brookhaven national laboratory

newsletter

national synchrotron light source

Spring 2006

X25 Cryo-Capable Mini-Gap In-Vacuum Undulator Installed in the X-Ray Ring

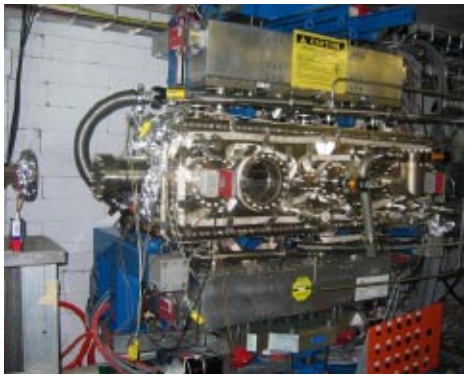
Lonny Berman, BNL-NSLS

At the start of 2004, beamline X25's programmatic focus shifted completely to monochromatic macromolecular crystallography, following 14 years of operation as a mixed-use high-brightness beamline. Thus, the NSLS was presented with an opportunity to renovate the beamline, as well as the radiation source, to optimize them for a dedicated macromolecular crystallography program. To this end, the BNL Macromolecular Crystallography Research Resource (PXRR), a collaboration between the BNL Biology Department and the NSLS, submitted a funding request in late 2002 as part of its proposal to the National Institutes of Health's National Center for Research Resources and the Department of Energy's Office of Biological and Environmental Research (DOE BER) to renew its five-year grant. The proposal was well received, and $2.2M in funds was awarded by DOE BER beginning in late 2003, to be dispensed over the course of three fiscal years.

Some of the X25 MGU project staff gathered around the newly assembled device in the Magnetic Measurements Facility prior to its move to the NSLS.

During the December 2005 shutdown, the original hybrid wiggler, which served as the radiation source for beamline X25 since its inception in 1990, was replaced by a custom-designed in-vacuum miniature-gap hybrid undulator (MGU). At a photon energy of 6.3 keV, the new radiation source will be 15 times brighter than the old one, and will be six times brighter at a photon energy of 10.5 keV. Its design consists of 0.99 meter-long planar hybrid magnet arrays with a period length of 18 mm (55 periods total) and a minimum attainable gap of 5.6 mm, with a corresponding maximum deflection parameter, K, of 1.5. The NdFeB-type permanent magnet material, which has been used in this insertion device, can have a higher magnetic field and a higher radiation resistance simply by cooling: Operation at 150K will likely produce a 13-14% higher magnetic field (and higher K), resulting in a larger photon energy tuning range. Therefore, this undulator design also incorporates a provision for

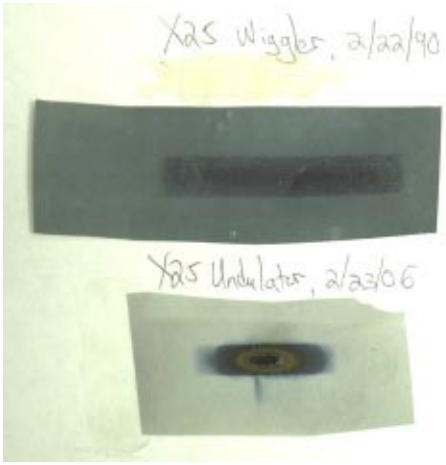
INSIDE THIS EDITION



January 12, 2006: The new X25 MGU installed in the NSLS x-ray ring.

cryogenic operation, which might be pursued in the future. Unlike previous miniature-gap undulator designs in use at the NSLS, the one now implemented for X25 will be continuously tunable from 2 to 20 keV by employing all harmonics up through the 9th. The undulator vacuum and gap separation system was manufactured by Advanced Design Consulting of Lansing, New York. In conjunction with the installation of the undulator, certain components in the front end of the beamline, and the active interlock system that protects the x-ray ring exit chamber, were upgraded in order to be able to cope with the much higher power density of the undulator beam.

In addition to the new radiation source, upgrades to the beamline optics will also be implemented in order to exploit the properties of the new source. The current double crystal monochromator will be replaced by one that incorporates cryogenic cooling of the first crystal and sagittal bending of the second crystal to permit horizontal focusing. It will be followed by a new bendable mirror, containing multiple coating stripes, to permit vertical focusing.



X-ray burns taken using the original wiggler (top) and the new undulator (bottom), in the same location, show that the undulator beam is much smaller than the wiggler beam, as expected.

NEWS

Joint Photon Sciences Institute at BNL

Steve Dierker, Associate Laboratory Director for Light Sources

A new initiative in photon sciences will capitalize on the unique capabilities of NSLS-II.

A partnership between the DOE and New York State, the Joint Photon Sciences Institute (JPSI) will serve as an intellectual center for development and application of the photon sciences and as a gateway for NSLS-II users. It will enhance scientific programs that use the powerful photon beams by cultivating and fostering collaborative, interdisciplinary R&D.

New York State Governor George Pataki recently committed to providing $30 million for the JPSI building, which will be located next to NSLS-II and provide office space, meeting areas, and specialized state-of-the-art laboratories. The operating expenses of the institute and its research programs will be covered by funding from the federal government, including the Department of Energy, the National Institutes of Health, the Department of Defense, and others. Research will be focused around several multi-year scientifically and technologically relevant research initiatives.

New York State Capitol Building, Albany

Over the past few decades, the power of photon sources has increased dramatically, and they are now used for a broad spectrum of research. Modern research increasingly requires interdisciplinary work that either spans multiple scientific disciplines or falls at the boundaries between them. JPSI will be an interdisciplinary institute devoted to basic research in areas of the physical sciences, engineering and the life sciences that are united in employing synchrotron-based methods. JPSI will also develop new methods and applications that exploit the unique capabilities of NSLS-II.

JPSI will have great flexibility in making scientific appointments, encompassing both Brookhaven scientists and faculty from universities. Junior and senior fellowships and sabbatical programs will draw the best photon scientists from institutions worldwide for interactions with the resident staff and user communities. An important element of the institute's mission will be training new researchers and enabling established researchers to embark on new directions in interdisciplinary research. JPSI will also host interdisciplinary workshops that highlight new opportunities, foster new collaborations, and promote JPSI initiatives in emerging areas of photon science.

Chairman's Introduction

Chi-Chang Kao, NSLS Chairman

Recently, everyone at the NSLS was very happy to learn that, as part of the president's American Competitiveness Initiative, the FY07 budget request shows a significant increase in funding for the physical sciences and engineering. This also includes a healthy increase in the operating budget for all synchrotron facilities, and will allow the facilities to provide better instrumentation and staffing for users. This increase is clearly a tribute to the scientific productivity of our user community, as well as their strong and continuing support.

In the area of operations, the 2005-2006 winter shutdown was carried out successfully, and both rings were back up and running without problems. It was an unusually long shutdown this time, due to the installation of both a new radio frequency (RF) cavity in the X9 straight section and a new undulator in X25. Undertaking two major projects in one shutdown is indeed very challenging, and it is a real testament to the ingenuity, dedication, and teamwork of the entire NSLS staff that both projects were completed on time, in spite of numerous problems encountered along the way.

The new X25 undulator is a cryogenic-ready in-vacuum undulator, the first of its type installed in an operational storage ring. It will significantly enhance the brightness of X25, the most productive macromolecular crystallography beamline at the NSLS. Initial commissioning results of this new undulator are very encouraging and normal operation is expected in April. Detailed descriptions of this new device can be found in the cover story of this newsletter.

Additionally, with the assistance of the NSLS Scientific Advisory Committee (SAC) and the Users' Executive Committee (UEC), we have been working hard to develop a five-year strategic plan for the NSLS. Input from the user community is a very important to the plan. If you have suggestions, please contact the UEC members, Special Interest Representatives, and NSLS staff. Or, bring your suggestions to the Annual Users' Meeting, where a draft of the plan will be presented and discussed.

There are also several noteworthy developments in our efforts to foster interactions between the NSLS and the Center for Functional Nanomaterials (CFN). First, we will have a joint users meeting this year, thanks to the hard work of the user executive committees of both facilities. Second, a low-energy electron and photoelectron microscope (LEEM/PEEM) has been successfully installed at the U5 undulator beamline, and commissioning of this instrument is underway. Third, the X9 small-angle scattering beamline project, a major construction project jointly funded by NSLS and CFN, got a good start with the installation of a new RF cavity in X9 during the shutdown.

In safety news, corrosive chemicals can now only be handled in designated chemical laboratories around the storage ring. This change was necessary in order to meet BNL requirements. We do not have adequate eye wash and shower facilities within our laboratories, according to OSHA requirements. BNL has allowed a temporary solution that requires having an eye wash/shower fixture within 50 feet of the work area, as long as we do some posting and provide an unobstructed path to the fixture. We are able to meet this requirement for most, but not all, of our laboratories, so please pay attention to the signs posted on the laboratory doors and work with corrosives only in the allowed designated areas. Contact Andrew Ackerman (ext. 5431) or Bob Chmiel (ext. 8141) with any questions or concerns.

Finally, I would like to extend my congratulations to several members of the NSLS community for various achievements. Nick Gmur, our ESH&Q Coordinator, and Peter Siddons, a staff physicist and leader of our Beamline Controls and Detector Development group, were recently honored, respectively, with a Brookhaven Award and a Science & Technology Award at the BNL Employee Recognition Award Ceremony. Additionally, the research group of NSLS scientist Elaine DiMasi won a "best poster" award at the fall meeting of the Materials Research Society. And, several NSLS student researchers recently presented the results of their research at the American Physical Society meeting in Baltimore.

The NSLS Scientific Advisory Committee (pictured above) and the Users' Executive Committee have been working with the NSLS to develop a five-year strategic plan for the facility.

Notes from the UEC

Peter Stephens, Users' Executive Committee Chair
Stony Brook University

When I wrote my last newsletter article, the NSLS-II project had just received CD-0 status. This means that the Department of Energy has, on the record, stated that there is a strong case for the nation to have such a facility. The good news keeps rolling in! The President's budget for FY07 contains a 14% boost for basic energy sciences, which funds construction and operation of the synchrotron radiation and neutron sources on which we depend for our research, as well as provides direct support for many of our research programs. This is exciting news, especially for us at the NSLS, because the budget contains $45M to start R&D for NSLS-II.

The landscape has changed, and we must work to take advantage of it. After years of essentially flat budgets for our research, there is suddenly a proposed 14% increase in the Office of Basic Energy Sciences (BES) in DOE's Office of Science. But first, a civics quiz: What will happen to that money between now and the next fiscal year? The answer: so many steps that it would exhaust the rest of my space here to discuss them. Moreover, there is so much uncertainty involved that it would be foolish to predict what could happen. But you can be sure that in this time of fiscal pressure, there will be lots of people looking to divert some of that increased funding to other areas. I believe that we will have to work harder than ever to make sure that money goes where we, NSLS users, want it to go. That boost is a crucial opportunity for our science, but we will have to present a strong case in order to get it.

One important impetus of this proposed increased funding is the report from the National Academy of Sciences, National Academy of Engineering, and Institute of Medicine, titled "Rising Above the Gathering Storm: Energizing and Employing America for a Brighter Economic Future." It is chock full of important data (543 pages) about the importance of science as a driver of the high standard of living that we enjoy in the United States, as well as some terrifying data about trends in education and research in this country. I strongly recommend that you download it from *www.nap.edu/catalog/11463.html* and read it carefully. If not the whole report, at least read the sixteen-page executive summary. The report has captured the attention of businesses and the federal government, and has led to the President's American Competitiveness Initiative, which includes the aforementioned increase in Office of Science funds for FY07.

By the time that you read this, the newly formed Synchrotron and Neutron Users' Group (SNUG) will have made a visit in April to Washington, D.C. to press our case for increased support of the DOE BES-supported facilities. We have designed SNUG to have a slower turnover than any of the individual facility user groups, in order to maintain continuity and coherence. We will be meeting with staff of individual members' senators and representatives, as well as key committee staff members.

The DOE Office of Science also supports high energy and nuclear physics, in part through user facilities such as Fermilab, the Stanford Linear Accelerator Center, and the Relativistic Heavy Ion Collider, along with other BES programs in environmental molecular sciences (Pacific Northwest National Laboratory), nanoscience centers, etc. We just had a meeting of the National User Facility Organization, which consists of user office heads and user group representatives, and received substantial advice, from Congressional staff members and others, on how to work with our elected representatives. The strongest lesson that I took from that meeting is the importance of building a continuing relationship with the government in order to win government support for science and technology — not just showing up to ask for money or argue for a program that is about to be canceled. We are planning a trip to Washington, D.C. early next fall, around appropriations time, and hope that many of you can join us. If you are interested in participating in this kind of effort, please get in touch with me.

One important focus of these education and outreach trips to Washington is to make it clear to senators and representatives that their districts contain strong constituencies for the DOE Office of Science, even if they do not house one of the facilities. Especially if you don't live in the First Congressional District of New York, your legislators should know that the NSLS is important in your life, that it is not a member item that could be cut without hurting you.

With that in mind, I have written you two emails in the past year suggesting that you contact your legislators, the head of the Office of Management and Budget, and the Secretary of Energy. Response appears to be about 4%, which I understand is typical of such requests within scientific societies. If looking at those two emails last year was burdensome, I apologize. If you are one of the few people who actually wrote, I thank

you, as does the rest of the NSLS community. If you didn't, there is still plenty of opportunity to make your voice heard in support of science.

In other news, the User Executive Committee voted at its last meeting to create two new Special Interest Groups: one with a focus on NSLS-II user issues, and one for high-pressure research. By the time you read this, representatives of those groups will have been elected and will be ready to work with the UEC at large.

The NSLS is working on a five-year plan for the future. The users and the DOE agree that it is crucial to keep the current NSLS operating at the cutting edge of science until NSLS-II is operating. This requires careful planning to make sure that limited resources are used in the best possible way. They must be divided among operations, stockpiling critical spares, hiring scientific and technical staff to work with users, and creating new beamline capabilities, etc. There will soon be a draft plan available for comment, and we will indeed be soliciting your input, especially at the Annual Users' Meeting in May. We are indeed grateful for the opportunity to participate in the long-range planning of the NSLS.

As many of you know, Mary Anne Corwin has left her position as head of the user office. While we will greatly miss her there, we will at least continue to see her as training coordinator. At the same time, I believe we have an excellent new friend and partner in Kathy Nasta; it is a pleasure to welcome her to the NSLS family.

As the NSLS-II project accelerates, Steve Dierker has stepped down as NSLS Chairman to devote his full attention to the new project. Chi-Chang Kao has assumed responsibility of chairing the NSLS. We are extremely grateful to both of them for their leadership and devotion, and excellent work on difficult tasks.

UEC Nominees

Joe Dvorak, Montana State University

Joseph Dvorak received his PhD from the University of Pennsylvania in 1998. During that time he conducted part of his research in the Chemistry Department at Brookhaven National Lab. After graduation, he accepted a post-doctoral position with Jose Rodriguez, where he did research on sulfur poisoning of model catalytic systems at U7A for two and one half years. He currently operates the U4B "double dragon" magnetics beamline for the Idzerda group at Montana State University. During his many years at the NSLS, he has been a benefactor of the outstanding resources, in terms of both equipment and people, that make the NSLS a truly unique and wonderful place to do research. As a member of the UEC, he would welcome the chance to serve the user community to maintain and improve the "useability" of the light source.

Benjamin S. Hsiao, Stony Brook University

Benjamin S. Hsiao is a Professor of Chemistry and an affiliated faculty member of Biomedical Engineering at Stony Brook University. He has been spokesperson of X27C since 1997, spokesperson of X3A2 from 2002-2004 and a long time user of the NSLS since 1989. He is a fellow of the American Physical Society. His research interests include polymer physics with an emphasis on soft materials. He has over 260 reviewed publications and book chapters. X27C routinely serves more than 80 researchers from over 20 international institutes every year and is the first dedicated small-angle scattering beamline with simultaneous SAXS/WAXD capability in the US. He is enthusiastic about bringing greater user friendliness, easier facility and software access, and more cutting-edge research opportunities to the NSLS community.

Dan Fischer, NIST

Dan Fischer is a group leader at the National Institute of Standards and Technology. His group operates a suite of spectroscopy materials science beamlines to study the structure and chemical nature of diverse materials at the NSLS. Research areas currently being investigated, include model catalyst systems, polymer surfaces and their interfaces, hard disk lubricant chemistry, self assembled monolayers and high temperature superconductors. For the past 22 years at the NSLS, Dan Fischer has engaged in materials characterization through the development and application of in situ synchrotron radiation spectroscopies via novel detection methods.

Howard Robinson, BNL

Howard Robinson is a Biophysicist in the BNL Biology Department/PXRR having come to BNL in 2001 from the University of Illinois. He collected protein crystallography data at all the US synchrotrons prior to coming to BNL. Many observations from these experiences have been applied to improvements in the user programs here at the NSLS. He has promoted rapid access to short project-driven data collections at the high flux beamline x29. In addition he is developing coordination of access to the crystallography insertion device lines for users on the bendmagnet lines. He has strived to expand the access to the NSLS for crystallography users via the PXRR Mail-in data collection program, which has in turn led to a number of long term collaborations.

Jeff Fitts, BNL

Jeff Fitts is an Associate Geochemist in the Environmental Sciences Department at BNL. He has been a synchrotron user for more than 10 years, beginning at SSRL, ALS and APS and for the last 5 years mainly at the NSLS. His interests are in the application of spectroscopy and imaging methods in environmental science. He is a co-PI in the Stony Brook/BNL Center for Environmental Science (CEMS), and spokesperson for the EnviroSuite Initiative. EnviroSuite is dedicated to developing resources for environmental science users at the NSLS and currently manages the PRTs at X11A/B and X15B and is a Contributing User at X27A. He is very interested in seeing the continued development of facilities and user support at the NSLS while also supporting efforts to provide user input into NSLS II.

Jose A. Rodriguez, BNL

Jose A. Rodriguez is a Senior Scientist in the Chemistry Department of Brookhaven National Laboratory and an Adjunct Professor at the Department of Chemistry at Stony Brook University. His main research interests are in the areas of surface science, catalysis, and solid state chemistry. He got a PhD in physical chemistry at Indiana University and did postdoctoral work at Texas A&M. He has been very active at the NSLS since 1992, doing experiments in high-resolution photoemission (U3,U4,U7 and U12), time-resolved XRD (X7B) and X-ray absorption spectroscopy (X11, X19A, X18B). He is interested in joining the UEC to facilitate and promote the use of the synchrotron in chemistry, physics and materials science.

Please vote online at: http://www.nslsuec.org/elections/uec-vote.asp

A Redox Reaction in Axon Guidance: Structure and Enzymatic Activity of MICAL

M. Nadella, M.A. Bianchet, S.B. Gabelli, and L.M. Amzel

Department of Biophysics and Biophysical Chemistry, Johns Hopkins University School of Medicine

During development, neurons are guided to their final targets by external cues. MICAL, a large multidomain cytosolic protein, is a downstream signaling molecule required for repulsive axon guidance. We have determined the structure of the N-terminal FAD-binding domain of MICAL to 2.0 Å resolution. This structure shows that $MICAL_{fd}$ is structurally similar to aromatic hydroxylases and amine oxidases. We obtained biochemical data that show that $MICAL_{fd}$ is a flavoenzyme that, in the presence of NADPH, reduces molecular oxygen to H_2O_2. We propose that the H_2O_2 produced by this reaction may be one of the signaling molecules involved in axon guidance by MICAL.

Neurons are required to make pathfinding decisions throughout their development and are guided to their final targets by a variety of environmental cues. Semaphorins are a family of guidance molecules that act as repellents in a variety of axon development processes. Repulsive guidance by Semaphorins is mediated through their interaction with Plexins, a family of transmembrane receptors. Biochemical and genetic analysis indicate that a large multi-domain cytosolic protein, MICAL (Molecule Interacting with Cas-L), is required for the repulsive axon guidance mediated by the interaction of Semaphorins and Plexins. MICAL proteins contain a large amino-terminal FAD-binding domain ($MICAL_{fd}$), followed by a series of protein-protein binding domains. $MICAL_{fd}$ is of great interest since it offers a novel link between redox reactions and an axon guidance response. Using x-ray crystallography, we determined the structure of murine MICAL1 FAD-binding domain, $MICAL_{fd}$ **(Figure 1)**.

Authors (from left) L.M. Amzel, S.B. Gabelli, M.A. Bianchet, and M. Nadella

$MICAL_{fd}$ is a mixed α/β globular protein that contains a Rossmann β-α-β fold, two conserved FAD-binding motifs, and a third conserved sequence motif. The first conserved GXGXXG dinucleotide binding motif resides within the Rossman fold. The second conserved GD motif has been observed in flavoprotein hydroxylases and forms part of a strand and a helix. A search of known structures reveals that the $MICAL_{fd}$ protein is most similar to aromatic hydroxylases, especially the *p*-hydroxybenzoate hydroxylase (pHBH) from *P. fluorescens* (rms 1.79 Å for 199 out of 484 aligned α-carbons).

The strong structural similarity of $MICAL_{fd}$ to PHBH suggests that the two proteins might have similar enzymatic activities. Since purified $MICAL_{fd}$ contains oxidized FAD, reduction of the cofactor was tested using either NADH (nicotinamide adenine dinucleotide) or NADPH (nicotinamide adenine dinucleotide phosphate). Although no net reduction of the FAD was detected, a steady, time-dependent oxidation of reduced nicotinamide dinucleotide was observed

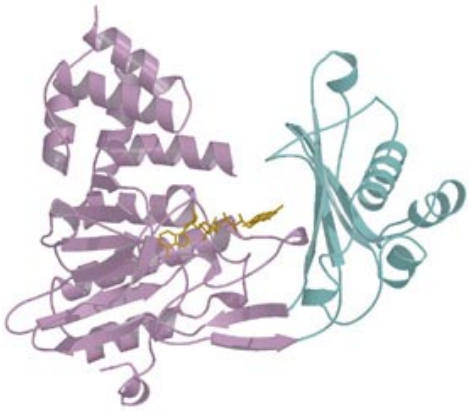


***Figure 1**. Ribbon representation of the tertiary structure of $MICAL_{fd}$. $MICAL_{fd}$ is a mixed α/β globular protein composed of two sub-domains of different sizes linked by two β-strands. Subdomain-1 is colored in magenta and subdomain-2 is colored in light blue. The observed FAD molecule is colored in yellow. The large sub-domain (subdomain-1; residues 1 to 226 and 373 to 484) contains the two known FAD sequence motifs (residues 84 to 114 and 386 to 416) and a third conserved motif typically found in hydroxylases (residues 212 to 225). The first motif is part of a Rossmann β-α-β fold (β1-α5-β2 in $MICAL_{fd}$). This is a sequence commonly found in FAD and NAD(P)H-dependent oxidoreductases. The second motif, which contains a conserved GD sequence in hydroxylases, forms part of a strand and a helix. In $MICAL_{fd}$ this second conserved sequence makes contacts with the ribose moiety of FAD.*

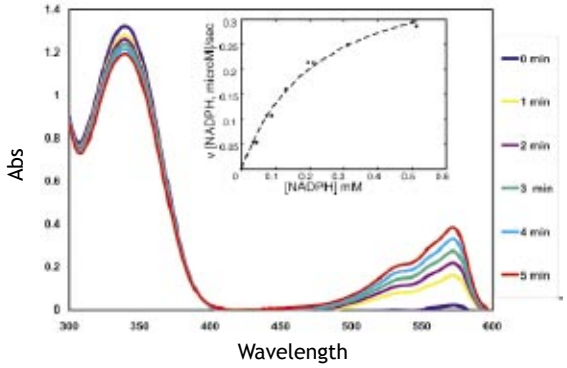
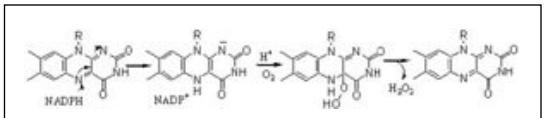


***Figure 2**. Kinetics of NADPH oxidation and H_2O_2 production. The absorbance peak at 340 nm is characteristic of reduced NAPDH and the peak at 560 nm the concentration of H_2O_2. The experiment ran for five minutes after the addition of the enzyme. The inset shows the initial rates as a function of NADPH concentration.*

(Figure 2). This observation suggested that enzyme-bound $FADH_2$ was formed but was then reoxidized by oxygen. The resulting production of H_2O_2 was confirmed by monitoring its formation with horseradish peroxidase in a coupled spectrophotometric assay **(Figure 2)**. The rate of the reaction is over 10 times faster with 200 μM NADPH than with 200 μM NADH, suggesting that MICAL is probably an NADPH-dependent enzyme.

The observation of this enzymatic activity can be explained by one of three cases. First, H_2O_2 is the physiological product of the enzyme and is a component of the avoidance signal. Second, as with other FAD hydroxylases, in the absence of substrate the hydroperoxide form of the enzyme (the $MICAL_{fd}$-FADH-O_2H intermediate) decomposes, producing hydrogen peroxide and oxidized enzyme-bound FAD (**Scheme 1**). Third, the enzyme may actually be an amine oxidase in which the $FADH_2$ is reoxidized by molecular oxygen, and the reduction by NADPH is a fortuitous, non-specific reaction. Although this last case is unlikely, discrimination among these possibilities requires further experimentation.



Scheme 1

The synthesis of a specific metabolite and the production of reactive oxygen species have been previously proposed as possible mechanisms of MICAL signaling. We have shown here that the FAD-binding domain of MICAL can generate at least the second kind of signals: MICAL reduces molecular oxygen using NADPH to produce H_2O_2.

*For more details of this work see: M. Nadella , M.A. Bianchet , S.B. Gabelli, J. Barrila, and L.M. Amzel, "Structure and Activity of the Axon Guidance Protein MICAL," Proc. Natl. Acad. Sci. USA, **102(46)**, 16830-5 (2005).*

DOE User Facilities Highlighted in Elements Magazine

The February issue of *Elements*, a magazine devoted to the fields of mineralogy, geochemistry, and petrology, highlights how scientists are utilizing User Research Facilities worldwide, including U.S. Department of Energy user facilities, such as the NSLS. This special issue, edited by Stephen R. Sutton (University of Chicago), describes x-ray, neutron, and mass spectrometry facilities worldwide and details many scientific advances made possible by these facilities.

As a part of this special issue, geochemists Antonio Lanzirotti (University of Chicago) and Richard J. Reeder (Stony Brook University) have authored an article in this issue titled "Accessing User Facilities and Making Your Research Experience Successful." It is written as a practical and comprehensive guide for *any scientist* who may want to boost their research by accessing user facilities that provide research tools not available at their home institutions.

To view the entire February issue of *Elements,* see:
http://www.elementsmagazine.org/Elements_online/ELEM_V2n1.pdf

X-Ray Ring Long-Range Schedule

May 2006

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June 2006

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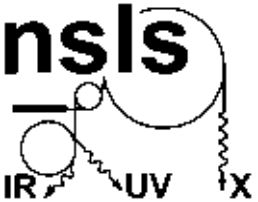


VUV-IR Ring Long-Range Schedule

May 2006

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

June 2006

Sun	Mon	Tue	Wed	Thu	Fri	Sat
				1 0000 Ops.	**2** 0000 Ops.	**3** 0000 Ops.
4 0000 Ops.	**5** 0000 Ops. 1800 Timing	**6** 0000 Ops.	**7** 0000 Ops.	**8** 0000 Ops.	**9** 0000 Ops. 1800 Studies	**10** 0000 Ops.
11 0000 Ops. 1800 Studies	**12** 0000 Maint.	**13** 0000 Maint.	**14** 0000 Ops.	**15** 0000 Ops.	**16** 0000 Ops. 1800 Timing	**17** 0000 Ops.
18 0000 Ops.	**19** 0000 Ops. 1800 Timing	**20** 0000 Ops.	**21** 0000 Ops.	**22** 0000 Ops.	**23** 0000 Ops. 1800 Studies	**24** 0000 Ops.
25 0000 Ops.	**26** 0000 Ops.	**27** 0000 Studies	**28** 0000 Studies	**29** 0000 Ops.	**30** 0000 Ops. 1900 No User Beam	

July 2006

Sun	Mon	Tue	Wed	Thu	Fri	Sat
						1 Lab Holiday No User Beam
2 Lab Holiday No User Beam	**3 Lab Holiday** No User Beam	**4 Lab Holiday** No User Beam	**5** 0000 Maint.	**6** 0000 Maint.	**7** 0000 Cond.	**8** 0000 Cond.
9 0000 Cond./Ops.	**10** 0000 Ops.	**11** 0000 Ops.	**12** 0000 Ops.	**13** 0000 Ops.	**14** 0000 Ops. 1800 Timing	**15** 0000 Ops.
16 0000 Ops.	**17** 0000 Ops. 1800 Timing	**18** 0000 Ops.	**19** 0000 Ops.	**20** 0000 Ops.	**21** 0000 Ops. 1800 Studies	**22** 0000 Ops.
23 0000 Ops.	**24** 0000 Ops.	**25** 0000 Studies	**26** 0000 Studies	**27** 0000 Ops.	**28** 0000 Ops.	**29** 0000 Ops.
30 0000 Ops.	**31** 0000 Ops. 1800 Timing					

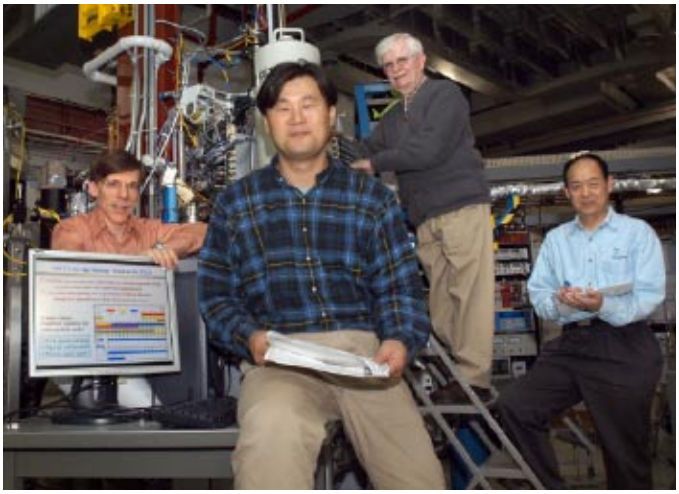
August 2006

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

At the NSLS, Scientists Working Toward Better Batteries

Laura Mgrdichian, NSLS Science Writer

As more and more people rely on cell phones, laptop computers, personal organizers, and even hybrid electric-gas vehicles, scientists are working to develop rechargeable batteries that are ever smaller, cheaper, lighter, safer, and longer-lasting. At the National Synchrotron Light Source, a collaboration of scientists is deeply involved in this effort. They are investigating a group of promising new materials for use in lithium-ion batteries, the most common type of battery found in portable electronics and the most promising type for hybrid cars.



Authors (from left) Daniel A. Fischer, Won-Sub Yoon, James McBreen, and Xiao-Qing Yang

Lithium-ion batteries work by shuttling positively charged lithium ions between the "cathode" (the battery's positive terminal) and "anode" (the negative terminal). As the battery is charged, lithium ions are forced out of the cathode and moved into to the anode through the "electrolyte," the solution inside the battery. When the battery is in use, the process reverses. The scientists are studying a group of new cathode compounds consisting of the elements lithium, cobalt, nickel, manganese, and oxygen.

"Despite the wide use of lithium-ion batteries, there have been very few studies on exactly how the cathode material behaves in the charging process," said the study's lead researcher, Brookhaven chemist Won-Sub Yoon. "How are the oxygen atoms involved? What is the relationship between the oxygen atoms and the other metal atoms in the compound? To design a better cathode material, and thus a better battery, these questions must be answered. An in-depth understanding of these problems will provide a road map for the development of these new materials."

Using various x-ray techniques, Yoon and his colleagues have done just that. They discovered that as lithium ions leave the cathode material during the charging process, changes occur on the manganese and cobalt atoms that are quite different from those that occur on the nickel atoms. Specifically, the manganese and cobalt atoms do not lose electrons as the lithium ions are removed, while the nickel atoms, in contrast, do lose electrons. The group also learned more about how the cathode material compensates for the positive charge it loses as the lithium ions move to the anode. They found that empty regions with positive charge, called "holes," are created in the cathode. In addition, their x-ray data show just where these holes are located: within the electron orbitals of oxygen atoms that are bound to cobalt atoms.

Gathering these details on the cathode's electronic behavior is an important step in lithium-ion battery research. This new knowledge will help the material become a common component of a new series of better lithium-ion batteries. More detailed information on this research can be found in the group's scientific paper, which is published in the December 14, 2005, edition of the Journal of the American Chemical Society.

The other scientists involved in this research are Kyung Yoon Chung, Xiao-Qing Yang, and James McBreen (BNL Chemistry Department); Mahalingam Balasubramanian (Argonne National Laboratory); Clare Grey (Stony Brook University); and Daniel Fischer (National Institute of Standards and Technology).

Call for Science Highlights

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- on the NSLS homepage
- in the Annual Activity Report
- in the NSLS Newsletter
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To apply:
Just send the publication reference and abstract to NSLSinfo@bnl.gov

The Word from User Administration

Kathleen Nasta, NSLS User Administrator

The calendar change to 2006 brought another change: I began my tenure here as your new User Administrator! I have been enjoying getting to know the staff (thank you for being so welcoming), and I have been learning about the many procedures our office must follow to meet our goal: assist users in gaining access to conduct their experiments. I welcome your ideas and concerns; please e-mail, phone, or stop by (NSLSUser@bnl.gov or nasta@bnl.gov; 631-344-5763).

I would also like to officially introduce Mercy Baez, who joined the NSLS in August 2005. Mercy has taken over responsibilities previously held by Melissa Abramowitz as well as additional opportunities.

Additionally, I would like to extend a personal thanks to Mary Anne Corwin for turning over an office that runs so efficiently, and for her continued cooperation during both of our transition periods.

Progress on PASS continues:

- Rapid Access – Two prerequisites are complete, and each will be helpful to users on its own. First, a Principal Investigator (PI) can name a delegate for a PASS form. PIs can designate another PASS user (e.g., a professor can name a student) to prepare, submit, and receive status updates. Second, a system of Envelope Safety Approval Forms (SAFs) has been established. Macromolecular crystallography users are asked specific questions prior to a full SAF. If answers indicate the experiment meets the criteria of a predefined Safety Envelope, no further SAF information will be required. Approval of the SAF will be greatly expedited.
- Contributing User (CU) – A new type of PASS form has been created for this new type of user. Similar to a PRT form, most information required is related to safety. It is expected that by the September cycle new features will be added to PASS for CUs to declare their intention to use their allotted beam time within the system.

Foreign Visits and Assignments:

A few up-and-coming requirements from the Foreign Visits and Assignments (FVA) office were discussed at the Town Meeting in March. Now, hosts will also receive an e-mail notification if a user is approaching a required renewal date. Further, hosts will receive an e-mail message at the close of a user's experiment, and the host will click on the applicable link within the e-mail to verify any known occurrences.

2006 Users' Meeting:

Finally, this year, the NSLS Annual Users' Meeting will be a joint meeting between users of the NSLS and the CFN, and will be held on May 15-17. We hope this joint meeting will provide many opportunities to network and to discuss collaborations for the future. I personally look forward to meeting many of you then!

Weekly NSLS Activities

TUESDAY

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

WEDNESDAY

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

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

THURSDAY

Student/Postdoc Pizza Get-Together: 1:00 p.m., NSLS Library (across from stockroom) every other Thursday. Funded by the Users' Executive Committee (UEC). All local and visiting students and postdocs are invited to attend. For more information, please contact Meghan Ruppel at (631) 344-2209 or ruppel@bnl.gov.

FRIDAY

Friday Lunch Seminars: 12:00 to 1:00 p.m., Seminar Room. Learn about the exciting research being done at the NSLS. Two unannounced, informal, half-hour presentations are made weekly by experimenters. Attendees can bring their own lunch or can place a sandwich order by contacting Joan Marshall at (631) 344-3887 or jmarshall@bnl.gov by 10:00 a.m. on Friday. Orders must be paid upon delivery.

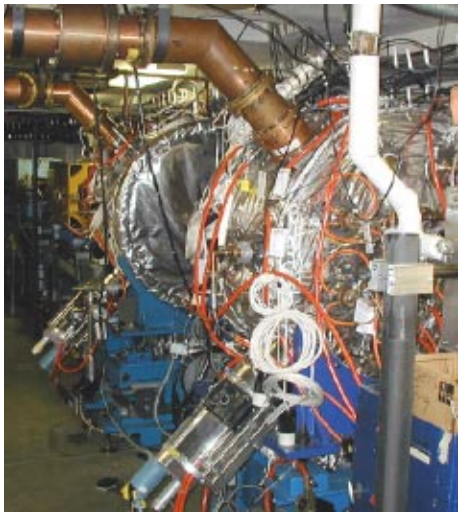
NSLS Accelerator Complex Update

Erik Johnson, Associate Chair for Operations and Engineering

As of March 1st, reliability of both the VUV and X-ray rings exceeded 95% for Fiscal 2006, although coming out of the winter shutdown was a bit rocky for the first week. The winter shutdown we just completed was one of the longest in recent memory because it included two major installations. As noted elsewhere in the newsletter the new insertion device for X25 was installed and will soon be moving into routine operations. We also installed the last of our new radio frequency (RF) cavities which makes way for the installation of an insertion device in the straight section that serves beamline X9.

Because the winter shutdown was long, we have scheduled a very short (but busy) May shutdown. The work planned includes starting the relocation of the existing X9 beamline to it's new home at X3. Over the next several shutdowns, installations will take place at X9 to provide an insertion device based beamline for the Center for Functional Nanomaterials. During the spring shutdown we have planned for the replacement of klystron 3, maintenance and rebuilds of the X17 cryogenics plant, chiller maintenance, and general preventative maintenance. In addition, servicing of the electrical substations in the center of the x-ray ring is scheduled for May 20th which will require powering down a substantial part of the building.

As part of our continuing effort to improve electrical safety at the facility, the Electrical Equipment Inspection (EEI) program for the Light Source is in place and inspection of our operating equipment has begun. This program is intended to ensure safe operation of our electrical equipment. The scope of the program includes currently owned equipment as well as future purchases. Equipment owners should visit the EEI website and begin the process of inspection for their equipment. More information on this program can be found on the NSLS website at *http://www.nsls.bnl.gov/organization/OpsEng/ElectricalSys/EEI/*.



The X9 RF straight section, showing the newly installed XRF-1 RF cavity (furthest away), along with the previously installed XRF-2 cavity (closest). In addition to improving the reliability of the x-ray ring RF systems, these new cavities provide additional free space in the straight section for the installation of an insertion device, as was done at X29 where the other pair of RF cavities in the x-ray ring reside.

Finally, thanks again to all who provided input for the Summer 2006 schedule. As with last year, working around the holidays resulted in an unusual schedule sequence, but it actually provides about the same user time as comparable schedules in the past. The Winter 2006 schedule was the first run with reduced studies time, resulting in 1.25 days of additional scheduled x-ray operations. I would be interested in comments on that change as well as the input for the Fall 2006 sched-

Identification and Tagging of Equipment

The Department of Energy requires that all non-expendable property at BNL have bar codes or tags to indicate ownership. If your organization does not have tags (logo's, etc.) we will supply blank tags (see sample on bottom).

Tags are available at the NSLS stockroom or with Anna Seda (rm. 2-176) free of charge. Please obtain tags, fill in your organization in the space provided and apply to all unidentified equipment belonging to your organization. The serial numbers on the blank tags are for your optional use in recordkeeping.

BNL's Supply & Material Division will be conducting periodic inspections to ensure proper identification of all equipment.

If you have any questions or need assistance, please call Anna Seda at (631) 344-7132.

Safety Update: PASS and ISM

Andrew Ackerman, NSLS Safety Officer

I chose two topics to discuss in this article: our improvements to the Proposal Allocation Safety Scheduling (PASS) system, which are aimed at providing a better safety review for our protein crystallography (PX) users, and our recent efforts to ensure good use of the concepts that constitute the Department of Energy (DOE) Integrated Safety Management (ISM) program. The changes to PASS were envisioned some time ago, so we are pleased to see that progress is being made. Our recent focus on ISM is important for everyone at the NSLS, as all of our planning is organized around that system.

PASS and PX

We are collecting a considerable amount of PX data at the NSLS, with many users bringing many samples and needing short runs and quick access to our PX beamlines. Almost all of these experiments involve harmless samples that are analyzed on a standard equipment setup for which the risks and controls are well defined. Making the most efficient use of the available beam time requires flexible scheduling and, since this work is so consistent and well defined, we have been able to change the Safety Approval Form (SAF) part of PASS to accommodate that. At the same time, we have been able to much improve our review and documentation of these projects.

When entering the SAF portion of PASS, users are now given the option to identify their work as fitting the new "standard PX envelope" by answering a set of eight questions that define that envelope. The standard PX envelope includes data collection on macromolecules with no wet chemistry, no gasses, no toxins, and nothing viable, and sample transport in dry shipping dewars. If your experiment fits this profile, you are asked to acknowledge that by answering the PX questions, after which your SAF is automatically approved and you may proceed at the beamline. Only standard PX experiments may use this new review path. Our intent is to provide a mechanism for PX users to report standard experiments, to allow that work to move easily among the PX beamlines, and to ensure that experiments that exceed the envelope are identified and given any necessary additional scrutiny.

Nothing has changed at the beamlines. You must still call the Operations Coordinator to start and finish your experiment, the envelope SAFs will be posted, and you must meet all the other requirements in place to enable the beam. You must still have a separate SAF for each experiment and for each beamline you use. All that has changed is the mechanism you must use to report your work at the NSLS. Our hope is that this new system will provide more flexibility and a better definition of the standard PX experiments at the facility.

ISM

Let me turn now to Integrated Safety Management (ISM) implementation at the NSLS. Here there is a good story to tell, with mature programs in place for planning our work, determining requirements, and working safely within those requirements. We have programs in place to ensure attention to worker qualification, to define individual roles and responsibilities, and to collect feedback for constant improvement. All work at the NSLS is planned and conducted with a well integrated consideration and review of safety. SAFs are the tools that most users are familiar with for ensuring experiment planning, but we do far more to control the risks at the NSLS that together make up our overall ISM program.

We will be working over the next several months to refine and improve those programs and to remind everyone of the ISM "Five Core Functions" and "Seven Guiding Principles" because, in addition to maintaining and improving these programs, we must also be able to explain them. A DOE audit of ISM implementation at BNL is expected sometime in the spring of 2007. We will prepare for this audit with discussions of experiment review, enhanced work planning, R2A2s, training and qualification, and feedback and improvement. The audit will likely go well and, while we will prepare, we are most interested in continuing to stress safety and keep the NSLS programs effective and sensible. More to come …

The NSLS Newsletter is printed on paper containing at least 25 percent recycled materials, with 10 percent post-consumer waste.

Highlights from the COMPRES-Sponsored Workshop on Synchrotron Infrared Spectroscopy for High Pressure Geoscience and Planetary Science

Zhenxian Liu, Geophysical Laboratory, Carnegie Institution of Washington

In recent years, infrared (IR) microscopy and spectroscopy have greatly benefited from new synchrotron techniques. This has opened up new directions in many fields, including physics, biology, chemistry, materials science, high-technology, and forensics. One of the most exciting areas is high-pressure geoscience and planetary science. High-pressure synchrotron IR spectromicroscopy is an ideal coupling of the diamond anvil cell and synchrotron IR radiation. The technique is also useful for studying minerals quenched from high pressures and temperatures, and natural samples at ambient conditions.

Participants of the Workshop on Synchrotron Infrared Spectroscopy for High Pressure Geoscience and Planetary Science.

Sponsored by COMPRES (the Consortium for Materials Properties Research in Earth Sciences) and the NSLS, the workshop on Synchrotron Infrared Spectroscopy for High Pressure Geoscience and Planetary Science was held at the NSLS on November 3-5, 2005. The conveners were Zhenxian Liu and Russell J. Hemley (Geophysical Laboratory, Carnegie Institution of Washington). The workshop was a great success, and more than 50 attendees — the maximum allowed by the budget and size of the lecture room — took part.

The workshop consisted of five sessions. The Friday morning session was for attendees who were new to the IR spectroscopy techniques used in this field. For experienced users, it was also a useful review of the fundamentals and new developments. Q. Williams (University of California at Santa Cruz) gave an overview of IR spectroscopy and its applications in the Earth sciences. G. Rossman (California Institute of Technology) gave a talk on hydrous components in nominally anhydrous minerals, which was important for users who are interested in calibrating the water content in minerals. A. Hofmeister (Washington University) discussed the high-pressure far-IR spectroscopy of mantle candidate minerals. Finally, J. Tse (University of Saskatchewan) described theoretical methods for vibrational spectroscopy and many other applications.

Friday's afternoon session was started by L. Carr (NSLS). He gave a very comprehensive talk on Fourier transform spectroscopy techniques and an overview of the IR programs at the NSLS. Seven additional speakers (A. Goncharov, V. Struzhkin, and S. Jacobsen, Geophysical Laboratory; D. Klug, Canadian Research Council; H. Scott, Indiana University at South Bend; G. Lager, University of Louisville; and Y. Lee, Brookhaven National Laboratory) discussed different topics related to the work they have done at NSLS beamline U2A.

The third session, held Saturday morning, focused on imaging techniques combined with synchrotron sources. L. Miller (NSLS) gave an extensive overview of chemical imaging at high spatial resolution using a synchrotron infrared microscope. Other speakers (L. Wang, Stony Brook University; L. Dobrzhinetskaya, University of California at Riverside; M. Koch-Müller, GeoForschungsZentrum Potsdam, Germany; and S. Clark, Advanced Light Source) discussed the applications of imaging techniques as well as high-pressure IR studies at other synchrotrons. The facility tour and hands-on session on Saturday afternoon attracted more than 30 people. At the IR beamline, new users received detailed information on the beamline facility and its capabilities, as well as first-hand experience on how to perform high-pressure IR experiments.

The last session, for student/post-doc experiments at U2A, started right after the workshop. Two students and one post-doc submitted their research proposals and one day of beamtime was allocated per proposal. This new session offered a great opportunity to learn how to use the synchrotron IR facility and collect valuable data. The experiments went very well and the IR data they obtained are publishable in scientific journals.

For more information about the IR workshop, please visit the web site at: *http://www.nsls.bnl.gov/newsroom/events/workshops/ir/Default.htm.*

NSLS Researchers Produce a Praiseworthy Poster

Laura Mgrdichian, NSLS Science Writer

At the Materials Research Society Fall 2005 meeting, held November 27 – December 1 in Boston, a poster created by an NSLS research group was chosen as one of only six (out of hundreds) to receive a "best poster" award.

The group is studying "biomineralization," the process by which organisms create mineralized tissues, such as bones, teeth, and shells. Biominerals are typically much stronger than ordinary minerals and may one day be used to create new nanoscale composite materials. The collaboration includes NSLS scientist Elaine DiMasi, Karthikeyan Subburaman (Stony Brook University), Nadine Pernodet (SBU), Seo-Young Kwak (BNL), Shouren Ge (SBU), Nan-Loh Yang (City University of New York), and Miriam Rafailovich (SBU).

The group's poster is a summary of their research on eggshell protein mineralization, which they use as a model to study biomineralization. First, the shell's support membrane is formed and proteins are deposited onto it. Then, the minerals begin to form and grow around the protein deposits. Finally, the mineral forms a crystal structure on the protein-fiber network.

The researchers studied this process using "extracellular matrix proteins" — the type of proteins that make up skin tissue, for example. Their results show that only the fibrous portions of the proteins accepted calcium carbonate, the mineral.

Elaine DiMasi (left) and poster presenter Karthikeyan Subburaman.

Two NSLS Staff Members Awarded for Jobs Well Done

Laura Mgrdichian, NSLS Science Writer

Congratulations are due to Peter Siddons and Nick Gmur, who, respectively, recently were honored with a Science & Technology Award and a Brookhaven Award at the Fiscal Year 2006 BNL Employee Recognition Award Ceremony on February 2.

Peter Siddons

NSLS physicist Peter Siddons is cited for his outstanding contributions to developing detectors for use in synchrotrons. His ideas are recognized as innovative and original, resulting in new and unique detectors that make new experiments feasible. Over the last several years, Siddons has directed the NSLS detector and control group and, in collaboration with BNL's Instrumentation Division, has developed a suite of detectors. The detectors have been delivered to users with great success, and have made significant impact on scientific programs at the NSLS and elsewhere. Also, the detector group under Siddons' direction has gained worldwide recognition for the NSLS and BNL. For example, recently BNL was awarded a multi-year project to construct two imaging detectors for the Linear Coherent Light Source project at the Stanford Linear Accelerator Center. Facilities in England, Australia and Taiwan as well as at Argonne National Laboratory are interested in or already actively collaborating with Siddons' group.

Nick Gmur

Gmur is cited for his outstanding work as the NSLS Environmental Safety & Health (ESH) Coordinator. He is involved in many activities within the department that carry into almost every part of all programs. He has been a key contributor to challenging ESH issues at the NSLS that include implementing requirements for BNL's Integrated Safety Management program and the internationally recognized ISO 14001 and OHSAS 18001 programs. Other major achievements included writing, conducting, and coordinating reviews and implementing the accelerator authorization basis documents for the Deep-Ultraviolet-Free Electron Laser, the NSLS and Accelerator Test Facility, and the NSLS Environmental Assessment required by the National Environmental Policy Act. Widely respected at BNL, he is recognized for his leadership, for bringing great attention to quality and detail, and for always getting the job done on schedule.

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

Call for NSLS General User Proposals

For Beam Time in Cycle	Deadline
September - December 2006	Wednesday, May 31, 2006

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

Proprietary Proposal Forms with instructions can be found at:
http://www.nsls.bnl.gov/users/usersguide/BT-proprietary.htm

Safety Approval Forms

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

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

NSLS User Administration Office

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

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

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