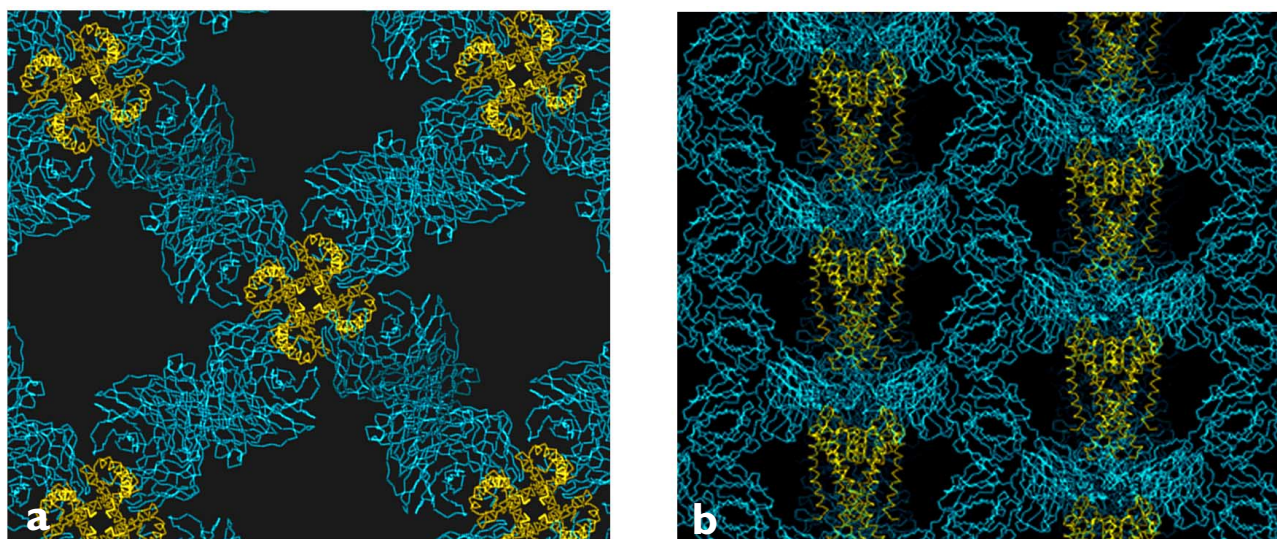


Figure 1. Crystal packing. KcsA (yellow) was crystallized as a complex with an antibody Fab fragment (blue). **a**, View down the four-fold crystallographic axis of the I4 cell, which corresponds to the molecular four-fold axis of the K⁺ channel. **b**, View perpendicular to the four-fold axis.

In order to obtain a high-resolution structure of KcsA, we raised monoclonal antibodies against the channel and selected clones that recognized the tetrameric but not the denatured, monomeric form of the channel. This selection step ensured us that we would obtain an antibody directed against the native structure. The Fab fragment of the antibody was easily produced by standard papain proteolysis followed by ion exchange chromatography. A KcsA-Fab complex with stoichiometry of one Fab fragment per channel subunit was produced and crystallized in space group I4. Frozen crystals diffracted up to 2.0Å at the National Synchrotron Light Source, beamline X25, and the phases were solved by molecular replacement using a published Fab structure [5]. All Fab fragments contain a well-conserved constant domain and an antigen binding variable domain, and the

by the presence of Fab fragments. The structure revealed detailed chemistry of ion coordination and hydration in the channel [6]. It shows how the K⁺ channel displaces water molecules around an ion at its extracellular entryway, how it holds a K⁺ ion in a shell of 8 water molecules in its central cavity, and how the selectivity filter mimics the hydration shell around each K⁺ binding site (Fig. 3). This unprecedented view of a hydrated potassium ion is made possible by the high-resolution data obtained through co-crystallizing KcsA with an Fab.

The high-resolution structure of the KcsA-Fab complex not only has revealed valuable information about the mechanism of K⁺ conduction, but it also offers important possibilities for membrane protein crystallography in general. First, although one additional example

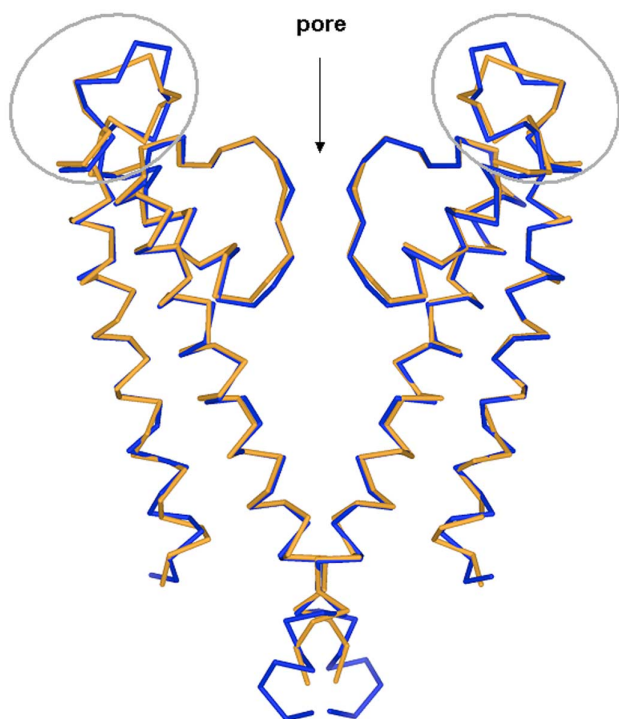


Figure 2. The presence of Fab has little effect on the conformation of KcsA. KcsA structures in the absence (yellow) and presence (blue) of Fab are shown. Gray circles mark the Fab binding region. The arrow indicates the ion pathway. For clarity, only two diagonally opposed subunits of the channel are shown.

is hardly proof, it seems that using antibody fragments to assist crystallization should be applicable to many membrane proteins. Second, it has been argued that Fab fragments should be less suitable than Fv fragments in crystallization because of the flexible hinge region between the two domains [1]. This work shows that in the crystal packing a fixed relationship between the two domains of the Fab can occur, yielding very ordered crystals. Moreover, it is relatively easy to produce Fab fragments. Third, Fab co-crystallization might, as in the KcsA K^+ channel, offer a simple, straight forward solution to the phase problem through molecular replacement using the Fab structure.

This structure was recently published [6], and the coordinates and structure factors are available under PDB code 1K4C. R.M. is an investigator in the Howard Hughes Medical Institute. We thank the staff at the National Synchrotron Light Source beamline X25 for assistance. Research carried out at the National Synchrotron Light Source, Brookhaven National Laboratory, which is supported by the U.S. Department of Energy, Division of Materials Sciences and Division of Chemical Sciences, under Contract No. DE-AC02-98CH10886.

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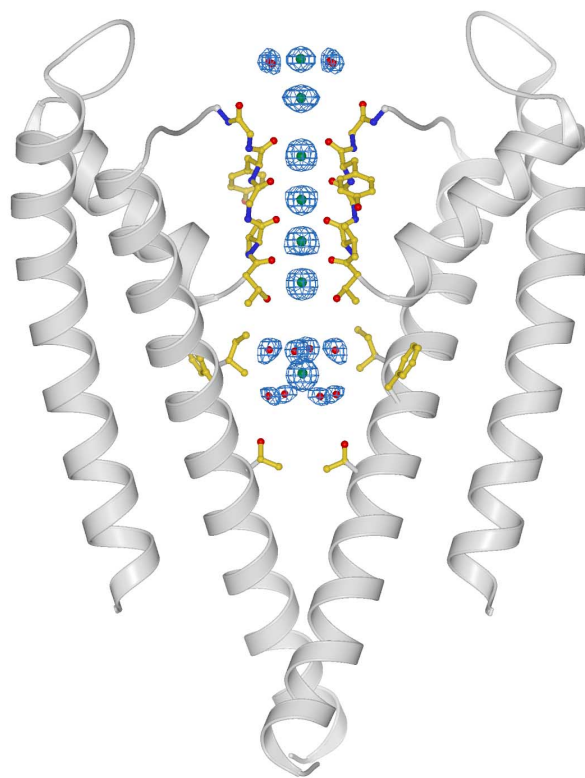


Figure 3. Structure of potassium channel KcsA at 2.0 Å resolution. Two diagonally opposed subunits of the tetrameric channel are shown in ribbon representation. Residues forming the selectivity filter and residues facing the central cavity are shown in ball-and-stick representation. The $2F_o - F_c$ electron density map (contoured at 2 σ) covers the potassium ions (green spheres) along the ion pathway and water molecules (red spheres) in the vicinity.

Chairman's Introduction

Steve Dierker
NSLS Chairman

Recent months have been a time of transition at the NSLS. We have undergone a major change in organization and management. This was done in order to improve our strategic planning, insure strong linkage between our goals and accomplishments, and increase the coordination of our activities. It will also facilitate placing increased emphasis on effective use and development of beamline programs.

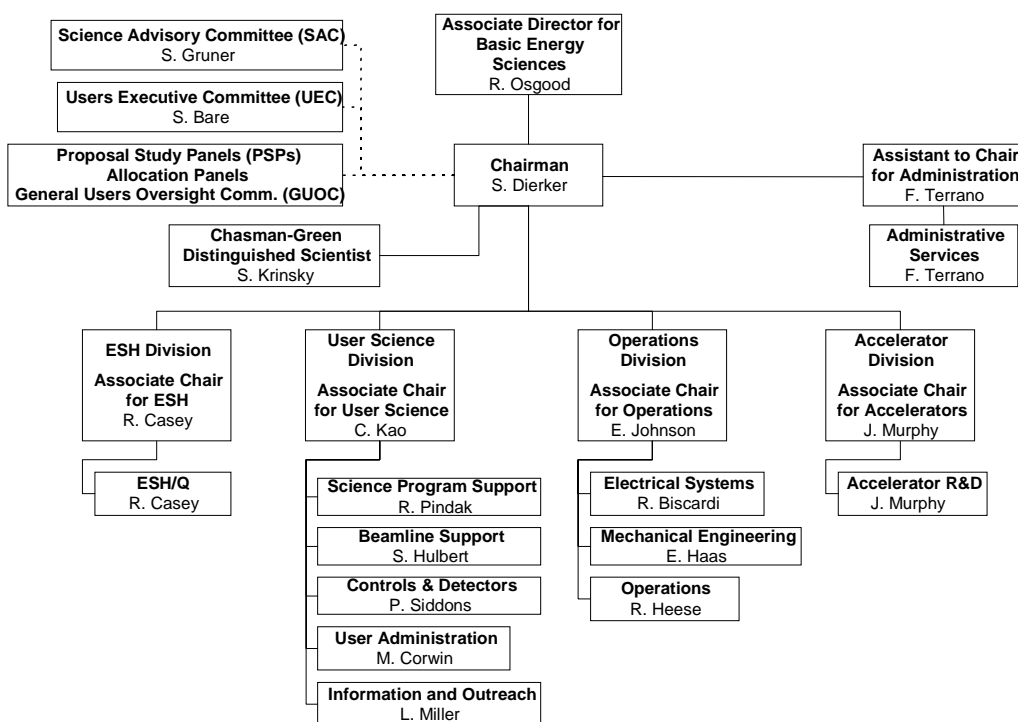
The NSLS is now organized as four divisions, with each lead by an Associate Chairman. Chi-Chang Kao is the new Associate Chair for User Science and oversees the User Science Division, consisting of the Science Program Support, Beamline Support, Controls and Detectors, User Administration, and Information and Outreach Sections. For further information on the expanded user support goals and mission of the User Science Division, see the focus article on page 18 of this Newsletter. Erik Johnson is the new Associate Chair for Operations and oversees the Operations Division, consisting of the Operations, Electrical Systems, and Mechanical Engineering Sections. Jim Murphy is the new Associate Chair for Accelerators and oversees the Accelerator Division consisting of the Accelerator

R&D Section. Bob Casey continues as Associate Chair for ESH and oversees the ESH Division, consisting of the ESH/Q Section. The Accelerator Test Facility is moving from the NSLS to the Physics Department, where it will have increased ties to the Center for Accelerator Physics and the Collider Accelerator Department.

This has been a difficult budget year. We lost 10 valued staff members via a voluntary reduction in force. We have implemented new budgeting procedures in order to maximize our effectiveness within the constraints of a tight budget and to insure proper emphasis on our strategic goals. The outlook for next year is considerably brighter: the President's FY03 budget has NSLS slated for a \$2.2M increase.

The user program, and especially the PRT system, is also in transition at the NSLS. There is growing consensus that an alternative model, that of facility operated General User (GU) beamlines, would better serve the needs and interests of many user groups. In this model, the NSLS would upgrade, maintain, and operate GU beamlines and support the general users. These would include both programmatic efforts, requiring substantial beamtime over an extended period, as well as one-time experiments. The users would focus their efforts and resources on carrying out their science programs. Our ability to support such GU beamlines would require substantial increases in our operating

NSLS Organization Chart



budget, which depends on acceptance and support of this approach by our users. It is essential that we are flexible in order to accommodate different user needs and interests and it is likely that the optimum arrangement will involve a mix of PRT and GU beamlines. There are many issues to be resolved as we consider such a transition and we are actively engaged in discussions with our users as to how best to proceed.

Finally, we continue to develop our concept for a major upgrade in the scientific capabilities of the NSLS. In the short term, we are working to develop superconducting in-vacuum undulators, which would provide higher brightness and full tunability from 2 to 20 keV. In the long run, we are developing a proposal for a two-stage upgrade. In the first stage, we would build a 3 GeV superconducting linac which would be

used for top-off injection to a new or rebuilt 3 GeV low emittance x-ray storage ring. The storage ring would have at least 16 superconducting in-vacuum undulators with a 1000 fold increase in brightness over our existing brightest beamline, X25. The linac would also feed a soft x-ray FEL for medium rep rate, ultrashort, high peak power pulses. Our existing injection system would be dedicated to top-off injection to the VUV ring. In the second stage, a return leg for operating the linac in energy recovery mode would be constructed. This would contain long undulators for even greater brightness, round beams, and short pulses. We believe the scientific opportunities enabled by the combination of these capabilities are truly compelling. We will continue to work with the user community in the coming months to further refine this concept so as to maximize its scientific potential.



A User's Perspective

Simon Bare

UOP LLC

Users' Executive Committee Chairman

This is my last Users' Perspective column in my term as chair of the UEC. I begin by thanking all the members of the UEC for their participation, support, and encouragement over the last year: Mark Chance, Leemor Joshua-Tor, Steve Almo, Dan Fischer, Tony Lanzirotti, and Michael Vaughan. Erik Johnson and Mary Anne Corwin, are thanked for the time and efforts as *ex-officio* members, and Dave Mullins as secretary. Thanks also to all the SplG representatives. A special thanks is due to all the staff in the User Administration Office for all their work and dedication. They have worked with the UEC to not only maintain the excellence of the NSLS but also to make it a more user-friendly environment for you to conduct your research.

At the recent UEC and Town meetings on February 11th Steve Dierker presented his macroscopic vision for both the evolution of the PRT system and plans for the NSLS upgrade (see his column in this issue for details). This followed on from his earlier announcement of the reorganization of the NSLS staff. First, the UEC fully supports the reorganization. We believe that it puts far more emphasis on you, the users of the facility. Conceptually the evolution of a PRT system into one of facility owned and operated beamlines is attractive – but clearly there are many details to be discussed before this is put into practice. This issue is primarily a PRT, and not directly a UEC, issue. However, the UEC represents **all** users of the NSLS and as this proposal

will impact **all** users of the facility we welcome an open and honest dialogue with the Chair and his staff. We have a common goal – the continued success and vibrancy of the NSLS in synchrotron-based research. We believe that it will be by working together that whatever issues arise as the facility transitions to the new mode of operation that these will be resolved to the benefit of all.

The proposal for the upgrade of the NSLS is truly exciting. The new breakthrough science that could be done at such a facility is inspiring. At this stage, however, it is simply a plan. There are many details to be finalized. At this early stage the UEC is fully supportive, and excited, about the potential of such an upgrade. It is also important to remember that it is only a proposal – with opportunity for input by you, the user. It is also critical to realize that this upgrade is not yet funded – and this is where your help will be needed. Stay tuned for more details.

The planning for this year's Users' Meeting are in full swing (see separate article in this Newsletter for details, or <http://nslsweb.nsls.bnl.gov/nsls/users/meeting/Default.htm> for all the latest information). I am very pleased with the job that Leemor Joshua-Tor and all the members of her Organizing Committee have done in getting ready for the meeting in May. There are literally thousands of details to attend to for a meeting of this size. We owe them a tremendous debt of gratitude. This year's meeting has the promise of being the best ever. Please give them your support. Write the date in your planner, and ensure that you are there to give your support to the NSLS, and to show the representatives from DOE, NIH and the President's Science Advisor that the NSLS is vibrant and full of life!

I am very pleased to announce the initiation of a new award at the NSLS this year: the **NSLS User Community Award**, sponsored by the UEC. There are many people around the NSLS whose contribution often goes unrecognized, or is not widely known. The purpose of this award is to specifically recognize an individual from the NSLS user community in recognition of her/his service, innovation, and/or dedication to the 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 annually at the NSLS User's Meeting. Any member of the NSLS user community with an active appointment is eligible to receive this award, except current UEC/SPIG members. A UEC Award plaque will be on display in the NSLS lobby and will be engraved with the name of each year's winner. In addition the winner will receive a \$250 cash award. Nominations are accepted through a web-based nomination page, which can be found at: <http://nslsweb.nsls.bnl.gov/nsls/users/uec/uec-award-noms.asp>. The deadline for nominations this year is March 29. So, take the time right now to nominate someone!

The UEC has been working on a major revision of NSLS Users' Association Charter – the charter that governs the workings of the UEC. In order for these revisions to take effect, the current charter states that “this charter shall be amended at the annual meeting or by ballot as needs emerge. Two-thirds of the membership responding to a proposed amendment shall be required for its passage”. The UEC will thus present the revised charter at the NSLS Annual Users' Meeting on May 21 and a vote will be taken there. I think that it is important for you to understand the revisions that are being proposed, and the reasons behind them. The current charter is outdated –for instance it was written well before there was even a thought of conducting ballots electronically, contains sexist language, and contains many inconsistencies and grammatical errors. There is not space in this newsletter to print in detail the full text of the charter, but the new version, with the proposed changes will be made available on the UEC page of the NSLS website before the Users' Meeting so that you can examine in detail the changes. I hope that you will take the time to read through the proposed new charter, and be at the Users' Meeting on May 21 to vote its passage. The UEC is recommending that you vote for passage.

There have recently been some significant improvements affecting the quality of life that have occurred recently at the NSLS. First, there has been a very positive improvement in the User Registration and Training. Users can now complete user training online both onsite and offsite via web-based training and registration. This will shorten the amount of time that you will have to

spend in User Administration – and will get you onto the experimental floor in a shorter amount of time. Furthermore, hopefully by the time you read this the NSLS database will be linked to the BNL Guest Information Services database, and therefore will allow you to complete all registration prior to your arrival. The icing on the cake for the whole registration process will be the installation of a badge printing system allowing User Administration to immediately print badges at the time of registration – this is awaiting approval from BNL Security. Mary Anne Corwin and her staff deserve special recognition from all the users for these significant changes to make the registration process easier for us all. Second, the NSLS has purchased five bicycles for use by users during their stay. Third, through the BNL Quality of Life Committee, of which Mary Anne Corwin is a member, there have been some significant improvements throughout the lab – which we are all enjoying; for example, new lighting along Yale Road, and upgrades to the swimming pool and changing rooms. If you have any suggestions for additional improvements for quality of life at NSLS and BNL be sure to let me, or Mary Anne know!

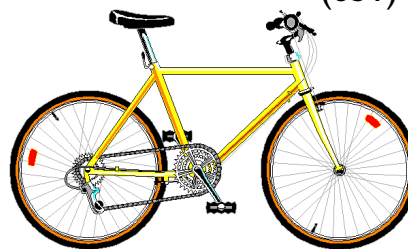
There is one project that the UEC fully supports that I was hoping to be able to include discussion of in this column: an on-line proposal submission process that would also allow rapid accesses to beamtime. However, while this project has been submitted to NSLS management for consideration, it is awaiting approval. Comments on this system will await Leemor Joshua-Tor, the incoming chair of the UEC.

I would like to close by saying that the UEC exists to provide an independent forum for the interests of you, the User of the NSLS. Please do not hesitate to contact me if you have any concerns, questions, or ideas about all aspects of the NSLS. We can't act on your concerns if we don't know about them. Please send comments to me at srbare@uop.com.

Need a Bicycle at BNL?

the NSLS has 5 new bicycles available

call Michelle Herman
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User Administration Report

Mary Anne Corwin

User Administrator

As we close out 2001 and begin the new fiscal year, we anticipate many new positive experiences for our users. Various projects within User Administration, described below, have moved through the blueprint stage to implementation. We expect several other efforts launched last year to come to fruition in 2002.

User Statistics

Our final tally on badged researchers who conducted experiments at the NSLS in FY01 was 2523, of which 720 were first-time users. Our users come from a variety of organizations including academia, industry and government. Here's the breakdown:

1357	U.S. academic institutions
350	U.S. DOE (including BNL) staff
146	U.S. Other government users
189	U.S. Industrial users
116	U.S. Other
32	Foreign government users
245	Foreign academic institutions
17	Foreign industrial users
71	Foreign Other
2523	Total

The 2523 users who visited our facility in FY01 are affiliated with 436 unique institutions or organizations including 30 federal government agencies, 156 U.S. academic institutions, 72 U.S. industrial institutions, 133 foreign institutions (academic, industrial, government, etc.), and 45 other institutions.

Based on data submitted during registration, the fields of research for our 2523 users are categorized as follows: 822 (or 33%) in the materials sciences field, 987 (or 39%) in the field of Biological/Life Sciences, 214 (or 8%) in Chemistry, 197 (or 8%) in Physics, 184 (7%) in Geosciences/Ecology, 117 (or 5%) in Applied Science/Engineering, and 2 (<1%) in unspecified fields.

Of the 1167 experiments performed by general users and Participating Research Teams (PRTs) with reported beamtime, 34% of the experiments were performed in the Materials Sciences field and 37% in the Biological/Life Sciences field. Physics, Chemistry, Polymers, Earth sciences, Environmental Sciences, and Instrumentation development made up another 23% of the experiments. Roughly 6% were performed in the fields of Medical

Applications, Optics, Engineering, Particle Accelerator research and development, Radiation Source research and development, and other non-specific fields.

During FY01, 86 beamlines were in operation, 10 designated diagnostic. Of the 76 non-diagnostic beamlines, 52 are x-ray and 24 are VUV.

Organizational Changes

Following the change in the management structure of the NSLS organization was the repositioning of User Administration (now a section) under the newly formed User Science Division and the creation of the NSLS Information & Outreach Section headed by Lisa Miller. A number of responsibilities within User Administration, primarily related to publications and the NSLS website, have been redistributed to this new section.

The changes have resulted in some staffing modifications. Nancye Wright will retain her role as Production Assistant processing abstracts, science highlights, and publication references in the production of the activity report and the tri-annual newsletter while working in the Information & Outreach Section. Nancye will also remain active with the NSLS Users' Meeting as Vendor and Exhibit Coordinator. Among her many other duties, Lydia Rogers is busy in her role as Deputy User Administrator training our new staff member, Liz Flynn, who recently joined the User Administration staff. Liz has worked onsite with the DOE Brookhaven Group for over 13 years, as did Gretchen Cisco before coming on board with us. Liz will be quite an asset to our little group and her database skills will benefit the office considerably. She replaces Wendy Spaeth who recently accepted a position with the NSLS Budget Group. Initially, Liz's principal roles will be to assist users in their appointments, registration, training, badging and in processing user agreements. She will maintain the BLOSA and Safety Approval Form data. Gretchen continues to be in charge of the proposal system as its coordinator and has provided significant input to developing the foundation for our proposed online proposal system, described later in this report.

User Obligations

Following publication of any work based on research carried out in whole or in part at the NSLS, users are obligated to provide the NSLS with a full citation. Early in the fiscal year, the Inspector General's (IG's) Office performed an audit of DOE's Office of Scientific & Technical Information (OSTI) and each of the four synchrotrons were required to participate in the audit to provide citations for articles appearing in peer-reviewed journals collected from users and staff by the facilities over the past few years to compare them with those maintained in OSTI's online system. The IG's findings

were that, on average, only 44% of the citations were reported to OSTI. Their initial recommendations were somewhat extreme and inappropriate in that users would be required to submit pre-publication abstracts to the facility, which would in turn submit them to OSTI.

These unpublished works would be available online. For obvious reasons, these recommendations needed to be addressed quickly. User Administration and scientific staff from the four synchrotrons scrambled on short notice to respond to the draft report, as did staff at DOE's Basic Energy Sciences. The outcome was about the best that we could have expected. While some of the minor recommendations remained intact (having no consequence to users and little effect on the facilities), the recommendation to provide pre-published abstracts was modified to require only the collection of reference information *after publication*. We consider this outcome a significant achievement.

On the topic of publication references, User Administration put into production an online database for the submission of citations in FY00. The system has worked extremely well for our office, reducing staff effort significantly, especially eliminating the need to reformat references. More effort is now focused on gathering information on published but incomplete citations. We have had a small number of complaints that one section of the online form has too many fields—the authors' names. The form is designed to ask for a first initial and separately the last name for each author. The purpose is to allow formatting of citations for inclusion in the activity report and for submission to OSTI in the various formats needed. While it may be desirable to reduce the requested information to just one field, this will result in going back to manual reformatting by our staff. The other fields users would like to see modified are those pertaining to the submitter so information does not have to be duplicated for additional references. This request is very reasonable and we will attempt to have this completed during the fiscal year with the assistance of an application developer.

Office Automation

Late last year, User Administration formed a committee consisting of users who are members of Participating Research Teams (PRTs), Proposal Study Panels (PSPs), the General User Allocation Committee, User Administration and other staff members at NSLS to define the criteria for an online proposal system. Thanks to members of the committee, Andrew Ackerman, John Aloji, Michael Becker, Lonny Berman, Gretchen Cisco, Dan Fischer, Liz Hicks, Tony Lanzirotti, Craig Ogata, Kumi Pandya, Howard Robinson, Lydia Rogers, Peter Stephens and Vivian Stojanoff, the new system is being designed to reduce lead time between proposal submission and

scheduled beamtime from three months to one, provide rapid access in the current cycle (1-7 days lead time) by back filling unallocated beam time, capture users who receive beam time but do not process proposals and are not therefore counted for reporting purposes, provide a paperless web-based system reducing considerable copying and freight charges for proposal distribution to committees, reduce proposal processing and routing time by approximately 50%, allow for immediate online panel reviews, and allow for an accurate count of all experiments at the NSLS versus only general user experiments. This project has been submitted to NSLS management for consideration and is awaiting approval at this time. It is hoped that once the project is approved, developed and in production, the next step would be to revise and connect the safety approval form system to the proposal system thereby eliminating extensive redundancy of information currently requested by both systems.

User Support, Services and Accessibility

A large undertaking this past year involved the creation of a web-based beamline guide to provide users and those submitting proposals to easily find information about each beamline, its staff, equipment and techniques from one source and to access each beamline's homepage. Information was gathered from the NSLS database and the beamline annual progress reports. To ensure the beamline guide is always accurate, contact User Administration with any updated information.

Participating Research Teams (PRTs) may now secure and maintain their own website in BNL's public domain. Refer to the User Administration webpage (under Computer Set Up) for more information.

The parameters for our FTP site set up for users to transfer files created while performing their experiments here at the NSLS have been modified to delete files at the expiration of 120 hours, instead of 72 to provide more time for users to return to their home institution for file retrieval.

BNL's Quality of Life Committee, which was established last year to improve the quality of services for our guests, completed several projects over the last few months. Shuttle services around the laboratory and on weekends for shopping have been increased. A pilot program for lending out BNL vehicles to user groups has been implemented (at RHIC at this time). Lighting to provide a safe environment during the evening hours was installed on Yale Road to the apartments. The BNL pool and weight lifting facility were upgraded. A game room was constructed in Building 50. Users with suggestions on improving services for guests at BNL may contact me.

Facility Update

Gerry Van Derlaske

NSLS Building Manager

Thanks to all for your patience and adherence to the stringent security controls implemented since the attacks on America on September 11th. As security levels change, staff and users will be updated with the latest available information. We ask you to continue to cooperate and abide with these new rules and regulations, as we await a resolution to these "minor inconveniences".

Many office moves have taken place recently within the NSLS Department. Numerous users are now relocated and fully situated in Bldg. 535A and 535M. The long awaited transition is nearly completed. Save for a few labs and storage areas, NSLS staff and users have vacated Building 510E. When acquisition of remaining 535A office space deemed to the NSLS becomes available, final completion of the transfer of affected NSLS users to their new locations will take place.

Portable storage trailers and shipping containers located to the south and east of Bldg. 727 have been

emptied and excessed following the relocation of equipment stored within these units to the new NSLS Warehousing facility at Bldg. 820A. Each Trade and Technical Section of the NSLS Dept. has been assigned an area in this facility for storage of their equipment. Similarly, the NSLS trailer park section has been trimmed down to only four units- one unoccupied trailer and three occupied office trailers.

Preparations have begun for the relocation of liquid nitrogen transfer and delivery lines near the West Roll up door. Repositioning of these utilities is necessary to provide uninterrupted service of our LN₂ system during the construction phase of the new 2nd floor offices, to be built above the Structural Biology wing. Preliminary indications are of late Spring 2002 startup, with a construction duration of between 12 to 18 months.

Lastly, the winter shutdown of 2001 has come to a close. A few of the projects completed range from increasing the deliverable water pressure on the experimental water system and multi faceted upgrades to the X12 beamlines along with upgrading the X18A & X18B interlock systems.



VUV Ring Status

Stephen Kramer

VUV Ring Manager

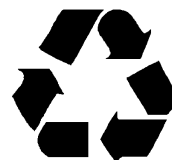
The VUV ring came back from the winter shutdown in record time. This was partly due to the lack of an opening of the vacuum chamber. The major change to the ring was a new of the 4th harmonic amplifier. This new amplifier replaces the vacuum tube amplifier with a solid state amplifier. This will provide a ready source of spare parts and ease of maintenance.

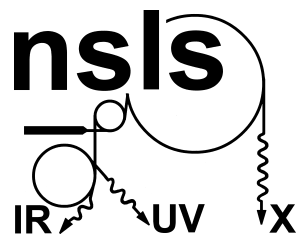
This system will provide only 6Kwatts of power compared to the 10Kwatts available from the older system, but that capability has never been used.

Work has also been continuing on replacing the old front-end interlock system with the newer programmable logic control system. This new system, besides being better documented, will provide greater flexibility and control for the new beamlines being installed. The control circuit will be installed on each operating beamline front-end at the rate of about one per shutdown.

The VUV ring continues operating with one of the highest (if not the highest) currents and reliability levels of any storage ring in the world. Next year (2003), will mark the start of the second decade of operation of this work horse in the synchrotron radiation field. This maturity and flexibility of the VUV ring allows it to continue to lead the way in many new directions of scientific research. The availability of the IR beamports has provided measurements of the high frequency beam impedance of the ring, that have not been possible on other storage rings. The affect of this impedance has been seen only indirectly on the bunch beam properties. This new capability should help address the estimation of this impedance that will dominate the properties of the beam in the proposed new facilities.

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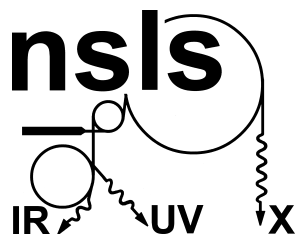
X-Ray Ring Long Range Schedule

X-RAY SCHEDULE - May 2002						
Sun	Mon	Tue	Wed	Thu	Fri	Sat
			1 00-1200 Studies 12-2400 Ops.	2 00-2400 Ops.	3 00-2400 Ops.	4 00-2400 Ops.
5 00-2400 Ops.	6 00-0800 Ops. 08-2400 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 Maint.	18 00-2400 Maint.
19 00-2400 Maint.	20 00-2400 Equip. Commissioning	21 00-2400 Equip. Commissioning	22 00-2400 Equip. Commissioning	23 00-2400 Cond.	24 00-2400 Cond.	25 00-2400 Cond.
26 00-2400 Cond.	27 Holiday	28 00-2400 Cond.	29 00-2400 Cond./Ops.	30 00-2400 Ops.	31 00-2400 Ops.	

X-RAY SCHEDULE - June 2002						
Sun	Mon	Tue	Wed	Thu	Fri	Sat
						1 00-2400 Ops.
2 00-2400 Ops.	3 00-2400 Ops.	4 00-0800 Template 08-2400 Ops.	5 00-2400 Ops.	6 00-2400 Ops.	7 00-2400 Ops.	8 00-2400 Ops.
9 00-2400 Ops.	10 00-1200 Ops. 12-2400 Studies	11 00-2400 Studies	12 00-1200 Studies 12-2400 Ops.	13 00-2400 Ops.	14 00-2400 Ops.	15 00-2400 Ops.
16 00-2400 Ops.	17 00-1200 Ops. 12-2400 Studies	18 00-0800 Studies 08-2400 Maint.	19 00-2400 Maint.	20 00-1200 Studies 12-2400 Ops.	21 00-2400 Ops.	22 00-2400 Ops.
23 00-1200 Ops. 12-2400 Studies	24 00-0600 Studies 06-1200 Intlk. 12-2400 Studies	25 00-1200 Studies 12-2400 Ops.	26 00-2400 Ops.	27 00-2400 Ops.	28 00-2400 Ops.	29 00-2400 Ops.
30 00-2400 Ops.						

X-RAY SCHEDULE - July 2002						
Sun	Mon	Tue	Wed	Thu	Fri	Sat
	1 00-2400 Ops.	2 00-0800 Ops. Template 08-2400 Ops.	3 Holiday 00-2000 Ops.	4 Holiday	5 Holiday	6 Holiday
7 Holiday	8 09-2400 Studies	9 00-2400 Studies	10 00-1200 Studies 12-2400 Ops.	11 00-2400 Ops.	12 00-2400 Ops.	13 00-2400 Ops.
14 00-2400 Ops.	15 00-1200 Ops. 12-2400 Studies	16 00-0800 Studies 08-2400 Maint.	17 00-2400 Maint.	18 00-1200 Studies 12-2400 Ops.	19 00-2400 Ops.	20 00-2400 Ops.
21 00-1200 Ops. 12-2400 Studies	22 00-0600 Studies 06-1200 Intlk. 12-2400 Studies	23 00-1200 Studies 12-2400 Ops.	24 00-2400 Ops.	25 00-2400 Ops.	26 00-2400 Ops.	27 00-2400 Ops.
28 00-2400 Ops.	29 00-2400 Ops.	30 00-0800 Ops. Template 08-2400 Ops.	31 00-2400 Ops.			

X-RAY SCHEDULE - August 2002						
Sun	Mon	Tue	Wed	Thu	Fri	Sat
				1 00-2400 Ops.	2 00-2400 Ops.	3 00-2400 Ops.
4 00-2400 Ops.	5 00-1200 Ops. 12-2400 Studies	6 00-2400 Studies.	7 00-1200 Studies 12-2400 Ops.	8 00-2400 Ops.	9 00-2400 Ops.	10 00-2400 Ops.
11 00-2400 Ops.	12 00-1200 Ops. 12-2400 Studies	13 00-0800 Studies 08-2400 Maint.	14 00-2400 Maint.	15 00-1200 Studies 12-2400 Ops.	16 00-2400 Ops.	17 00-2400 Ops.
18 00-1200 Ops. 12-2400 Studies	19 00-0600 Studies 06-1200 Intlk. 12-2400 Studies	20 00-1200 Studies 12-2400 Ops.	21 00-2400 Ops.	22 00-2400 Ops.	23 00-2400 Ops.	24 00-2400 Ops.
25 00-2400 Ops.	26 00-2400 Ops.	27 00-0800 Ops. Template 08-2400 Ops.	28 00-2400 Ops.	29 00-2400 Ops.	30 00-2400 Ops.	



VUV Ring Long Range Schedule

VUV SCHEDULE - May 2002						
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 Ops.	6 00-2400 Maint.	7 00-2400 Maint.	8 00-2400 Maint.	9 00-2400 Maint. Hardware Equip. Comm.	10 00-2400 Maint. Hardware Equip. Comm.	11 00-2400 Maint.
12 00-2400 Maint.	13 00-2400 Cond.	14 00-2400 Cond.	15 00-2400 Cond. and/or Ops.	16 00-2400 Ops.	17 00-2400 Ops.	18 00-2400 Ops.
19 00-2400 Ops.	20 00-2400 Ops.	21 00-2400 Ops.	22 00-2400 Ops.	23 00-2400 Ops.	24 00-1800 Ops. 18-2400 Studies	25 00-2400 Ops.
26 00-2400 Ops.	27 Holiday 00-2400 Ops.	28 00-0800 Ops. 08-2400 Studies	29 00-2400 Studies	30 00-2400 Ops.	31 00-2400 Ops.	

VUV SCHEDULE - June 2002						
Sun	Mon	Tue	Wed	Thu	Fri	Sat
						1 00-2400 Ops.
2 00-2400 Ops.	3 00-2400 Ops.	4 00-2400 Ops.	5 00-2400 Ops.	6 00-2400 Ops.	7 00-1800 Ops. 18-2400 Studies	8 00-2400 Ops.
9 00-2400 Ops.	10 00- 2400 Ops.	11 00-0800 Ops. 08-2400 Studies	12 00-2400 Studies	13 00-2400 Ops.	14 00-2400 Ops.	15 00-2400 Ops.
16 00-2400 Ops.	17 00-2400 Ops.	18 00-0800 Ops. 08-2400 Studies	19 00-0800 Studies 08-2400 Maint.	20 00-2400 Maint.	21 00-1800 Ops. 18-2400 Timing	22 00-2400 Ops.
23 00-2400 Ops.	24 00-1800 Ops. 18-2400 Timing	25 00-2400 Ops.	26 00-2400 Ops.	27 00-2400 Ops.	28 00-1800 Ops. 18-2400 Studies	29 00-2400 Ops.
30 00-2400 Ops.						

VUV SCHEDULE - July 2002						
Sun	Mon	Tue	Wed	Thu	Fri	Sat
	1 00-2400 Ops.	2 00-2400 Ops.	3 00-2000 Ops. 20-2400 Maint.	4 Holiday	5 Holiday	6 Holiday
7 Holiday	8 00-2400 Cond. and/or Ops.	9 00-2400 Ops.	10 00-2400 Ops.	11 00-2400 Ops.	12 00-1800 Ops. 18-2400 Studies	13 00-2400 Ops.
14 00-2400 Ops.	15 00-2400 Ops.	16 00-0800 Ops. 08-2400 Studies	17 00-2400 Maint.	18 00-2400 Maint.	19 00-1800 Ops. 18-2400 Timing	20 00-2400 Ops.
21 00-2400 Ops.	22 00-1800 Ops. 18-2400 Timing	23 00-0800 Ops. 08-2400 Studies	24 00-2400 Studies	25 00-2400 Ops.	26 00-2400 Ops.	27 00-2400 Ops.
28 00-2400 Ops.	29 00-2400 Ops.	30 00-2400 Ops.	31 00-2400 Ops.			

VUV SCHEDULE - August 2002						
Sun	Mon	Tue	Wed	Thu	Fri	Sat
				1 00-2400 Ops.	2 00-1800 Ops. 18-2400 Studies	3 00-2400 Ops.
4 00-2400 Ops.	5 00-2400 Ops.	6 00-0800 Ops. 08-2400 Studies	7 00-2400 Studies	8 00-2400 Ops.	9 00-2400 Ops.	10 00-2400 Ops.
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18 00-2400 Ops.	19 00-1800 Ops. 18-2400 Timing	20 00-2400 Ops.	21 00-2400 Ops.	22 00-2400 Ops.	23 00-1800 Ops. 18-2400 Studies	24 00-2400 Ops.
25 00-2400 Ops.	26 00-2400 Ops.	27 00-0800 Ops. 08-2400 Studies	28 00-2400 Studies	29 00-2400 Ops.	30 00-2400 Ops.	31 00-2400 Ops.

X-Ray Ring Status

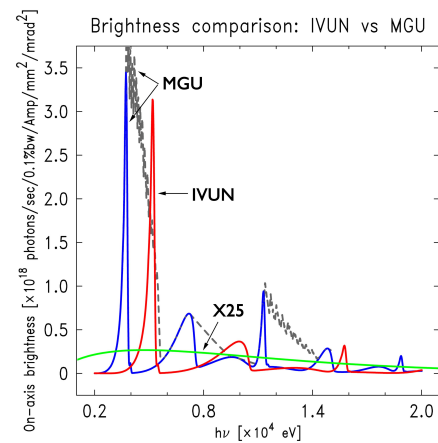
Jeff Rothman

X-Ray Ring Manager

During the winter shutdown, the mechanical group removed the IVUN from the X-13 straight section and disassembled the unit. The support structure was reinforced and a new magnet array was installed. The new array is a hybrid structure of magnets and ferromagnetic vanadium poles. After the mechanical group installed the magnet array it was shimmed to optimize electron trajectory and spectral performance. The upgraded undulator, known as the Mini-gap Undulator (MGU), was then installed in the ring.

The relative performance of these two devices and the X25 wiggler is shown in figure 1. X25 is shown in green, the IVUN is red, the MGU is blue and the tuning range of the MGU is shown as a dashed gray line. The X-ray energy of interest to most users is in the region of 12.4 KeV, corresponding to a 1-angstrom atomic spacing. The third harmonic of the MGU provides a factor of three improvement in brightness at this energy over the second harmonic of the IVUN.

The NSLS plans to install another MGU in the X29/X30 straight section. In preparation, the mechanical group disconnected an upstream trim magnet from the high-pressure copper (HPC) water system, removed the dipole vacuum chamber in that area and disconnected the front-end components. The X29 front end was replaced by a water cooled cap and a small leak in the X30 front end was repaired. The group then installed and surveyed a new dipole chamber. After new lead shielding was designed and installed on the outboard side of the magnet, the water was reconnected to the chamber and trim magnet. The ion pumps and NEG pumps were then reconnected. Finally the vacuum group baked out the entire superperiod. Dry nitrogen was pumped into the superperiod that had been open to air during the shutdown to prevent contaminants from entering the ring. As a result of the care taken by



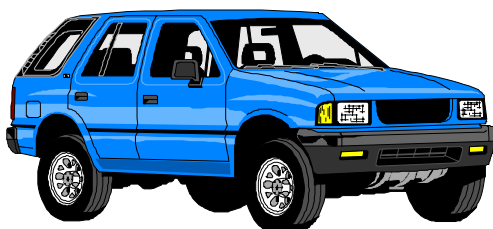
the mechanical group, commissioning proceeded smoothly. We encountered no vacuum related problems such as ion trapping or beam drop-outs.

The RF group replaced the 3 kW tube amplifier on RF system 1 with a solid-state amplifier. A circulator was installed between the new amplifier and the 150 kW transmitter to protect the output stage of the solid-state amplifier. The new configuration should be less expensive to maintain. The Imac tubes were replaced in the transmitters of RF systems 1 and 2a. During commissioning the large circulator on RF system 2 failed and was removed and bypassed as a temporary measure. The RF group expects to repair it and reinstall it in the near future.

The HPC water system, used by the ring magnets and RF cavities, has been running near maximum capacity for many years. The LEGs experiment at X5 has been disconnected from the HPC water system and connected to the experimental water system to alleviate this problem. After the LEGs magnets were disconnected from the HPC water system, the water systems group added booster pumps to improve flow at X5. They also upgraded the experimental water main pump to improve the flow rate for all other users. Other plumbing work was done on the X12 mirror, front end, and compressed air system.

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Catalysis at the NSLS: Importance of Oxygen Vacancies in the Behavior of Oxide Catalysts

J.A. Rodriguez^a, J. Hrbek^a, J.C. Hanson^a, A.I. Frenkel^b, Z. Chang^a, J. Dvorak^a, T. Jirsak^a, J.Y. Kim^a, and G. Liu^a

^a Department of Chemistry, Brookhaven National Laboratory

^b Department of Physics, Yeshiva University

Introduction

Metal oxides are widely used as catalysts in environmental chemistry and commercial processes that deal with the conversion of hydrocarbons [1]. Thus, oxide catalysts are useful in the destruction of the SO₂ and NO_x species produced during the combustion of fuels in automobiles, factories and power plants. By preventing the emission of SO₂ and NO_x into the atmosphere, they help to minimize the negative effects of acid rain on the environment [1,2]. Selective oxidation, ammoxidation, and dehydrogenation probably constitute the most important industrial applications of oxide catalysts active for the conversion of hydrocarbons [1]. Each year these processes produce millions of dollars in revenues.

Over the years there has been a considerable interest in obtaining a fundamental understanding of phenomena responsible for the good performance of oxide catalysts [1,3,4]. Part of the problem in explaining the behavior of these systems arises from the fact that they are complex and very difficult to characterize, in many cases containing several interacting phases and a small fraction of active sites [1]. Useful knowledge in this subject can be obtained through synchrotron based techniques, which nowadays allow the detailed study of the interaction of molecules with surfaces (photoemission, x-ray absorption spectroscopy, infrared spectroscopy, etc) or the evolution of catalytic materials under reac-

tion conditions (x-ray diffraction and scattering, extended x-ray absorption fine structure, etc) [5-8]. These techniques become particularly powerful when combined with state-of-the-art density function (DF) calculations [9]. Using such an approach, recent studies carried out at the NSLS (U7A, X7B, X16C, X19A beamlines) have shown the importance of oxygen vacancies in the behavior of oxide catalysts [10-14].

DeSOx and DeNOx reactions on Titania

Titania (TiO₂) is used as a catalyst/sorbent for the Claus reaction (SO₂ + 2H₂S → 2H₂O + S_{solid}) and the destruction of NO_x species [10,13]. High-resolution photoemission (U7A beamline) has been used to study the interactions of S₂, SO₂, NO, N₂O and NO₂ with a TiO₂(110) surface [10,11,13,14]. Figure 1 shows the structural geometry of this surface. In a perfect

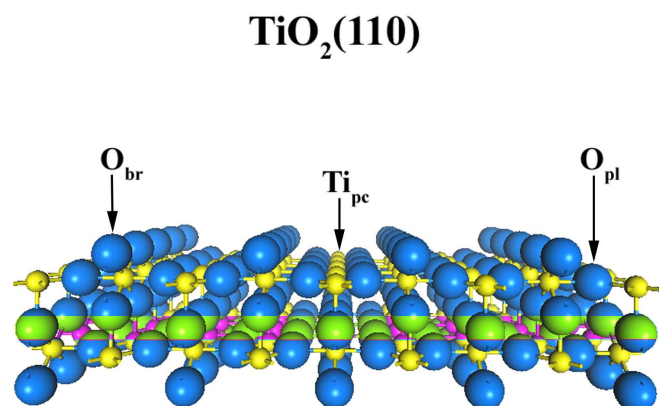


Figure 1. A perfect TiO₂(110) surface. The O atoms are represented as blue spheres, while yellow spheres denote Ti atoms.

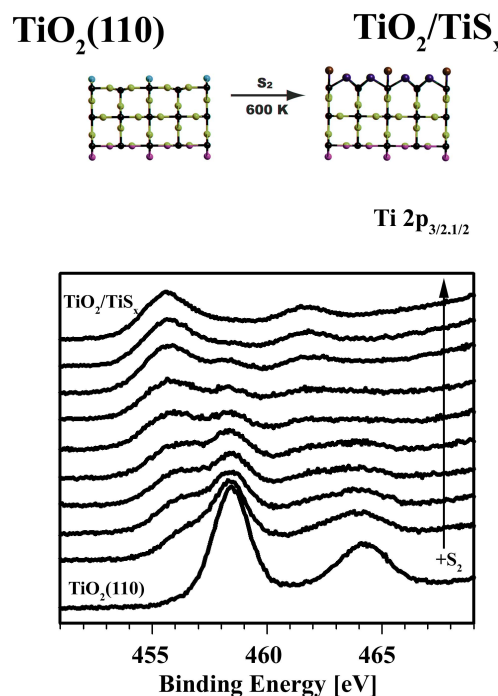


Figure 2. Ti 2p core level photoemission spectra for the reaction of sulfur with a TiO₂(110) surface at 330 °C [11]. Photon energy= 625 eV

TiO₂(110) surface, adsorbates can interact with pentacoordinated Ti sites (Ti_{pc}) or atoms in the O bridging rows (O_{br}). In addition O vacancies can be present in the O bridging rows or the bulk of the oxide sample [10,13]. Photoemission data and first-principles DF calculations indicate that these vacancies play a dominant role in the chemical properties of the TiO₂(110) surface [10,11,13]. When present on the surface they offer adsorption sites which are more reactive than Ti_{pc} or O_{br} sites [10,11,13]. Furthermore, the exchange of O vacancies between the surface and bulk of the sample can lead to unexpected chemical transformations [11,13]. Figure 2 shows Ti 2p core-level spectra for the adsorp-

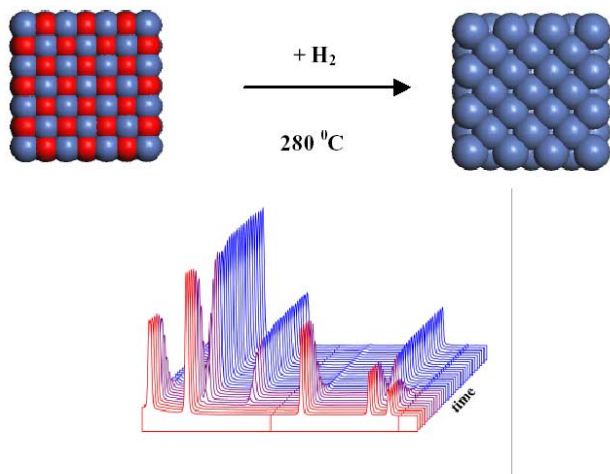


Figure 3. Time-resolved x-ray diffraction results for the reaction of a NiO powder with H₂ at 280 °C [14]. X axis is 2 θ , Y axis is time, and Z is intensity.

tion of S₂ on TiO₂(110) at 330 °C [11]. As sulfur is dosed, the peaks for TiO₂ completely disappear and new features appear for titanium sulfide. There is a complete TiO₂ → TiS_x transformation in the surface and near subsurface regions. This is surprising since oxides are much more stable than sulfides and a S₂(gas) + TiO₂ → TiS + SO₂(gas) reaction does not occur on the surface [11]. The key to the TiO₂ → TiS_x transformation is a S induced migration of O vacancies from the bulk of the oxide to the surface [11]. Adsorbates like Au and NO_x species can also induce a migration of O vacancies in TiO₂, thus producing an important enhancement in the chemical reactivity of this oxide surface [11-13].

Reduction in Hydrogen and Activation of Oxide Catalysts

In most cases, pure stoichiometric oxides do not exhibit high catalytic activity [1]. One method frequently employed for the preparation of active oxide catalysts consists of partial reduction under hydrogen at elevated temperatures [1]. In this process, it is important to identify well-defined suboxides that can have high catalytic activity and are stable at the elevated temperatures typi-

cal of many catalytic reactions [1,11]. Experiments at beamline X7B have shown that *in situ* time-resolved x-ray diffraction is a powerful technique to study the reduction/activation of oxides [11,15]. Figure 3 displays time-resolved XRD data for the reaction of hydrogen with a NiO powder at 280 °C [14]. During the first 50 min, no major changes are seen in the intensity of the diffraction lines for NiO (in red). The NiO lines then begin to disappear, and simultaneously lines for metallic Ni appear (in blue), without any well-ordered intermediate phase. An induction or delay time was also found in photoemission experiments (U7A) for the reduction of a NiO(100) single-crystal, in NEXAFS/EXAFS

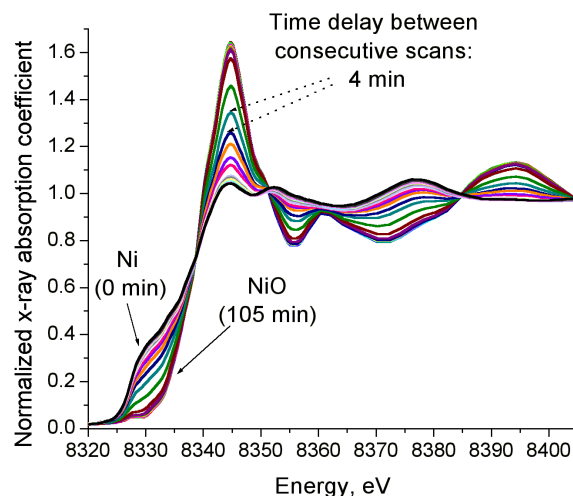


Figure 4. Time-resolved edge-step normalized NEXAFS data for the reduction of NiO powder at 280 °C under a flow of hydrogen [14].

measurements (X16C) for the reduction of NiO powder [14], and in time-resolved XRD data (X7B) for the reduction of cobalt and nickel molybdates [15]. Thus, such phenomenon must be taken into consideration when aiming at the activation of oxides via reduction in hydrogen.

In Figure 3, it could be argued that the induction time is associated with the formation of an amorphous NiO_x phase with special chemical properties. This possibility was ruled-out after analyzing NEXAFS/EXAFS data (Figure 4, for example) using the principal-component-analysis (PCA) method. The PCA results indicated that only two components (NiO initial phase, Ni final phase) were present in the system [14]. Photoemission and DF results for the adsorption of H₂ on NiO(100) indicate that O vacancies play a key role during the induction time, generating the necessary sites for the dissociation of the adsorbate. A perfect NiO(100) surface, the most common face of nickel oxide, exhibits a negligible reactivity towards H₂ [14].

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Tom Dickinson Retires

Bob Casey

Assoc. Chair for ESH&Q

It is important to note the retirement of Tom Dickinson from the NSLS on 12-21-2001. Tom has worked at the NSLS from its early days and contributed in so many important ways to the safety program. His perceptiveness, enthusiasm, and dedication will be sorely missed. Bill Thomlinson, the long-time NSLS Associate Chair for ESH at the NSLS, who now works at the ESRF, made the following comments in a letter to Tom sent just before his retirement:



"Your contributions extend far beyond the walls of BNL in our community of accelerators and synchrotron science. It is fair to say that I have not been in a synchrotron facility anywhere in the world where I do not feel your presence in the design, implementation and operation of safety systems, and safety operations in general. That is especially true here at the ESRF where the systems are modeled directly on those you so significantly helped to develop. I think that every facility built after NSLS, and those upgraded as well, use the system that we developed together with so many outstanding people at NSLS.

When we started with the development of the NSLS personnel protection systems, it was a green field cluttered with absolutely horrible examples at some of the other facilities. They were safe in their own ways since they effectively prevented anyone from doing any science. We took a different approach. You argued always and effectively for safety. I argued for efficient access to the experiments. It was then that the world of synchrotron research changed. We built a system that was, and is, efficient and inherently safe. We had to convince

DOE that the efficient use of the beams by scientists was not counter to the principles of safety first. It was a tough sell, but we prevailed. The outstanding safety record at synchrotron facilities is the best testimony to our success.

Much more was at stake than building hardware. As I look back, your principal contribution was perhaps not the engineering of the hardware, but something far, far more important. For lack of better words, I will invent an oxymoron and say that you created a policy of "rigid flexibility". That may seem strange but what I mean is that you had a rigid approach, a no-compromise approach, to safety. But, at the same time, you also had a no-compromise approach to making sure that good science could be done if the proper safety concerns were addressed. You gained the utmost respect of the Users and often had to work one on one with them to assure that their experiments could go forward, but safely.

A great deal of flexibility was, and is, required. That support by the User Community allowed us to go to NSLS, BNL and DOE with our ideas and in return we always had the full support of management. That was long before such things were popular. Because of that trust and support, we built systems and created operational principles that became the hallmark of synchrotron safety around the world."

I couldn't agree more with Bill's comments. The NSLS safety program has the stamp of Tom Dickinson in every fiber of its character, and it is widely recognized within the Laboratory and beyond as being uncommonly effective. I recently read the following comment made by a user at the end of his run at the NSLS: "I wish the rest of the Laboratory had the same common sense approach to safety that the NSLS does!" I can't think of a better tribute to the program that has had Tom at its center for the last 20 years.

Best wishes and good health to our colleague on his retirement. He will be missed!

NSLS Annual Users' Meeting

May 20-22, 2002

Leemor Joshua-Torr

Cold Spring Harbor Laboratory and UEC Vice Chair

The NSLS Annual Users' Meeting is a forum, organized by the NSLS Users' Executive Committee, for reporting new research results and advances in experimental capabilities that utilize synchrotron radiation. The meeting brings together scientists from many diverse disciplines to share their recent accomplishments and visions of the future. It also provides them with the opportunity to visit with old friends and to forge new relationships.

Because the focus of our meeting is on the science produced using synchrotron radiation, we especially encourage the infrequent or new synchrotron user to attend. Through workshops, invited talks, the poster session, and the informal interactions, there will be numerous opportunities to learn about new frontiers in synchrotron-based experimentation and how these will impact your research interests.

The Users' Meeting is an ideal time to interact with the wide variety of scientists who make the NSLS a most productive user facility. Below are brief descriptions about each workshop. Full details about the meeting and workshops (including speakers and their topics), and *all the latest information*, can be found at the following website: <http://nslsweb.nsls.bnl.gov/nsls/users/meeting/default.htm>.

We hope to see you at this year's meeting, May 20-22.

SCHEDULE FOR THE MEETING

Monday May 20

9:00 a.m. – 5:00 p.m. Workshops (see details below)
5:30 – 8:00 p.m. Welcome reception, Poster session, Vendor exhibit

Tuesday May 21

8:15 a.m. – 5:30 p.m. Main Users' Meeting (see details below), Poster session, Vendor exhibit
6:30 – 10:00 p.m. Entertainment (comedy and more)

Wednesday May 22

8:30 a.m. – 5:00 p.m. Workshops (see details below)

Poster Session

All scientists, researchers, post docs and students are encouraged to submit posters exhibiting their research at the NSLS for the Poster Session to be held during Annual Users' Meeting. Multiple entries by the same

author are permitted. In addition, post docs and students may enter their poster(s) in the Poster Contest. Cash prizes will be awarded and the winning posters will be exhibited in the NSLS Lobby after the close of the Users' Meeting and Workshops. Deadline for poster registration is April 26.

Main Meeting

We will have a full day of both scientific talks and updates from numerous funding agencies. Our keynote speaker will be Dr. John Marburger, the director of the Office of Science and Technology. Confirmed speakers from funding agencies include: Dr. Pat Dehmer (DOE), Dr. Judith Vaitukaitis (NIH-NCRR) and Dr. Richard Swaja (NIH-NIBIB). In addition, Congressman Felix Grucci will be speaking. We will have a BNL and BES update and a facility update from NSLS chair, Dr. Steve Dierker.

Workshops

Monday, May 20

The Environmental Sciences: Synchrotrons Providing Powerful Tools for a New Science

(organized by Douglas Hunter, Savannah River Ecology Laboratory)

The environmental sciences encompass all the traditional branches of science in the study of man's impact on this planet. This workshop will highlight ways in which a wide variety of synchrotron-based spectroscopies are being applied to a wide range of problems in the environmental sciences. Talks will span the spectrum ranging from the infrared, soft x-rays to hard x-rays. Techniques will include SR-FTIR, diffraction, spectro-microscopy, x-ray fluorescence, x-ray absorption spectroscopy and others. Applications will range from the geological, soil, biological sciences and more. The workshop promises to be an exciting blend of demonstrations showing the many diverse ways that NSLS can be used to study the complex research problems faced by environmental scientists.

X-Ray Sources for Studies of Ultrafast Processes

(organized by John Sutherland, BNL)

New technologies are appearing that make possible studies of the structure and dynamics of matter on time scales of pico- and femtoseconds. Extending the spectral range of such studies into the X-ray region will increase significantly the information that can be obtained. This workshop will review briefly the scientific case for the use of X-rays in the study of ultrafast processes. The main focus will be on the resources available for such studies at present and those that are expected to become available over the next decade. The latter group

includes new time resolved capabilities obtainable by adding new experimental facilities (beamlines) to existing accelerators as well as sources that can only be realized by the construction of new accelerators.

EXAFS Studies of Nanoscale and Nanostructured Materials

(organized by Vincent Harris, Naval Research Lab)

In recent years the evolution of nanoscience and technologies has taken the scientific community by storm. Reports of advances in nanotechnology routinely appear in the mainstream press and are touted by public officials as examples of the success of government investments in science and technology. X-ray absorption fine structure is a technique that is ideally suited to describe and address the nanoscale properties of these materials. This workshop is designed to highlight the successful use of XAFS in the study of biological, chemical, and physical systems that are defined by their length scales as nanomaterials. In addition, it is anticipated that obstacles to a complete characterization and understanding of these systems will emerge revealing opportunities for a greater role of XAFS and synchrotron radiation techniques in the understanding of nanomaterials.

Practical Aspects of Membrane Protein Crystallography: From Overexpression to Crystallization

(organized by Larry Shapiro and Filippo Mancina, Columbia University)

Integral membrane proteins perform some of the most important functions of living cells, yet understanding their molecular mechanisms through structural studies presents unique challenges. The aim of this workshop is to discuss the technical aspects of overexpressing, purifying, and crystallizing membrane proteins for structural studies by x-ray crystallography.

Wednesday, May 22

Recent Advances in the Application of Synchrotron Radiation to Catalysis

(organized by Simon Bare, UOP)

Over the last 30 years, research performed using synchrotron radiation has proven to be of clear value to understanding the structure-function relationships of heterogeneous catalysts, from probing the structure of adsorbed species on model single crystal catalysts, to solving the structure of highly dispersed bimetallic clusters. A diverse program has been assembled for this workshop, covering a variety of synchrotron radiation-based techniques that are used to study heterogeneous catalysts, with a focus on x-ray absorption spectroscopy and *in situ* studies. In a follow-up to last year's ca-

talysis workshop, part of this year's workshop will report progress made on ways that the NSLS can attract more users from the catalysis community. Representatives from the NSLS and government agencies have been invited to provide perspective on this initiative.

Combining Synchrotron Infrared and X-Ray Micro-Spectroscopy and Imaging

(organized by Lisa Miller, NSLS, and Antonio Lanzirotti, Univ. of Chicago)

The goal of this workshop is to introduce and describe the many microspectroscopy and imaging techniques that are available at the NSLS, including infrared microspectroscopy, hard x-ray microprobe, soft x-ray scanning transmission x-ray microscopy, x-ray micro-diffraction, diffraction-enhanced imaging, and x-ray microtomography. During the morning session, speakers will describe the "in's and out's" of each technique. The afternoon session will focus on various applications of the different techniques, emphasizing the complementary information that can be obtained by using multiple techniques to solve scientific problems in many fields of interest. A "Guidebook of Microspectroscopy and Imaging Techniques at the NSLS" will be distributed to every participant.

In-Situ Studies of Materials Processing

(organized by Karl Ludwig, Boston University, Randy Headrick, University of VT, and Chi-Chang Kao, NSLS)

Advanced materials continue to be at the forefront of science and technology. In many cases, the formation of these materials requires increasingly sophisticated thin film growth techniques, surface modification regimens, or carefully controlled phase transformations. Synchrotron-based real-time x-ray studies offer the ability to examine the evolution of materials structure under many processing conditions, either in a surface-sensitive or a bulk-sensitive mode, with microsecond resolution on length scales from 0.1-100 nm. This workshop will examine efforts utilizing synchrotron radiation for in-situ studies of materials processing. These include wide-bandgap, oxide and organic thin film growth, surface modification by sputtering/plasma processing and thin silicide film formation via solid phase epitaxy. A brief overview will also be given of ongoing efforts to construct an in-situ x-ray scattering facility at the NSLS for real-time studies of surface processing.

Advanced Detectors Development

(organized by D. Peter Siddons, NSLS)

This workshop is of interest to both detector developers and synchrotron radiation users wishing to hear about new developments in the field of advanced detectors for synchrotron radiation.

Focus On . .

User Science Division

In the new NSLS organization, the User Science division consists of the following sections: User Administration (Mary Anne Corwin), Information and Outreach (Lisa Miller), Scientific Program Support (Ron Pindak), Beamline Development and Support (Steve Hulbert), and Detector and Control (Peter Siddons). The goal of the new structure is to identify and coordinate the major activities related to user science so that we can be more effective in strengthening the existing user programs, fostering the growth of new user programs, and raising the visibility of the exciting science produced by our users.

The User Administration section continues to carry out most of the functions served by the previous User Administration office, such as user registration, administering safety training, the general users proposal program, PRT agreements, and addressing all aspects of user quality of life issues. In addition, it also serves an increasingly important role in providing vital statistics to NSLS management, DOE, and various user organizations.

The Information and Outreach section is responsible for all publications related to user science activities, in-

cluding the NSLS website, annual activity report, newsletters, science highlights, online news, etc. It also oversees a number of outreach programs, including the newly revived Faculty Student Research Support program, visiting scientist programs, topical and training workshops, regular seminars, and tours.

The Scientific Program Support section works with users to develop new and expand existing science programs and coordinates with the Beamline and Detector/Control sections to implement and refine new synchrotron techniques. The mission of the Beamline Development and Support section is to support the NSLS beamlines on the VUV-IR and X-ray storage rings and to develop new beamlines and new beamline capabilities.

Finally, the Detector and Control section is responsible for the development and implementation of beamline control systems, and the development and support of detectors. With anticipated increases in funding, the Beamline section and the Detector/Control section will also expand its mission to include support of PRT beamlines.



Members of the User Science Division at the NSLS. Chi-Chang Kao (front row, center) is the Associate Chair for User Science.

News and Notables

NSLS users elected into the National Academy of Sciences

Congratulations to NSLS users John Kuriyan (Howard Hughes Medical Institute, Rockefeller University) and Rus Hemley (Geophysical Laboratory, Carnegie Institution of Washington) upon their election into the National Academy of Sciences in May 2001. Election to membership in the Academy is considered one of the highest honors that can be accorded a U.S. scientist or engineer. The total number of active members is 1,874.
<http://www4.nationalacademies.org/nas/nashome.nsf>

Faculty Student Research Support Program begins again

The NSLS is happy to announce the resumption of its Faculty Student Research Support Program. This program is designed to encourage new users to the NSLS by supporting faculty/student research groups by covering expenses incurred during exploratory visits to the NSLS and while performing initial experiments. Expenses covered may include travel, housing, per diem, and some incidental costs. For more information, please see the NSLS website at:
<http://nslsweb.nsls.bnl.gov/nsls/users/funding>

User Community Award initiated

The Users' Executive Committee (UEC) at the NSLS is instituting a new 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 21, 2002. The award winner will receive a \$250 cash award. In addition, a UEC Award plaque will be on display in the NSLS lobby and will be engraved with the name of each year's winner. For nomination and other information, please see the NSLS website:
<http://nslsweb.nsls.bnl.gov/nsls/users/uec/uec-award-noms.asp>

NSLS summer student becomes Intel Science Talent Search semifinalist

Congratulations to high school student, Jenanan Vairavamurthy (Shoreham Wading River High School), for becoming a semifinalist in the Intel Science Talent Search competition. During the summer of 2001, Jenanan worked with NSLS scientist, Lisa Miller, on a project entitled "Mineralization of Bone: Probing the Early Mineral Phases Using Infrared Microspectroscopy." Three hundred semifinalists were chosen from among 1562 entrants. Each semifinalist and their school received matching awards of \$1,000. At the age of 15, Jenanan is currently a high school senior and plans to major in biomedical engineering when he attends college this Fall.
<http://www.intel.com/pressroom/archive/releases/20020116corp.htm>

Student/Postdoc Pizza Get-Together resumes

Through funding from the Users' Executive Committee (UEC), the student/postdoc pizza get-togethers have resumed at the NSLS. Organized by NSLS scientist, Cecilia Sanchez-Hanke, the get-togethers take place every other Thursday evening at 4 pm. All local and visiting students and postdocs are invited to meet in the NSLS x-ray ring kitchen (across from the vending machines) for pizza and soda.

Upcoming Events

BNL Nanocenter Workshop

Brookhaven National Laboratory
March 8-9, 2002
<http://www.bnl.gov/nanocenter/>

Rapid Data 2002: A Practical Course in Macromolecular X-Ray Diffraction

Brookhaven National Laboratory
April 21-26, 2002
<http://www.px.nsls.bnl.gov/RapiData2002/>

Frontiers for Synchrotron Research on Soft Matter and Biomaterials Workshop

Tarrytown, NY
April 25-27, 2002
<http://nslsweb.nsls.bnl.gov/nsls/org/workshops/2002-SMB/>

NSLS Annual Users' Meeting

Brookhaven National Laboratory
May 20-22, 2002
<http://nslsweb.nsls.bnl.gov/nsls/users/meeting/Default.htm>
* Registration deadline: April 30, 2002
* Poster Session deadline: May 7, 2002

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Call for NSLS General User Proposals

For Beam Time in Cycle
September - December 2002

Deadline
Friday May 31, 2002

General User Proposal and Beam Time Request Forms including instructions can be found at:
<http://nslsweb.nsls.bnl.gov/nsls/users/procedures/proposals.htm>
Proprietary Proposal Forms including instructions can be found at:
<http://nslsweb.nsls.bnl.gov/nsls/users/procedures/proposals-prop.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. Do not send in SAFs with your proposal. Go to:
<http://130.199.76.52/safety/>

NSLS User Administration Office

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The *NSLS Newsletter* is published triannually by the Information and Outreach Office, National Synchrotron Light Source Department, Brookhaven National Laboratory

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For additional information about the NSLS (including this Newsletter in electronic format) see the NSLS Home Page on the World Wide Web at:

<http://nslsweb.nsls.bnl.gov>