

### November 2000

### Determination of the Atomic-Resolution Crystal Structure of the Large Subunit from the Ribosome of Haloarcula marismortui

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The ribosome is a macromolecular complex found in all living cells that is composed of protein and ribonucleic acid (RNA). It is the enzyme that catalyzes the synthesis of proteins from amino acids, and it is unusual in two striking ways. First, it is a programmed enzyme: information extracted by the ribosome from molecular data tapes determine the identity of the protein it makes. Proteins are linear polymers of 20 different kinds of amino acids. What distinguishes one protein from the next is its chain length, i.e. the total number of amino acids it contains, and the order in which the different amino acids appear in the chain. The data tape in this case is a molecule of messenger RNA, which is essentially an RNA copy of a DNA gene encoding a particular protein. Interactions between the ribosome and the messenger bound to it determine the sequence of the product it makes. The second unusual feature of the ribosome is that unlike almost all other enzymes, it is almost two thirds RNA, and as we will see below, ribosomal RNA contributes directly to the catalytic activity of the ribosome.

Two papers were published this August announcing the determination of the structure of the large ribosomal subunit from Haloarcula marismortui at 2.4 Å resolution [Ban, N. et al, (2000) The Complete Atomic Structure of the Large Ribosomal Subunit at 2.4 Å Resolution. Science 289, 905 - 920; Nissen, P. et al, (2000) The Structural Basis of Ribosome Activity in Peptide Bond Synthesis. Science 289, 920 - 930]. Most of the data for this work were collected at the National Synchrotron Light Source using Beamlines X12B, X12C, and X25, which are run by Malcolm Capel, Robert Sweet, and Lonnie

Berman, respectively. Knowledge of the structure of this subunit has taught us a lot about the functioning of the whole ribosome.

The crystals in guestion posed major technical challenges. The molecular weight of the large subunit from H. marismortui is 1,500,000 (that of the small one is 600,000), and since it lacks internal symmetry, this was the molecular weight of the minimum unit of unique structure that had to be determined. This is several times larger than that of the next most complicated biological macromolecule whose structure has been solved at atomic resolution. The unit cells of crystals of molecules this big are quite large, in this case 210 x 300 x 570 Å, and because they diffract X-rays weakly, data collection is impractical using X-ray sources less bright than those available at

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synchrotron light sources. Adding to the difficulty was the fact that the packing of ribosomal subunits in the crystals is extremely sensitive to ionic conditions, and several crystal forms can be produced that have superimposable reciprocal lattices. The crystals we solved have the symmetry C222<sub>1</sub>. The variant most commonly encountered belongs to the lower-symmetry space group P2<sub>1</sub>, but is usually twinned so that its diffraction pattern has the same symmetry as the C222<sub>1</sub> crystals [Ban, N., Nissen, P., Capel, M.S., Moore, P.B., and Steitz, T.A. (1999), A The Large Ribosomal Subunit at 5Å Resolution: Identification of Protein and RNA Structures. Nature 400:841-847].

It is difficult to determine phases for macromolecular crystals like these using conventional isomorphous replacement techniques, or any of the other approaches commonly employed by macromolecular crystallographers. All of them require that the positions be determined of a small number of atoms having unusual scattering properties that have been introduced into the crystals by one strategy or another. For example, difference-Patterson methods often are used to locate heavy metal atoms in macromolecular crystals that have reacted with standard, single atom, heavy-metal compounds, provided the number of sites of reaction is small. However, if the number is small, the heavy-atom contribution to the diffraction pattern of derivatized crystals is likely to be too small to measure, and no positional information will result. If a heavy metal compound that reacts at a large number of sites is used so that the diffraction differences are easy to measure, the difference Pattersons that result are likely to be too complicated to solve, and again no useful positional information will be obtained. Similar problems confront the crystallographer attempting to obtain phases experimentally by other routes.

The phasing problem was solved for these crystals in two stages. In the first stage, only low resolution phase information was sought [Ban, N., Freeborn, B., Nisssen, P., Penczek, P., Grassuci, R.A., Sweet, R., Frank, J., Moore, P.B. & Steitz, T.A. (1998). A 9 Å resolution X-ray crystallographic map of the large ribosomal subunit. Cell 93, 1105-1115]. Cluster compounds that contain large numbers of metal atoms (for example, 18 tungsten atoms) were used to make derivatives, and the resulting difference data were analyzed initially at low resolution. In this case the contribution each cluster makes to the diffraction pattern is roughly that of a single atom having the same number of electrons as the total number in the cluster compound. When heavy-metal compounds like these are used, derivatization at a small number of sites can produce measurable changes in diffraction intensities, and difference Pattersons will be soluble. Use was also made of the remarkably accurate three-dimensional reconstructions of macromolecular structures that one now can generate by analysis of two-dimensional electron microscopic images. Using molecular-replacement techniques, these electron density maps - and that is approximately what results from such an analysis - can be used to phase the low-resolution reflections of X-ray diffraction patterns containing the same objects. (For another example of the use of this approach, see [Cate, J.H., Yusupov, M.M., Yusupova, G.Zh., Earnest, T.N. and Noller, H.F. (1999) X-ray crystal structures of 70S ribosome functional complexes. Science 285, 2095-2104].)

Low-resolution phases were critical for obtaining experimental phases at higher resolution. Conventional, single-atom, heavy-metal compounds that bind to the ribosome at many locations were soaked into crystals, and diffraction differences were measured. Because low resolution phases were available, the sites where these compounds bind to the ribosome could be determined approximately by difference-Fourier methods, and their positions then were refined using the higher resolution difference data. Both isomorphous difference data and anomalous difference data were used for this purpose.

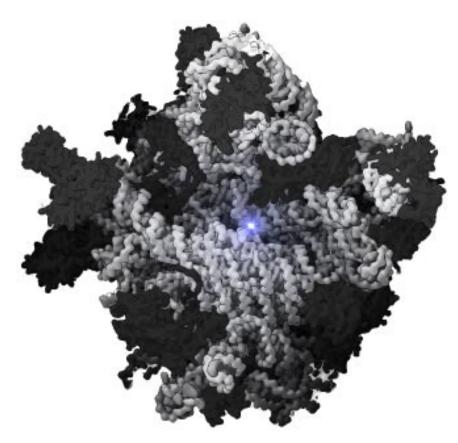
The ribosome was well-enough imaged in the electron density maps generated using such phases that solvent-flipping and histogram-matching methods could be used to improve phase quality and extend the resolution of the phase set. The first, well-phased electron density map having a resolution high enough so that its features could be interpreted chemically was obtained in the middle of November, 1999, using data measured at X25 with a MAR345 imaging-plate detector. The native data set that made it possible to extend the resolution to 2.4 Å was obtained at APS the following spring.

The structure that has emerged reveals that the large ribosomal subunit from *H. marismortui* consists of 31 proteins and two RNA molecules (see **Figure 1**). The RNA forms a monolithic matrix that has a shape similar to that of the whole particle. The globular bodies of the proteins are inserted into gaps and crevices in the surface of the RNA mass, and many have irregularly structured extensions that reach into the center of particle through interstices in the folded RNA. The predominant function of the protein appears to be stabilization of the fold of the RNA, which constitutes two-thirds of the mass of the overall assembly.

Structures also have been obtained of the large ribosomal subunit complexed with two substrate analogues. These structures reveal that the site in the subunit where peptide bond formation takes place is at the bottom of a deep cleft. This is the origin of a tunnel that passes all the way through the body of the particle. It appears that proteins are synthesized at one end of this tunnel, pass through its length, and then emerge complete at its far end. No portion of any protein comes closer to the site where peptide bonds form than 18 Å. **There can be no doubt that the active site of this enzyme is entirely composed of RNA.** For the benefit of non-biochemists, one hastens to add that the overwhelming majority of enzymes are composed entirely of protein.

On the basis of the placement of nucleotides in the neighborhood of the active site, a proposal has been formulated for the way ribosomes catalyze peptide-bond

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**Figure 1**. The image represents the active site view of the large ribosomal subunit showing its RNA/protein architecture. The subunit is shown in a surface filling representation, RNA is shown in lighter shading and the proteins are the darkest regions of the structure. The location of the substrate analogue bound to the active site of the ribosome is shown as a source of light. The active site of the ribosome is formed exclusively by ribosomal RNA revealing that the ribosome is a ribozyme.

formation. It postulates that a specific adenine in ribosomal RNA acts as a general acid/base during peptide bond formation, and the structure suggests why the pK<sub>a</sub> of that adenine is approximately 7.0, as it must be if it is to function catalytically, rather the roughly 1.0 that is observed for adenines in more ordinary environments.

This structure is providing insights into the way RNA molecules fold, how proteins interact with RNA, and the mechanism of peptide-bond formation. It also will be informative for those interested in antibiotics, many of which kill pathogenic bacteria by blocking the activity of their ribosomes. Unpublished studies, done so far only at low resolution, show that antibiotics can be soaked into these crystals, and then visualized bound to the ribosome using difference-Fourier techniques. Insights into the mechanism of antibiotic action, the ways bacteria become resistant to antibiotics, and, more speculatively, strategies for synthesizing new antibiotics may well emerge.

### Acknowledgements

Image courtesy of N. Ban, Institute for Molecular Biology and Biophysics ETHZ, Switzerland, Science, and Yale University.

### Structural Genomics at the NSLS-NIH Awards Major Grants to BNL

Mark Chance Albert Einstein College of Medicine

The National Institute of General Medical Sciences (NIGMS) has developed a major new initiative to determine the structures of thousands of proteins over the next decade. Work toward this goal will be divided into two phases: a five-year pilot stage and a subsequent five-year full-scale production phase. The initial phase began on September 27, 2000 with the announcement of funding for Structural Genomics centers.

BNL and NSLS staff and beamlines are closely involved with two of the centers, which were awarded after an international competition. The first, the New York Structural Genomics Research Consortium, includes a partnership between five New York institutions including: the BNL Biology Department, which runs crystallography beamlines X12B and X12C, Albert Einstein College of Medicine, which runs X9A and X9B, as well as Rockefeller, Mt. Sinai, and Cornell Weill Medical College. The TB Structural Genomics Consortium will also utilize beamline X-8C through the connection with Los Alamos National Lab.

"These research centers are true pilots," said Dr. John Norvell, director of the NIGMS Protein Structure Initiative. "Each will include every experimental and computational task of structural genomics and will develop strategies for use in the subsequent large-scale research networks. By the fifth year of the award, we expect each pilot center to reach a production level of 100 to 200 protein structures annually, which is significantly greater than the current rate of protein structure determination." Users may remember that Dr. Norvell was the keynote speaker at the NSLS Annual meeting in 1999. Based on the generous funding for the structural genomics centers, and the key role to be played by the NSLS, it appears that Dr. Norvell remembers us.

### **Users' Perspective**

Mark Chance UEC Chair, Albert Einstein College of Medicine

The UEC met in the morning on August 7<sup>th</sup> and conducted a town meeting that afternoon. During the UEC meeting, the 2001 annual Users' Meeting plan was presented by Simon Bare and approved for the dates of May 21-23 (see adjacent article). To better plan for the 2001 and future meetings, the UEC requested that Mary Anne Corwin, our User Administrator, attend the ALS meeting in October. She will report on that meeting at the Nov. 15, 2000 UEC and Town Meetings coming up. We are eager to see what other light sources are doing and hope to adopt the best practices of those facilities (as well as avoid the worst!).

The UEC also discussed election procedures and decided the current system of electing candidates at the annual meeting to be satisfactory. Getting good candidates to run for the UEC has sometimes been a problem. Users are encouraged to consider running for the UEC to help make the NSLS a better facility for all users. Please e-mail me (mrc@bnl.gov) if you are interested in becoming more involved.

The Town meeting included presentations on Computer Security, Long term facilities planning for BNL, UEC lobbying efforts, and the Chair's report. In Michael Hart's absence, Richard Heese reviewed the status of the machine and the continual improvements that have been seen in recent years. At the time of the Town Meeting, the permanent shift to a ring energy of 2.8 GeV at lower emittance was imminent. Since that time it has been accomplished with few problems. Users are encouraged to contact the UEC with comments on the higher energy, low emittance beam and its effect (both positive or negative) on their user programs.

A report on Computer Security changes at BNL elicited significant concern from the users. The loss of telnet and FTP access from outside may cause problems for some users although access from BNL to the outside (e.g. sending your data home and logging onto your computer at your home institution) should continue unaffected. A further update on Computer Security issues will occur at the town meeting on November 15. If you are affected adversely, please contact me with examples of problems you are encountering and they can be brought up at the meeting for discussion.

Tom Sheridan, Deputy Director of Facilities gave a presentation on long term plans for BNL, including construction projects under consideration. This long term planning process is to give DOE an idea of where BNL is going and what significant additional resources in terms of space and infrastructure will be required. This planning process is ongoing and at the Town Meeting the users emphasized their needs for lab and office space that are currently hindering research progress.



Users' Executive Committee (including Special Interest Group Representatives): Lisa Miller, Larry Carr, Michael Dudley, Shane Stadler, Mary Anne Corwin, Barbara Illman, Mark Chance, Tony Lanzirotti, Mark Lucas, Leemor Joshua-Tor, Michael Vaughan, Simon Bare, Chris Jacobsen, and Kenneth Evans-Lutterodt.

In addition, a presentation on UEC lobbying activities in Washington, DC was given by yours truly. These activities were coordinated with DOE officials as well as with BNL lobbyists. Most encouraging is that this was a joint effort of user representatives from each of the four DOE synchrotrons. This effort will be continued this year and a visit to DOE to discuss the proposed 2002 budget will be formalized soon. On the "results" side, it appears that Congress has funded the DOE budget at or near the President's request. This includes a significant increase for the NSLS as well as for a number of important basic science programs.

### One View of the NSLS from the Perspective of SRI 2000

Erik Johnson

Head, NSLS Experimental Systems Group

'The NSLS continues to be a vibrant international center for synchrotron radiation research. Continuous machine improvements coupled with a broad spectrum of technique and instrument development at the NSLS contribute to this vitality. With 70 beamlines and more than 5000 hours of scheduled operation on each of its two storage rings, last year over 2400 users from around the world came to conduct their research at the NSLS. The community is guite dynamic with nearly 800 new users each year while the life sciences has become a leading constituency comprising nearly 1/3 of NSLS users. The poster on the following page provides a small selection of some of the activities and trends at the facility'. This was the way the NSLS introduced itself in the facility poster prepared for the SRI 2000 meeting held in Berlin this summer. But more about that later...

The 7<sup>th</sup> International Conference on Synchrotron Radiation Instrumentation was hosted by BESSY and the TU Berlin with Wofgang Gudat and Peter Zimmermann as co-chairmen. It ran from August 21st to the 25th and was attended by over 700 people from around the world. A broad range of topics were presented by 109 speakers in 31 sessions, and in the 440 posters discussed during the two poster sessions. In addition, there were 60 vendor exhibits and 21 facility posters that ran throughout the week. The technical meetings were held in the historic Hauptgebäde (Main Building) of the TU Berlin and on one afternoon the new 'third-generation' BESSY II facility was showcased in a tour and reception in its Berlin-Adlershof (East Berlin) location. Housed in an elegant new building the BESSYII machine is more than equal to the architecture, and is already supporting an active scientific program. Between their new facility and their highly successful conference, our hosts have much of which they can be justifiably proud and have set a very high standard for organizers of the 2003 SRI meeting in San Francisco.

With a large scientific community, now over 2500 active users, providing a representative view of the NSLS presented something of a challenge. Within the context of the meeting, it seemed most appropriate to focus on the science driven instrumentation developments supported by the department. As a guide for what to include we referred back to our mission statement for our users:

- Develop new capabilities to maintain the facility at state-of-the-art
- Encourage new communities from all fields to use the NSLS
- Operate key facilities for the benefit of the general user community

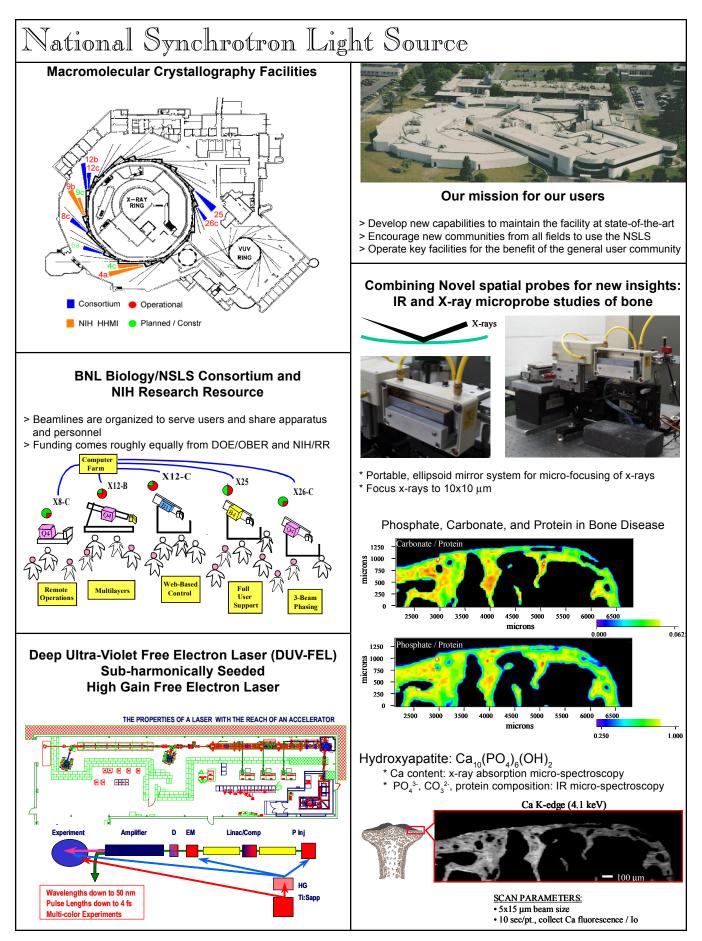
The result (reformatted for the newsletter) appears on the following pages. Two major facility improvements since the last SRI were an enhancement of the X-ray ring brightness by a factor of 5, and the completion of the beamline upgrade program on the VUV-ring.

The breadth of the NSLS research is also one of its greatest strengths. An example combining novel spatial probes for new insights was presented where complementary IR and x-ray microprobe studies were conducted on bone samples. Another illustration of novel science was a section of the poster devoted to the study of interface magnetism using soft x-ray magnetic scattering.

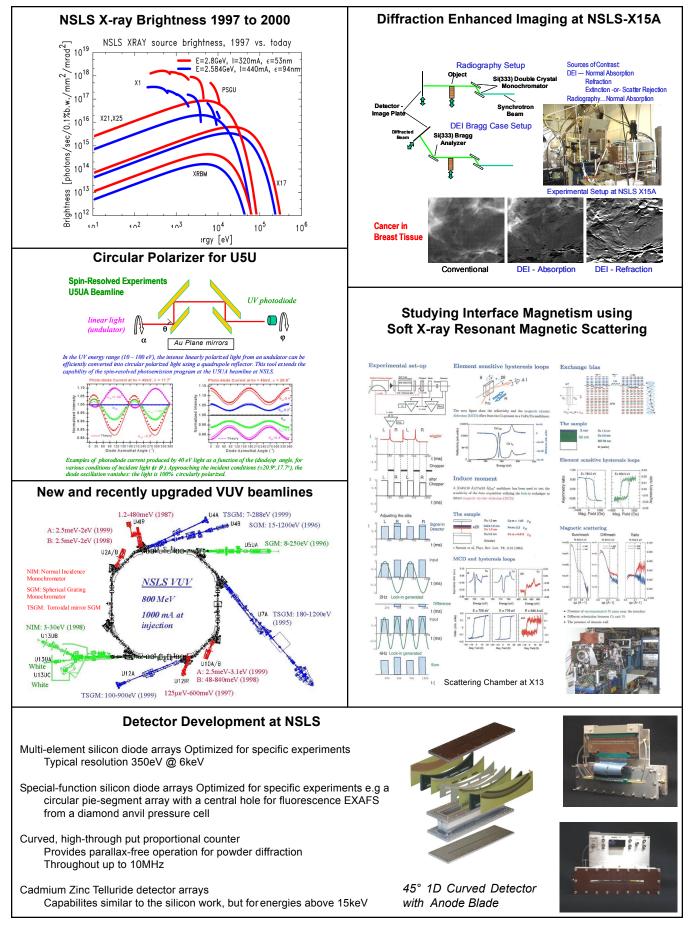


There have also been specific instrument enhancements such as the installation of a Circular Polarizer on the U5U undulator, and the ongoing development programs in detectors and diffraction enhanced imaging. The macromolecular crystallography consortium was also presented as an example of a growing community for the NSLS and looking toward the future, the Deep Ultra-Violet Free Electron Laser research program was outlined. Taken as a whole, the focus provided by the meeting underscores the fact that the NSLS is indeed a vibrant part of the synchrotron radiation based research community, and can remain so for many years to come.

> Breaking News!! 2551 users from 417 institutions visited the NSLS to perform 1132 experiments in FY2000



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### **NSLS Annual Users' Meeting and Workshops**

Simon R. Bare

Users' Meeting Chair, UOP

### http://nslsweb.nsls.bnl.gov/nsls/users/meeting

The 2001 National Synchrotron Light Source Annual Users' Meeting and associated Workshops will provide a scientific forum for the presentation and discussion of recent developments in many diverse areas of science where synchrotron radiation has been used to further the field. New research opportunities and significant accomplishments will be presented in both invited talks and contributed posters.

### Workshops

The program of one-day workshops will focus on specific scientific topics and techniques of interest to the synchrotron community. The following one-day workshops are currently planned:

- Environmental Molecular Sciences, Richard Reeder (SUNY Stony Brook) & Tony Lanzirotti (Univ. Chicago)
- Tricks and Know-How in Analyzing EXAFS Data, Anatoly Frenkel (Univ. Illinois). In conjunction with the EXAFS workshop there will also be a hands-on EXAFS analysis session in the use of WinXAS. This session will be given by Thorsten Ressler, the developer of WinXAS.
- Nanotechnology: Opportunities in Synchrotron Radiation, Peter Johnson (BNL Physics Department) & Chi-Chang Kao (NSLS)
- Applications of Infrared Microspectroscopy, Larry Carr & Lisa Miller (NSLS)
- Catalysis Research Using Synchrotron Radiation, Jiangguan Chen (Univ. Delaware)
- NEXAFS Theory: Techniques and Applications, Sue Wirick (SUNY Stony Brook) & Janos Kirz (SUNY Stony Brook)
- Frontiers in Biological Applications of Synchrotron Radiation, Mike Becker & Lonny Berman (BNL)

### **Poster Session**

A poster session will be held concurrently during Monday's opening Reception and Tuesday's Annual Meeting in Berkner Hall. All Users are encouraged and invited to present posters highlighting research activities conducted over the past year at NSLS. This is an excellent opportunity to showcase the caliber and diverse nature of the research performed at NSLS. Graduate students or postdoctoral associates submitting posters, and who are also registered for the Users' Meeting, are eligible to win one of three cash prizes that will be awarded for the best posters in three scientific categories. Representatives of the NSLS UEC will judge the posters. Detailed information will be available in the Registration Booklet and at our meeting website listed above. The deadline to submit an application for poster session submission is April 30, 2001.

### **Equipment Exhibit**

The ever-popular instrumentation and equipment exhibit will be held beginning on Monday evening at 5:30 p.m. in Berkner Hall with a reception for all registered meeting/ workshop attendees. A variety of vendors will be on-hand to showcase their latest instruments and equipment. All vendors interested in participating should contact Nancye Wright as soon as possible.

### **Social Functions**

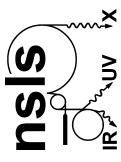
A welcoming reception will be held for all meeting/ workshop attendees on Monday evening in Berkner Hall. Both the equipment exhibit and poster session will be on display for viewing during this reception. A varied selection of hot and cold hors d'oeuvres will be served along with complimentary refreshments. A conference banquet will be held Tuesday evening, May 22. The location is yet to be finalized.

### Registration

Registration packets will be available on the web (see URL at top of page). Those registering on or before April 30, 2001 with full payment will receive a discount on the Users' Meeting registration fee. Don't miss out on this year's meeting!! If you have any questions, contact the Conference Coordinator at Isusrmtg@bnl.gov.

### **Planning Committee Members**

Simon R. Bare, UOP LLC	Chair
Chi-Chang Kao, NSLS	Program Chair
Dan Fischer, NIST	Workshops
Lisa Miller, NSLS	Posters
Sue Wirick, SUNY at Stony B	rook Publicity
Lydia Rogers, NSLS	Conference Coordinator
Nancye Wright, NSLS	Vendors
Mary Anne Corwin, NSLS	NSLS User Administrator



# X-Ray Ring Long Range Schedule

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### Reminders About User Obligations ...

personnel are notified of your arrival. To access the online pre-registration form, go to URL: http://nslsweb.nsls.bnl.gov/nsls/dbforms/user-regis.asp. Please Pre-Register for Every Visit: All NSLS Users are required to pre-register with NSLS User Administration prior to each visit so that BNL gate security provide this information at least 7 days prior to your arrival at BNL.

Foreign Nationals: All foreign nationals must file Form IA-473. Go to URL: http://nslsweb.nsls.bnl.gov/nsls/users/procedures/foreign.htm.

First-Time Users and Those with Expired Appointments: First-time users and users whose appointments or training have expired are requested to arrive at NSLS User Administration Monday through Friday before 3:00 p.m. to allow ample time to register and receive training. Thank you. X-Ray Ring Long Range Schedule

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## VUV Ring Long Range Schedule

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	Sun		5 00-2400 Oper		12 00-2400 Oper	-	10	00-2400 Oper	26 00-2400 Maint

BNL Weekend Food Service ... The Cafeteria serves breakfast and sandwiches from 7:30 a.m. to 2:00 p.m., Saturdays and Sundays.

BNL Onsite Shuttle & Courtesy Van Available ... An onsite shuttle is available weekday mornings from the apartment area to onsite facilities and door-to-door from 8:45 a.m. to 4:15 p.m. For more information, see their website: http://www.bnl.gov/bnlweb/shuttle.html

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### VUV SCHEDULE - April 2001

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VUV SCHEDULE - April 2001	Thu	5 00-2400 Oper	12 00-2400 Maint.	19 00-2400 Ope.	26 00-2400 Ope.	
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	Sun	1 00-2400 Ope	8 00-2400 Oper	15 00-2400 Ope	22 00-2400 Oper	29 00-2400 Oper

### Call for NSLS General User Proposals

### For Beam Time in Cycle May - August 2001

### Deadline is: Wednesday, January 31, 2001

### **Prior to Submitting a Proposal**

You must contact the beamline personnel responsible for the beamline(s) selected in order to verify technical feasibility on the beamline(s) and discuss any special arrangements for equipment. Your chance of getting beam time is improved by being able to use more than one beamline.

### **Preparing Your Proposal**

The same form is used for both new proposals and beam time requests against existing proposals. Follow the instructions on the information sheet and complete and submit all the required sections. Type or print all information legibly. MAIL OR FAX ONE COPY of the proposal form and any attachments to the NSLS User Administration Office. Only one copy is required - do not mail a hard copy if you have already faxed one.

### Macromolecular Crystallography (PX)

### Requirements

New Proposals: The proposal represents a two-year program. Provide an overall plan for your research according to the instructions on the proposal form. If you can, estimate the number of crystals you plan to measure over the two years. If you require the use of an insertion device beamline like X25, be sure to indicate your need for the enhanced performance. New proposals must also include your plans for the upcoming cycle for which you are requesting time (below).

Beam Time Requests: Be specific about what you plan to study in the upcoming cycle. Submit PX Forms only for the crystals you plan to study in that cycle. Answer all the questions, use the back of the form if you need more space. Be clear about what crystals you already have, which you expect to have, and how you would use the beam time you requested if you were unable to

### Update on FY 2001 Overhead Rates

Ken Koebel NSLS Administration

There have been some changes to the Laboratory's overhead rates for the Fiscal Year 2001.

The revised rate for General and Administrative (G&A) is down to 34.5% from 37%. This rate, which is broken down into traditional G&A rate of 10.5% and site support rate of 24%, is applied to total modified costs (all labor, material costs and burdens except for power burden). Material burden rate will remain the same at 6.5% and will be applied to all material (purchases, store issues, travel, etc.) costs. All BNL labor costs incur a burden charge of 14.8%. This burden is broken down into

obtain the planned crystals in time (i.e., other crystals described in your program).

### Proposal Deadline

The complete proposal package must be received by the User Administration Office on or before 5:00 p.m. Eastern Standard Time on the above date to be considered for beam time in this cycle. The fax machine is always extremely busy on the deadline date. Do not rely on faxing the proposal successfully on the deadline date. New proposals should be sent by mail or fax prior to the deadline. Beam time requests for active proposals will be accepted after the deadline, but will be allocated beam time only after requests are not eligible for a rating upgrade if beam time could not be allocated to them.

Each proposal will receive a prompt preliminary review to verify that it is complete and legible. If there is a problem with the proposal, you will be contacted immediately. Submitting your proposal well in advance of the deadline date assures that the User Administration Office has time to reach you and that you will have enough time to correct any deficiencies.

### **Proposal Forms and Additional Information**

Blank proposal forms and instructions are available on the World Wide Web. From the home page at http:// www.nsls.bnl.gov, go to User Information, then Forms. The PX form must now be completed online. A guide to the NSLS beamlines and more information about the General User Program can be found through our homepage, http://www.nsls.bnl.gov or by contacting the NSLS User Administration Office at (631) 344-7976. Office hours are Monday through Friday, 8:00 a.m. to 5:00 p.m. Eastern Standard Time (EST). Contact information is on the back page of this Newsletter.

two components: an organizational burden rate of 12.5% and a power burden rate of 2.3%. The rates applied to space are broken down into three components: office/ trailer space of approximately \$15 per square footage, industrial space of approximately \$11 per square footage, and storage space of approximately \$4 per square footage.

Please note that these rates are not established by the NSLS, but by the Laboratory's Budget Office.These rates are subject to change. Please direct any questions to Ken Koebel at (631) 344-7351.

### **VUV Ring Status**

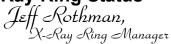
Stephen Kramer WV Ring Manager

The major improvement in the ring has been the commissioning of the new digital orbit feedback system. This new system has made it possible to increase the number of PUEs used in the orbit feedback system from the original 8 to all 24 PUEs in the ring. The number of Eigenvectors used in the correction algorithm has similarly increased from 6 to 8. However, due to the slow response of the additional trims, only the original 8 trims used in the old analog system are presently being used. Consequently the digital feedback has made only a minor improvement over the older system on the long-term current dependent orbit drift. However, the new system has higher frequency response and the ability to more easily modify the time dependence of the orbit correction algorithm, by filtering in the time domain in order to enhance the gain at certain frequencies, e.g. 60 Hz beam motion. In addition, the RF frequency feedback has been reactivated, in order to reduce the remaining current dependent horizontal orbit motion. Initial studies have shown a factor of 4 to 6 reduction in the 60 Hz frequency component on the beam. Work will continue on this system and on the development of a high speed monitoring system that will help debug the source of orbit glitches that have been so difficult to understand in the past.

Following the May shutdown, the ceramic gap in super-period one started to leak. This was quickly repaired with a vacuum sealant and a water cooling loop was clamped on to reduce the beam induced temperature rise of this component. Efforts are being made to understand why this ceramic gap has such a poor reliability record, three failures in 8 years. An improved ceramic gap will be installed during the winter 2000-2001 shutdown. While studying the problems with the ceramic gap, it was found that the stripline kickers used in the longitudinal damping system have been damaged. One is shorted to the vacuum chamber and one has an open circuit. These kickers will also be replaced during the winter shutdown, which should help improve the longitudinal stability of the beam.

The problem of large amplitude dipole oscillations of the beam with only one RF system, have continued to plague the operations during timing shifts. The current limits for the normal seven bunch fills has decreased to 200mA or less. Actually it was found that 3 three bunch and 5 bunch fills have a higher current threshold than the seven bunch fills. This has not been a problem during normal operations because the bunch stretching RF system provides adequate damping of this instability to levels greater than 1 Ampere. It is felt that the high frequency impedance of the ring has changed and the next shutdown will be used to look at the state of the damping antenna in the main RF cavity, to see if they are still damping the cavity modes properly. During the spring and early summer, the U3B diagnostic beam line has been commissioned for operations and the first data has been obtained on the frequency oscillations of the average energy of the bunches up to 15KHz. This average motion was found to be less than 10% of the natural energy spread of the bunches. New detectors are being installed to look at shape oscillations on the bunches, either as the average of the bunches or for individual bunches. This information should help to understand how the longitudinal frequency oscillations of the beam produce transverse motions of the beam at these high frequencies. It is felt that the amplitude modulation of these high frequency oscillations is the source of the user observed low frequency fluctuations of the photon beam flux.

### X-Ray Ring Status



The transition to low emittance 2.8GeV operations improved beam brightness substantially. Users on brightness limited beamlines have seen the improvements shown in **Table 1**. For typical experiments using 10KeV photons, the brightness has increased by a factor of 3 on the bending magnets and a factor of 4.85 on the X21 and X25 wigglers. X17 is up by a factor of 1.62. The Undulator brightness has gone up even further with X1 improving by a factor of 8.1. The most dramatic increase has been on the IVUN (In Vacuum Undulator) with peak improvements of 45.5 at 5.5KeV and 600 at 16.5KeV on the 1<sup>st</sup> and 3<sup>rd</sup> harmonics respectively.

Operating at low emittance and high energy pushes some of the trim dipole magnets close to their maximum current. This limits our ability to perform horizontal orbit corrections for users. The NSLS is now working on improved trim strength reduction algorithms to mitigate the problem in the short term. Upgraded trim magnets will be installed to solve the problem permanently.

Digital feedback studies with the new hardware will begin before the December shutdown. Initially the studies will focus on one plane, since the wiring for both planes will not be completed until the end of December. The new digital feedback system has been running successfully in the UV Ring since August, significantly reducing 60Hz beam motion. When implemented in the X-ray Ring, digital feedback should reduce both long-term drift and high frequency beam motion.

In addition to the preventative maintenance performed during the December shutdown, the X29 vacuum exit chamber will be replaced in preparation for the installation of an IVUN in the RF straight section. Beam loss monitors are also being installed downstream of the

dipole magnets inside the X-Ray tunnel. These monitors will allow optimization of injection and reduce fill times.

ENERGY (KeV)	X-ray Bend	X21, X25	X1	X17	IV UN
1	2.2	3.5	8.1	1.52	_
5	2.5	4.05	-	1.56	-
5.5	-	-	-	-	45.5 (1 <sup>st</sup> Harmonic)
10	3.0	4.85	-	1.62	-
15	3.6	5.9	-	1.69	-
16.5	-	-	-	-	600 (3 <sup>rd</sup> Harmonic)
20	4.4	7.1	-	1.77	-
25	5.3	8.5	-	1.85	-

Table 1. Improvement in Beam Brightness, 1997 vs. Today

### Facility Update

Gerry VanDerlaske Building Manager

Welcome to my first Facility report, where updates will be written to keep the User Community abreast of new changes and upgrades planned for the NSLS Facility. But first, please join me in wishing a happy retirement to Mike Kelly, who, as of September 9th, has decided to pursue his dream of spending days relaxing on his boat sailing the inter-coastal waterways of the Eastern Seaboard. Mike has been with the Light Source since its infancy and grew along with this facility to become a major participant in helping to bring the NSLS to the World Class recognition that it carries today. Mike's vacancy has left a huge void, which I will do my best to try and fill. Along with Mike's retirement, taking charge of the NSLS User Shop is Bob Kiss, a 23-year BNL employee who transferred to the Light Source from his duties as Reactor Maintenance Supervisor at the HFBR. Bob not only is very capable with the operations and supervision of Machine Shop workings--in his new position as the NSLS Alternate Building Manager--he takes responsibility for Crane and Forklift training, assigning short and long term storage, and has assumed the stewardship of Lab 1-117. You may find Bob in his office located directly adjacent the NSLS User Shop in Room 1-124. His phone is BNL X4926 and you may e-mail him at kiss@bnl.gov. Bob and I are presently working with Corinne Messana assembling a Building Manager's web page where we hope to offer a "one stop shopping" venue of information and services for the LS User Community. Look for us to be online in the near future.

Some planned work for this year's winter shutdown consists of the following: reconfiguration of the X6 A & B Hutches; complete inspection of the LS Overhead Crane inventory, and the X17 Angiography suite will be undergoing dramatic changes as the old comes down to make way for the new. Please be advised of construction crews working in and around these areas and read and obey any and all postings related to safety.

During the winter shutdown, Plant Engineering personnel may be busy working on or near your beamline or on the experimental floor. Please render them any requested assistance they may ask of you if there is a need for equipment (delicate or electronic) to be moved. Remember: Plant Engineering staff are not familiar with the nuances of your beamline and they will feel more comfortable having you present to supervise the positioning of such equipment.

Please Note: Although I will be retaining X3476 as the Building Manager's office phone number, please use 8222 (digital) when paging me.

### **Computer Security**

For users who require access to BNL computers, please read this important message concerning computer security and changes to computer access procedures from Tim Sailer (BNL's Information Technology Division):

A high priority of the Cyber Security Program Plan (CSPP) is to implement a Perimeter Defense Network (PDN). The plan to deploy the PDN was developed with the help of key System Administrators at Brookhaven. The PDN deployment plan has been reviewed and approved by the Cyber Security Advisory Council.

The initial deployment of the PDN will impact the following three types of network traffic. In future deployments, we will implement other classes of traffic such as ssh.

(1) HyperText Transfer Protocol (HTTP) - a method in which browsers and web servers communicate.

(2) Telnet - a text-based method of interactively communicating to remote servers.

(3) File Transfer Protocol (FTP) - a common method used to move files between different machines. The required deployment will not affect IDAS users, nor will they affect internal communication between BNL computers.

In deploying the PDN, users will be required to reconfigure their browsers, and web masters will need to register servers. Users requiring access to the Laboratory via FTP or telnet will also need to apply for a CryptoCard. The following directions explain the user actions required to support the deployment plan. If you need help in executing any of the steps below, please call the ITD Enterprise Service Desk at ext. 5522.

Telnet (For users requiring telnet access from outside of BNL network): To use the telnet proxy from other institutions, agencies, and users accessing the Laboratory from their private ISP, users will need a CryptoCard. For directions on how to obtain a CryptoCard, please go to http://www.bnl.gov/cybersecurity/ cryptocards.htm

Users requiring telnet access from BNL to outside will not be restricted, and traffic that leaves the Laboratory will not be blocked, as long as you access it through the proxy.

For documentation on proxies go to URL:

http://www.bnl.gov/cybersecurity/proxy.htm. This documentation will provide instructions on how to use the proxies for both gaining access to the Laboratory, and gaining access to outside systems from within the Laboratory.

Rationale: The PDN will restrict the telnet protocol coming into and leaving BNL via the Internet. The danger of a telnet connection is that both the user's name and password are transmitted across the network or Internet as plain readable text, making it a trivial matter for unethical parties anywhere to capture this information, and compromise the account.

Schedule: On October 16, 2000, telnet to and from BNL's network will be blocked, and access will only be allowed via the telnet proxy.

**FTP (For users requiring FTP access from outside of BNL network)**: To use the FTP proxy from other institutions, agencies, and users accessing the Laboratory from their private ISP, users will need a CryptoCard.

For directions on how to obtain a CryptoCard, please go tohttp://www.bnl.gov/cybersecurity/cryptocards.htm

Users requiring FTP access from BNL to outside will not be restricted, and traffic that leaves the Laboratory will not be blocked, as long as you access it through the proxy.

For documentation on proxies go to website:

http://www.bnl.gov/cybersecurity/proxy.htm. This documentation will provide instructions on how to use the proxies for both gaining access to the Laboratory, and gaining access to outside systems from within the Laboratory.

Rationale: The PDN will restrict the FTP protocol coming into and leaving BNL via the Internet. The danger of a FTP connection is that both the user's name and password are transmitted across the network or Internet as plain readable text, making it a trivial matter for unethical parties anywhere to capture this information, and compromise the account.

Schedule: On October 30, 2000, FTP access to and from BNL's network will be blocked, and access will only be allowed via the FTP proxy.

**HTTP (For all users)**: All users will have to reconfigure their browsers (e.g., Netscape, Internet Explorer) to use the HTTP proxy for accessing the Internet. Large portions of the browsers at the Laboratory have already been configured to use the proxy, but this must be expanded to include all browsers. Directions for this configuration can be found at http://secops.itd.bnl.gov/WebProxy.

Rationale: To hide the identity of BNL machines from hackers, screen the request for malicious code, and reduce the bandwidth generated by web surfing.

Action: (For Webmasters or people running web servers): Webmasters should register their server, and provide the information requested at http:// secops.itd.bnl.gov/cgi-bin/webserver.cgi. Direct access from the Internet to the unregistered web servers will be blocked.

Rationale: To eliminate the web servers to act as targets for the crackers all over the Internet.

Schedule: On October 9, 2000, all outbound HTTP traffic not going through the HTTP proxy will be blocked. On this same date, inbound HTTP traffic to unregistered web servers will be blocked.

If you require an exception to any part of the PDN deployment plan, please contact Cyber Security Operations at secmgr@bnl.gov with the rationale.

### A Message about Cryptocards from Mary Anne Corwin, NSLS User Administrator

For users requiring a Cryptocard, please go to the websites listed in Tim Sailer's message above. Follow the instructions and print out a form requesting a Cryptocard. After your form has been completely filled out, bring it to NSLS User Administration for approval. NSLS User Administration Office staff have been authorized to approve requests for Cryptocards for NSLS users only. However, please note the following:

1. Users requesting a cryptocard SOLELY for email use will be referred to ITD to secure an account on the Exchange email server and the account will reside in the BNL domain. No Cryptocard will be issued to any person whose only access will be for email.

2. Beamline Staff who need access to their computers at the NSLS from an offsite location may obtain a Cryptocard. We will verify that you are a current beamline staff member (i.e., Spokesperson, Local Contact, Safety Coordinator, Training Coordinator, etc.) before giving approval to obtain a cryptocard.

3. Persons who are NOT beamline staff members: The User Administrator will verify with the Beamline's Local Contact and/or Spokesperson that you should receive approval for a Cryptocard before granting approval. If the Local Contact or Spokesperson does not verify with me in writing that you should receive a Cryptocard or states that you are not entitled to access, no approval will be given.

If you have any questions concerning the cryptocard or other computer security related questions, please contact Eric Blum at blum@bnl.gov. Any questions regarding NSLS User Administration office procedures with regard to signature approval, please contact Mary Anne Corwin, NSLS User Administrator, at corwin@bnl.gov.

### Safety and Compliance: Use and Transport of Hazardous and Radioactive Materials at the NSLS

Bob Casey Assoc. Chair for Environment, Safety & Health

Many experiments at the NSLS involve small amounts of chemicals. Occasionally, small amounts of radioactive materials may be involved as well. It is very important that NSLS is aware of these materials before you arrive at the site and that these materials be properly transported to and from your home institution. Please consider the following points:

1. All chemicals as well as other hazardous or radioactive materials must be listed in detail on NSLS Experimental Safety Approval Forms. Some of these materials may require barcoding and entry into the BNL Chemical Management System database. Radioactive sources will need to be added to the NSLS Source Inventory and a source custodian will need to be identified.

2. If you have additional questions as to what constitutes a hazard OR if you plan to bring material of significant hazard, contact Andrew Ackerman (631) 344-5431; ackerman@bnl.gov) well in advance of your arrival to determine agreed upon procedures while at the NSLS. Lack of approved procedures could result in postponement of your experiment.

3. Packaging, labeling and transport of chemicals and hazardous materials to Brookhaven National Laboratory (BNL) must be done strictly according to Department of Transportation regulations. Contact your institution's Safety Office for guidance. Shipping of chemicals and hazardous materials from BNL must be done through BNL's Shipping Division and a Material Safety Data Sheet (MSDS) must accompany each item.

4. Transport of ANY radioactive material to, from and within BNL must be done through the BNL Isotopes & Special Materials Group. You are not allowed to transport these materials in your private vehicles or suitcases. Contact I&SM at least 2 weeks in advance of your arrival at BNL: (631) 344-5233. Federal law 49CFR170-180 governs transport of hazardous materials to and from BNL.

5. As a DOE-operated institution, BNL falls under the Price Anderson Amendment Act (PAAA). We must therefore follow the regulations set out in the Code of Federal Regulations 10CFR835, "Occupational Radiation Protection." Not following these regulations makes BNL or an individual liable for fines and penalties.

6. Some materials such as scientific equipment or samples can be legally transported by you during your travel to BNL. We advise that you always carry information on your institution's letterhead stationary describing the equipment or samples and what hazards they may pose to other individuals, if any. Presenting such information up front at airport terminals, for example, will make your travels considerably smoother.

Please contact any member of the NSLS ESH Staff if you have questions or comments on this topic.













NSLS Newsletter, November 2000

NSLS 2000 Annual Service Awards Barbecue and Farewell to Michael Hart, Chairman of the NSLS





Vayne Rasmussen and Rich Biscardi











NSLS User Administration Office Brookhaven National Laboratory NSLS Building 725B P.O. Box 5000 Upton, NY 11973-5000

### **Important Upcoming Dates**

Nov. 15, 2000	UEC Meeting 1:00-3:00 NSLS Town Meeting
Dec. 15, 2000	Deadline for Scientific Highlight Articles for 2000 Activity Report
Jan. 10, 2001	Deadline for submissions, March Newsletter
Jan. 31, 2001	Deadline for General User Proposals (May-Aug. 2001)
May 21-23, 2001	NSLS Annual Users' Meeting and Workshops

The NSLS Newsletter is published triannually by the	NSLS User Administration Office General Information, User Registration, Training:	
National Synchrotron Light Source Department,		
Brookhaven National Laboratory	Phone: (631) 344-7976	Fax: (631) 344-7206
Mary Anne Corwin, Editor	User Administrator	
Nancye Wright, Production Assistant	Mary Anne Corwin Annual Users' Meeting	corwin@bnl.gov
For additional information about the NSLS (including this Newsletter in electronic format) see the NSLS	Lydia Rogers	lrogers@bnl.gov
	General User Proposals	
	Lydia Rogers	lrogers@bnl.gov
Home Page on the World Wide Web at	Nancye Wright	wright1@bnl.gov
	Publications/Newsletters	
www.nsls.bnl.gov	Nancye Wright	wright1@bnl.gov