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National Synchrotron Light Source ◆ Brookhaven National Laboratory
Newsletter

July 2000

Malaria, Synchrotron Radiation, and Monte-Carlo

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Malaria presents a terrible public health problem. As many as half a billion people are sick with the disease, and several million die of it each year, mostly young children in Africa. The problem is exacerbated by the fact that the *Plasmodium* parasite which causes malaria is developing resistance to the drugs in wide use today.

The *Plasmodium* parasite has a complicated life cycle, with several developmental stages in mosquitoes, and several in its human victims. The most damaging phase of *Plasmodium* is the late trophozoite, where it infests the red blood cells, digesting the oxygen-carrying enzyme hemoglobin. In a massive infection, 80% of the victim's hemoglobin may be consumed. To any parasite, hemoglobin is a dangerously spicy dish. Its active site for oxygen absorption, the iron porphyrin ring, is a dangerous oxidizing agent in solution, and would prove fatal to the trophozoites if present in significant concentration in the digestive vacuole of the microorganism. Just as a diner in a Szechwan restaurant piles the hot peppers at a corner of the plate, *Plasmodia* immobilize the heme groups liberated by proteolysis into an insoluble crystalline material called hemozoin. The process by which hemozoin is formed is not known, and until our recent work at the NSLS, neither was its structure.

Approaches to controlling the disease may be made at many stages of its life cycle, e.g., controlling the mosquito vectors, or current efforts to develop a vaccine against the early infestation. In the 17th century, Jesuit missionaries observed indigenous peoples of Peru using the bark of the cinchona tree to treat fevers, observed that it had the ability to cure malaria, and brought the material to Europe. The active ingredient, quinine, is arguably the first drug known to treat a disease; the previous pharmacopoeia consisted of anesthetics, purgatives, etc. However, it has limited effectiveness, and is somewhat toxic in therapeutic doses. Synthetic drugs have been developed since the mid-20th century, and have largely replaced quinine.

Chloroquine has been the most successful antimalarial drug. There is a long history of models for the action of chloroquine and related drugs, many of them subsequently disproved. Various experiments, such as autoradiography of trophozoites growing in the presence of labeled chloroquine, show that it is associated with the crystallization of hemozoin. This suggests that the drug acts by interfering with the growth of the solid phase, and suggests avenues for the possible development of new drugs, especially ones that might sidestep the resistance of some *Plasmodium* strains to chloroquine. Progress toward these goals depends on understanding the precise nature of hemozoin. For a long time, it has been widely assumed that hemozoin is a polymer, consisting of covalently bonded chains of heme groups. Evidence for this has been the observation of iron-carboxyl bonds via infrared absorption in hemozoin and the low solubility of hemozoin, although neither of these proves the polymer model. However, the idea has been reinforced in the literature, so that most biochemical papers on hemozoin refer to it as heme polymer. Unfortunately, crystals of natural hemozoin, as well as synthetically produced material, are too small for single crystal analysis, even though microscopy shows that they are needles with well-defined facets (**Figure 1**.)

Traditionally, powder diffraction has been regarded as a technique useful for identification or quantification of phases in polycrystalline samples or for the determination of rather simple crystal structures. However, within

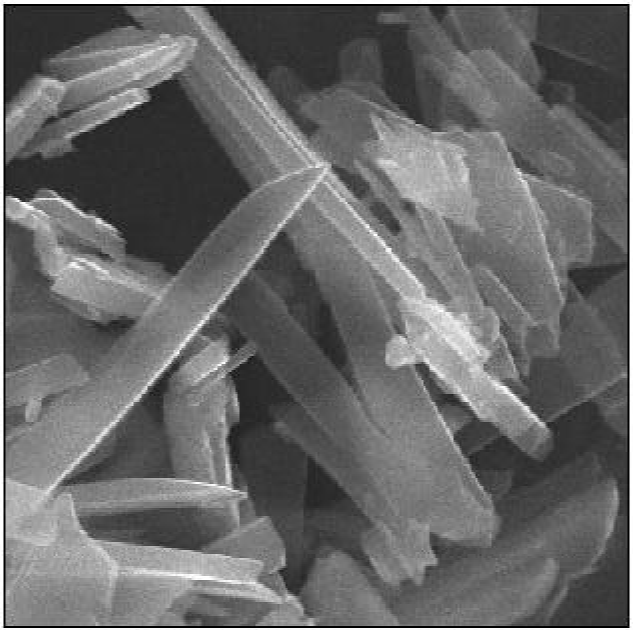


Figure 1. Scanning electron micrograph of synthetic hemozoin crystallites. The width of the image is about 50 microns.

the last twenty years, the power of powder diffraction techniques for structure solution has grown, so that now, the absence of single crystals of materials like zeolites and pharmaceuticals is no longer an overwhelming impediment to structure determination. Interested readers are referred to a structure determination from powder diffraction web site and discussion group, **http://sdpd.univ-lemans.fr**. One important development has been the use of high-resolution beamlines at synchrotron sources, based on using an analyzer crystal before the detector, to obtain angular resolution on the order of 0.01 degree with broad beams, free of parallax. This makes it possible to resolve much more information from a powder spectrum than is available from traditional techniques.

In our first powder diffraction measurements, in collaboration with David Cox and Robert Dinnebier, we used the powder diffraction peak positions alone to identify the dimensions of the unit cell. Powder diffraction measures only the *d*-spacings of Bragg peaks, and so their geometrical relationship into a reciprocal lattice must be inferred from combinations of accurate measurements. Fortunately, there are well-established and efficient search algorithms for that task, and we readily found that the hemozoin unit cell is triclinic, with a volume of 1416 Å^3. From the density, we inferred that there must be two molecules in the unit cell, and since the material is a racemate, we suspected that they would be related by inversion, so that only one molecule must be placed in the unit cell. In that initial work, we also showed that synthetic hemozoin (known as β-hematin) had a powder diffraction pattern identical to the crystalline component found in whole dried blood cells which had been infected with malaria.

The nature of the crystal structure solution problem, especially from powders, is that it is easy to see if given a candidate solution is compatible with experimental data, and to refine the details of a given model if it is essentially correct. However, there is no general procedure that will lead from powder data to a usable first approximation to the structure. For organic molecular solids, a large amount of structural information, e.g., most of the bond lengths and angles, can be predicted from the chemical structure of the molecule. Accordingly, the crystal structure of a molecular solid can be described by specifying the location and orientation of the molecule in the unit cell, and any remaining internal degrees of freedom. As long as this prior information is correct, all chemically possible structures can be summarized in a few parameters. **Figure 2** shows the molecular structure of the iron porphyrin molecule which comprises hemozoin, known from biochemical studies, including the aforementioned synthesis.

Since the molecule does not have any of the symmetry elements of the lattice (in this case, only inversion), it must occupy a general position and orientation in the cell. Accordingly, six parameters give its position and orientation, and the eight bond torsion angles shown in **Figure 2** specify the internal degrees of freedom. The correct structure can be determined by searching that fourteen-dimensional parameter space and finding the values that give the best agreement between experimental data and calculated diffraction pattern. While much simpler than finding each atom individually, this is still too large a task to solve by an exhaustive search. Further-

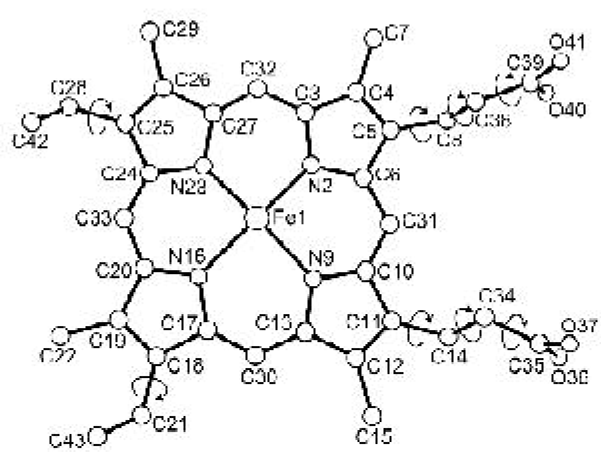


Figure 2. Representation of the Fe^{III}-protoporphyrin-IX molecule which crystallizes to form hemozoin. The arrows indicate torsional degrees of freedom which must be determined in order to obtain the intermolecular linkages.

more, the goodness-of-fit surface is so irregular that local methods such as following the gradient downhill will always get stuck in local minima, far from the global minimum which represents the correct solution.

The simulated annealing method is a general technique for obtaining approximate solutions to optimization problems, based on the analogy with finding a low-energy state of a physical system by annealing it: heating it to a high temperature and cooling it slowly. Several groups have independently applied this idea to the solution of crystal structures from powder data. Generally, one regards the parameter which is to be minimized, such as the familiar crystallographic weighted profile *R*-factor, as an energy, and performs Monte Carlo searches to sample the configuration space, initially at some high "temperature." This process is repeated as the temperature parameter is lowered, and eventually, the system should condense into a low energy state, i.e., a satisfactory solution. There are different approaches in practice, based on the choice of energy parameter, form of the Monte Carlo moves, tricks for accelerating the algorithm, etc. Our own program, PSSP (for Powder Structure Solution Program) has been used for several other problems, and is distributed, with several examples and tutorials, on the web at **http://powder.physics.sunysb.edu/ppsd**.

The results of a typical run of PSSP on one of our β-hematin data sets are shown in **Figure 3**. Starting at the upper right, the temperature parameter is so high that essentially every Monte Carlo step is accepted, and the value of the *S* parameter is large enough to indicate that the candidate structures probed are no better than randomly placed atoms. In this simulation, the algorithm computes 100,000 structures before lowering the temperature by 20%. The fit between experimental data and model structures gradually improves (proceeding from right to left) until it condenses into reasonable agreement. We typically repeat this procedure many times, and take seriously a structure only if it recurs frequently, and if it makes chemical sense. In the present case, the only solution that emerges is the one illustrated in **Figure 4**, in which the hematin molecules are dimerized. Besides the excellent agreement in the refinements of the diffraction data (**Figure 5**), the supporting evidence for this structure is

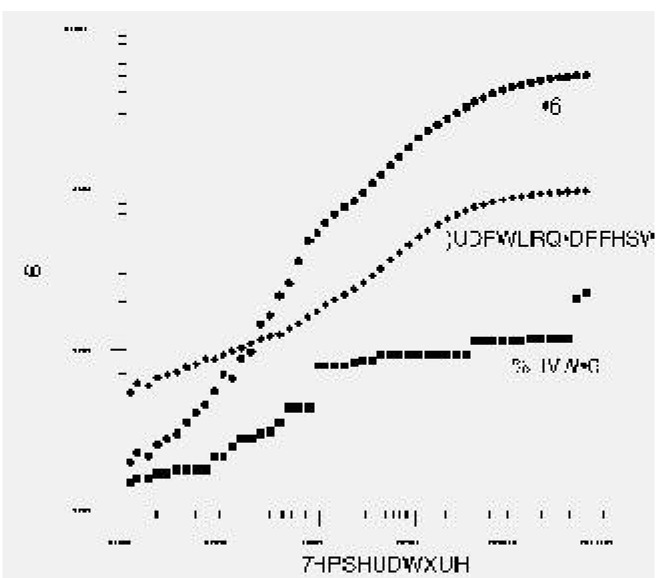


Figure 3. Progress of the quality of fit (*S*-factor) with annealing temperature (from right to left) during a typical run on β-hematin in the data analysis program PSSP.

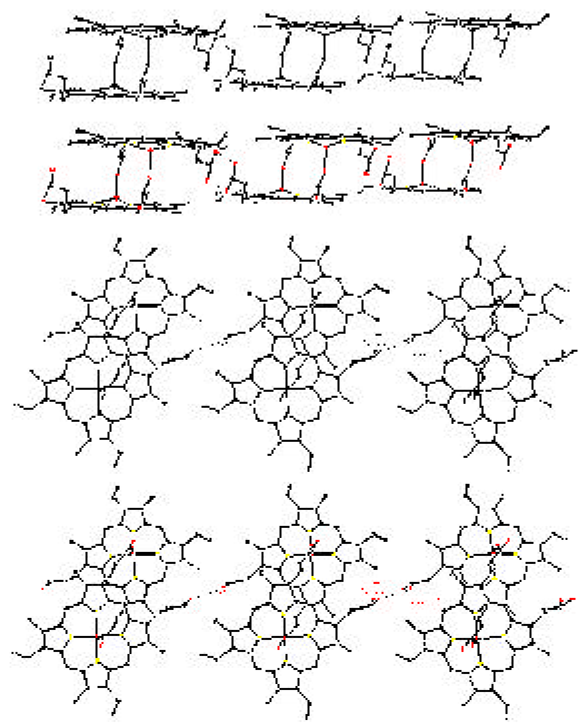


Figure 4. Drawings of the structure of hemozoin, determined from powder diffraction. Note that the molecules shown in Figure 1 are dimerized by reciprocal iron-carboxyl linkages at the end of the propionic acids, and that these dimers are assembled into the lattice by hydrogen and van der Waals bonds.

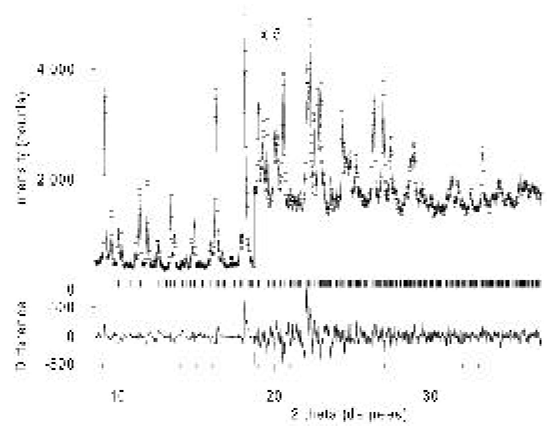


Figure 5. Observed (crosses) and calculated (solid line) X-ray powder diffraction patterns of β-hematin, using 1.162Å x-rays from NSLS beamline X3B1. The lower trace shows the difference between experiment and model.

that the solution has produced the iron-carboxyl bond observed in the infrared, which was not built into the individual molecule from the start.

What is surprising about this structure is that the iron-carboxyl bonds do not form the anticipated polymer chains, but instead dimerize the hemes, so that the crystal is held together only by hydrogen bonds and the van der Waals attraction between dimers. What are the consequences of this structure for understanding, and perhaps interfering with the sequestration of heme? Our work supports the hypothesis, originally voiced by Ridley and Goldberg, that the quinoline antimalarial drug action is due to its binding to high affinity sites on the surface of the hemozoin crystallites. It further suggests that appropriate studies of the morphology of the hemozoin crystallites will lead to improved understanding of the biological control of their formation, analogous to the current status of understanding of biomineralization. More broadly, it should call attention to the growing power of powder x-ray diffraction to research communities who might find other interesting applications for these techniques.

Reference

S. Pagola, P.W. Stephens, D.S. Bohle, A.D. Kosar, and S.K. Madsen, "The Structure of Malaria Pigment β-Hematin," *Nature* **404**, 307 (2000).

2000 Annual Users' Meeting

Mark Chance, UEC Chair, Albert Einstein College of Medicine

The National Synchrotron Light Source annual meeting was recently held at Brookhaven National Laboratory (BNL) on May 22-24, 2000. Over 260 registered attendees participated in workshops, a poster session, vendor exhibits, lectures, a reception and a banquet.

(Left to right): BNL Laboratory Director Dr. John Marburger, UEC Chair Mark Chance (AECOM), UEC Past Chair Barbara Illman (USDA-FS), and Associate Director for Department of Energy/Office of Science and Technology Policy Arthur Bienenstock

The festivities began Monday the 22nd with workshops on Environmental and Geological Sciences and X-ray Absorption Fine Structure Studies of Dilute Systems. As the 19 exhibitors set up their displays in the lobby of Berkner Hall, students and Post-Docs set up posters in the adjoining rooms, hoping to win cash prizes for 1st, 2nd or 3rd place in the poster competition. At 5:30, a welcoming reception and the poster session began, with live music and an open bar. Old friends got reacquainted and the author even met someone he knew in high school and hadn't seen in 25 years, who was in the synchrotron game!

On Tuesday, the main meeting began with an update of activities at BNL by Dr. John Marburger, Lab Director. Dr. Marburger painted an upbeat picture with the opening of the new high energy physics facility, RHIC, and the thousand or so new users that will be regularly coming to BNL. Although the closing of the reactor was admitted as a serious blow, relations with DOE were said to be improving significantly, and the importance of the Light Source within the lab framework as a "multi-facility" lab was emphasized.

Dr. Marburger then introduced the new Associate Lab Director for Basic Energy Sciences, Richard Osgood, Jr., a Professor of Physics from Columbia. Dr. Osgood oversees both the NSLS and the Chemistry Department and started his new position only in the last month with the retirement of Denis McWhan. Although, Dr. Osgood's expertise is primarily in lasers, his group has used the synchrotron and he seemed responsive to the concerns of a large user facility as well as the need for new directions.

Richard Osgood, Jr., Assoc. Lab Director for BES

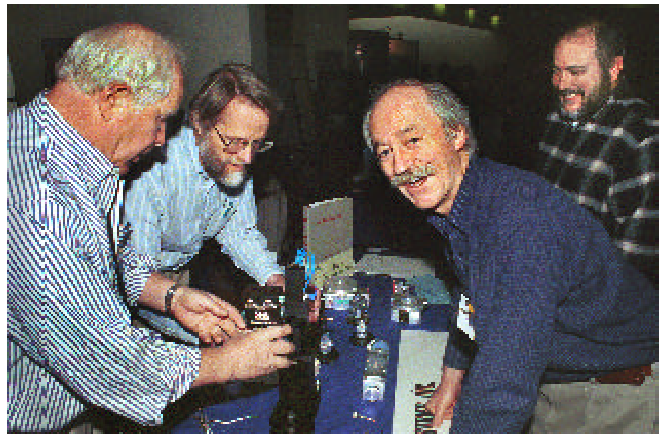
After Dr. Osgood, the audience was taken on a virtual ride of protein crystallography beamline X12-C worthy of Disneyworld. Using dual projection, a live 'telepresence' and remote operation, Dr. Robert Sweet of the Biology Department showed us all how it can be done from the low bandwidth comfort of your living room (How about from the beach Bob?). The demonstrated remote capability that Dr. Sweet and colleagues have developed with support from the National Center for Research Resources of the NIH immediately generated discussion of what other beamlines these techniques could be transferred to and how this could be expanded.

Subsequent to this first scientific talk, Michael Hart, Director of the Light Source gave an overview of another very good year, while yours truly, outlined how the User's Executive Committee is working hard to make the case for increased synchrotron funding in Washington, D.C. This included a joint visit by the UEC leadership of all 4 DOE synchrotrons to lobby members of Congress on April 11, 2000.

Excellent scientific highlights outlining the potential uses of femtosecond x-rays (Janos Hajdu, Uppsala University) and the potential for generating them (Igor Pogorelsky, BNL) rounded out the morning's activities. In UEC elections, Simon Bare, Leemor Joshua-Tor, and Michael Vaughan were elected to 2-year terms with Simon Bare assuming the position of vice chair of the UEC.

Prof. Janos Hajdu, Uppsula University, Sweden

After lunch under the tent, Arthur Bienenstock, Associate Director for Science of the Office of Science and Technology Policy, gave us a peek into the inner workings of Presidential science advising and emphasized the real concern in the Administration with respect to the funding lag for the non-biological sciences that has occurred over the last 25 years. The audience was reminded that only their direct efforts can effect change.



At the Users' Meeting, 19 exhibitors displayed synchrotron-related equipment and instruments.

The day concluded with a Science Advisory Committee (SAC) User Forum, chaired by Sol Gruner of Cornell University, where users posed questions about future directions for the NSLS. A lively discussion outlined a number of exciting directions and strong comments from the SAC about the health and strength of the facility. After the forum, the attendees retired to Giorgio's Restaurant for a banquet. Some attendees tried the valet parking with mixed success.

The meeting concluded Wednesday with additional workshops on Very Bright Infrared Sources and Applications, New Approaches to Solving Protein Crystal Structures, and Chemical Applications of Synchrotron Radiation. Overall, the meeting was a great success, both well attended and very informative.

2000-2001 Election Results

User Executive Committee

Newly Elected UEC Members are:

Simon Bare, UOP
Leemor Joshua-Tor, Cold Spring Harbor Lab
Michael Vaughan, SUNY at Stony Brook

Newly Appointed UEC Officers are:

Mark Chance, AECOM, UEC Chair
Simon Bare, UOP, UEC Vice Chair
David Mullins, ORNL, UEC Secretary

Existing UEC Members include:

Barbara Illman, U. of Wisconsin, UEC Past Chair
Kenneth Evans-Lutterodt, Lucent Tech., Inc.
Chris Jacobsen, SUNY/Stony Brook
Erik Johnson, NSLS, Ex-Officio
Mary Anne Corwin, NSLS, Ex-Officio

Special Interest Groups (SpIGs)

Newly Elected SpIG Reps are:

Zbigniew Dauter, SAI, Bio. Scattering and Diff.
Kumi Pandya, NCSU, EXAFS
Anthony Lanzirotti, U. of Chicago, Imaging
David Mullins, ORNL, UV Photo/Surface Sciences
Lisa Miller, NSLS, Infrared Users
Steve Ehrlich, NSLS, X-ray Scat./Crystallography
Larry Carr, NSLS, Time Resolved Spectroscopy
Michael Dudley, SUNY at Stony Brook, Topography

Interest Groups currently without representation:

Students & Post Docs
X-ray Crystallography and Scattering
Industrial Users

NSLS Bids Farewell to Michael Hart, NSLS Chairman 1995-2000

In September, Michael Hart's term as NSLS Chairman will come to a close.Having joined the NSLS Community in an official capacity in September 1995, Michael was appointed Chairman of the Light Source, succeeding Denis McWhan. His appointment followed numerous distinguished contributions in x-ray physics and many notable accomplishments. He earned his B.Sc., Ph.D. and D.Sc. in physics from the University of Bristol, England, in 1960, 1963, and 1972, respectively, and started his career in physics at Cornell. He has held distinguished positions at Bristol University and at the NASA Electronics Research Center. Michael served on the Central Policy Review Staff for the British government's cabinet and became Wheatstone Professor and Head of the Physics Department at King's College of London University.

Dr. Michael Hart
NSLS Chairman 1995-2000

Michael has won many honors including the American Crystallographic Association's Bertram Eugene Warren Award for Diffraction Physics in 1970 and the Charles Vernon Boys Prize from The Institute of Physics in 1971. In 1982, he was elected Fellow of the Royal Society of the United Kingdom, and in 1994, he was appointed by Queen Elizabeth as Commander of the British Empire for his service to physics.

As a consultant and research collaborator, Michael became a member of the NSLS User Community in 1991. He is well known in the synchrotron community for his contributions to x-ray physics in the development of monolithic multiple Bragg reflection devices such as the x-ray interferometer and the Bonse-Hart small-angle scattering camera and his pioneering work on x-ray polarization phenomena.

During his tenure as Chairman, despite strong competition from two new light sources, the number of users increased from 2200 to over 2400 annually, between 1994 and 1999. More importantly, publications in 1999 hit an all time high at 953, a 70% increase over 1994. NSLS users produced 875 of those writings (a record number).

A defining moment in the history of the NSLS came during the second year of Michael's term as Chairman. In the spring of 1997, the DOE's Basic Energy Sciences Advisory Committee (BESAC) established a panel led by Dr. Robert Birgeneau, Science Dean at the Massachusetts Institute of Technology. The charge of the panel was to recommend priorities for synchrotron radiation research in the coming decade and to make detailed budget recommendations. At the time, budget projections for Basic Energy Sciences (BES) were flat and prospects seemed ominous for the NSLS, as a "second generation" facility, in light of the two expensive new "third generation" facilities which had recently come online, and would certainly require large portions of the BES budget. Staff morale was beginning to reflect these concerns and recruitment was becoming more difficult. Undaunted, Michael Hart took up the challenge, rallied the User community and after some five months of dedicated effort, presented a case so compelling that in the "priority one" recommendations of the Birgeneau panel report, the NSLS was the only facility to receive an actual increase ($3M) over the Presidents budget for FY98. Perhaps even more significant, the perception of the DOE and the synchrotron community at large from that point on was revised from initially viewing the Light Source as an "aging facility," to ultimately recognizing it as one of the "Gems" of the DOE complex.

A notable turning point in synchrotron radiation at the NSLS that also_took place under Michael's leadership was a 75% increase in the number of life sciences users between 1994 and last year. For the first time, in 1999 the number of users registered at the NSLS in the field of life sciences topped those in the field of material sciences.

To Michael's credit, two other important objectives were achieved: the arduous task of securing a Memorandum of Understanding (MOU) from PRTs, detailing beamline construction, operations, management and financial support reached 97% compliance (up from 48%); and, the NSLS became the first synchrotron facility to provide BES with statistical data based_on experimental beam time rather than user registration information.

No, Michael Hart is not ready to retire yet! Some grand plans may be in store for his future. The NSLS Community of Staff and Users wish you the very best, Michael. [We will miss your English humor!]

Weekly Users' Meetings

X-Ray Users: Wednesdays
11:30 a.m., Conference Room A

VUV Users: Thursdays
11:30 a.m., Conference Room A

Denis McWhan Retires, Returns to NSLS as a User

Dr. Denis McWhan
ALD for BES 1995-2000

Following a long and distinguished career as a condensed matter scientist at AT&T Bell Laboratories, Denis joined Brookhaven National Laboratory (BNL) and served as Chairman of the Light Source from 1990 to 1995, and as Associate Laboratory Director for Basic Energy Science (BES) at BNL from 1995 to 2000.

While at Bell Laboratories, Denis was a frequent visitor to BNL, first as a user at the HIGH Flux Beam Reactor (HFBR) and later as a user at the Light Source. He was in charge of the planning of the first AT&T beamline at the NSLS, and later became responsible for all five AT&T beamlines.

Denis played a leading role in the development of the technique of magnetic x-ray scattering as well as other techniques that have facilitated the study of high-temperature superconductivity.

Denis has received Bell Laboratories' Distinguished Service Award, and is a Fellow of the American Association for the Advancement of Science and the American Physical Society.

Although retired from BNL, Denis has been active in pursuing his scientific interests as a user on Beamline X22C, a beamline managed by BNL Physics, Argonne National Laboratory (ANL) and the University of Maryland.

Appointment of New Associate Laboratory Director for BES

by Michael Hart - Chairman, National Synchrotron Light Source

Mark Chance, in his report of the 2000Annual User's Meeting, mentioned that Dr. Richard Osgood, Jr. had just taken up office, on 15 May 2000, as Associate Laboratory Director for Basic Energy Sciences in succession to Denis McWhan. The Director's announcement is reproduced here:

"Richard Osgood is currently the Higgins Professor of Applied Physics and of Electrical Engineering at Columbia University where he has forefront research programs in UHV surface physics and in integrated optics. Many of his research programs are in the growing area of nanoscience, which is one of the initiatives in the President's budget request for FY2001. Professor Osgood has had over 33 years of experience in basic research in the fundamental properties of matter using a wide range of experimental tools from femtosecond lasers to synchrotron sources to many methods of materials synthesis. He received his B.S. from the U.S. Military Academy in 1965, his M.S. in physics from Ohio State University in 1968, and his Ph.D. in physics from MIT in 1973. Before coming to Columbia in 1981 he was a scientist at the Lincoln Laboratory, MIT. During the past two years Professor Osgood has served as vice chairman of the BSA Science and Technology Steering Committee, and on many national advisory committees including the DOE Basic Energy Sciences Advisory Committee. I look forward to working with him to enhance and expand the BES programs at BNL.

I want to thank Denis McWhan again for his ten years of service to BNL first as Chairman of the NSLS Department and then as ALD for BES programs. I also want to thank Martin Blume and the search committee for conducting the national search that has led to the appointment of Professor Osgood."

Dr. Richard Osgood, Jr., Associate Laboratory Director for Basic Energy Sciences

Three Directorates are key to the future of the NSLS: Basic Energy Sciences for funding and physical science user programs, Life Sciences (Dr. Nora Volkow) and Environmental Sciences, Applied Science and Technology (Dr. Teresa Fryberger). The trio of new appointments made in the last year or so is now complete and we look forward to a period of renewed enthusiasm and direction in the Light Source portfolio and the formation of new links between the three areas of science and technology.

Synchrotron Measurements of Interplanetary Dust Particles

Lindsay P. Keller (MVA, Inc.), George J. Flynn (SUNY-Plattsburgh), John P. Bradley (MVA, Inc.) and Steve Sutton (Univ. of Chicago, and CARS)

The Earth is continually bombarded by interplanetary dust, accreting onto the planet at a rate of about 30,000 tons per year. Although dust particles greater than about 100 µm in size generally vaporize on atmospheric entry, producing meteors, smaller particles, ranging from 5 to 35 µm in size, radiate heat so efficiently that they decelerate without melting. These dust particles are collected from the Earth's stratosphere by impact onto small dust collectors carried aloft by NASA stratospheric sampling aircraft since the mid-1970s. These particles are mostly samples of asteroids and comets, providing the only comet samples available for laboratory analysis. Each particle can provide clues to the physical, chemical, and mineralogical properties of the asteroid or comet from which it came. However, since each particle may sample a different parent body, each ~10 µm interplanetary dust particle (IDP), weighing about 1 nanogram, must be analyzed individually for maximum scientific return. These small particles are ideal candidates for analysis by the high intensity, microfocused photon beams available at synchrotron light sources. We are using four beamlines at the National Synchrotron Light Source to characterize the IDPs. We measure the infrared (IR) and ultraviolet (UV) spectral properties of the IDPs at U10B and U9B respectively, the carbonaceous materials in the particles are mapped and characterized with the scanning transmission X-ray microscope (STXM) at X1A, and the element abundance patterns, particularly the volatile elements which provide clues to the formation conditions of the IDPs, are obtained at X26A. Because of our novel sample preparation techniques, many of these measurements are made on the same samples.

The NSLS delivers an infrared flux about 1000 times greater than that of conventional infrared sources, allowing us to obtain high-quality FTIR spectra of these small particles. The IR studies have focussed on the 10 µm silicate stretching region[1] and the 3.4 µm C-H (organic) features, and allow for the direct comparison to astronomical data obtained for dust in variety of astrophysical environments.

A population of glassy silicate grains known as GEMS (glass with embedded metal and sulfides) are found within the ultrafine-grained matrices of cometary IDPs. The properties of GEMS are exotic (e.g., they contain superparamagnetic metal inclusions) but similar to those inferred for astronomical "amorphous" silicate grains that are ubiquitous throughout interstellar (IS) and circumstellar (CS) space. Evidence of these grains is found in astronomical IR spectra where bands at ~10 and ~18 µm corresponding to the Si-O stretch and Si-O-Si bending mode vibrations in silicates are observed (in absorption and emission) along multiple lines of sight. We measured the infrared ~10 µm bands of GEMS and compared them with IS and CS silicates and silicates in solar system comets. Measuring the IR properties of GEMS is difficult because: (a) they are too small to analyze using conventional laboratory IR spectrophotometers and, (b) they are almost always found mixed with other submicrometer crystalline silicates. We compared the ~10 µm band from pure GEMS with those of IS and CS "amorphous" silicates (**Figure 1**). The pure GEMS spectrum (**Figure 1a**) was obtained from a thin section of IDP L2011*B6 where GEMS are the only silicates present. The band is broad and featureless (i.e. it lacks fine structure), and it peaks at ~9.8 µm with an IR excess or asymmetry on the long-wavelength side (**Figure 1a**). Elias 16 (in Taurus) and Trapezium (in Orion) are IS molecular cloud environments (**Figures 1b & 1c**). Their smooth asymmetric spectra with maxima at ~9.8 µm and an IR excess on the long wavelength side are remarkably similar to those of some GEMS. DI Cephei (a T Tauri star) exhibits a ~10 µm band typical of the dust around many young stellar objects (YSO's) (**Figure 1d**). µ-Cephei is an evolved (post-main-sequence) M type supergiant star (**Figure 1e**). Its CS ~10

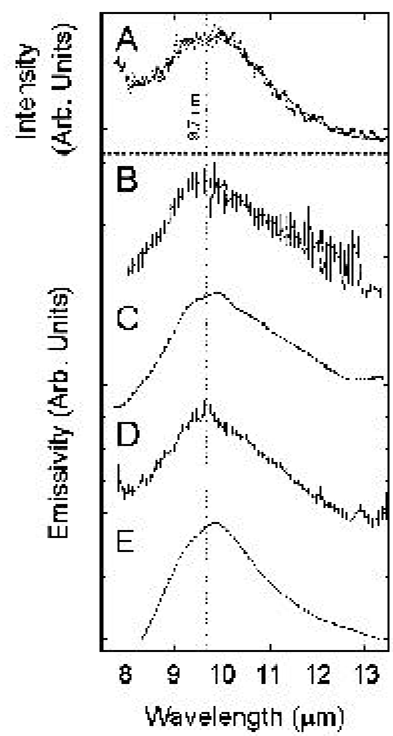


Figure 1. Comparison of the 10 micrometer Si-O stretch bands of pure GEMS with astronomical silicates. (a) GEMS (profile in KM units derived from transmittance spectrum); (b) Elias 16 molecular cloud; (c) Trapezium molecular cloud; (d) Pre main-sequence T Tauri YSO DI Cephei; (e) Post main-sequence M type supergiant µ-Cephei.

μm band is similar to but slightly narrower than GEMS, Elias 16, Trapezium, and DI Cephei.

The organic component of the IDPs may be of particular importance in understanding the origin of life on Earth. The relatively gentle deceleration these IDPs experience in the Earth's upper atmosphere allows some IDPs to carry organic matter to the surface of the Earth without significant thermal degradation. Modeling by Anders[2] indicates that IDPs may have contributed a significant amount of prebiotic organic matter, important for the development of life, to the early Earth. Using the FTIR instrument initially installed on U4IR and now at U10B, we have been studying the organic and silicate components of the IDPs for 2 years. Eight IDPs exhibited FTIR spectra significantly different from silicone oil (the collection medium) and from the terrestrial control particles. The strongest absorption in the 3 micron region in each of these 8 particles is at 2926 cm^{-1}, and a second, weaker, feature at 2854 cm^{-1} was also detected. This pair of absorptions is characteristic of $C\text{-}H_2$ symmetric and asymmetric stretching vibrations of aliphatic hydrocarbons. A weaker absorption was detected at 2960 cm^{-1}, a $C\text{-}H_3$ stretching vibration at a position slightly different from the silicone oil feature. The FTIR spectra of these 8 IDPs are very similar to the 3 micron absorption detected in the interstellar medium and to that of the organic matter extracted from carbonaceous meteorites. Our FTIR measurements at U10B provided the first unambiguous detection of aliphatic hydrocarbons in IDPs. These aliphatic carbon compounds may be a more important resource for the development of life than the aromatic compounds, which are relatively non-reactive, that were reported previously in IDPs.

In addition to the FTIR characterization of the IDPs we also use the STXM at X1A to make detailed measurements on the distribution and solid state environment of carbon in IDPs. We have mapped the absorption of ultramicrotome thin sections (~100 μm thick) of several IDPs at x-ray energies of about 275 eV and 310 eV. Since the absorption coefficient of carbon increases sharply at the carbon K-edge (~285 eV), while other elements have roughly constant absorption coefficients over this energy range, spots showing increases in absorption at 310 eV are carbon-rich. Each of the IDPs examined thus far showed some carbon-rich regions, which ranged from a few percent up to 90 percent of the area of the particle on the section. These carbon-rich regions were then examined by C-XANES (X-ray absorption near-edge structure) spectroscopy. In C-XANES spectroscopy we detect absorptions that correspond to photon induced transitions from core level electrons into various bound and virtual excited states. Variations in electron density surrounding the photoexcited states leads to well-resolved absorption bands corresponding to carbon in different functional groups. Organic carbon is easily distinguished from elemental carbon (graphite, amorphous carbon, or diamond) by the presence of C-H and/or C-O absorption features in the organic carbon. Two particles showed C-XANES spectra very similar to that of amorphous carbon. Eleven of 12 IDPs, including one which also showed amorphous carbon, showed C-XANES spectra quite distinct from graphite, amorphous carbon or diamond and very similar to the acid insoluble organic extract from the carbonaceous chondrite meteorite Murray (e.g. **Figure 2**). These C-XANES results indicate that organic carbon, similar to that extracted from the carbonaceous chondrite meteorites is a common component of both hydrated and anhydrous IDPs. Our STXM measurements have confirmed the high abundance of carbon in IDPs and further, we have identified most of that carbon as organic rather than elemental. Although our initial efforts have focused on carbon, because of the exobiology interest, the X1A monochrometer spans the energy range from 250 to ~800 eV energy range, including the K-edges of the elements C, N, and O, and the l-alpha lines of the elements from K through Fe. Thus, the STXM offers the possibility of performing element mapping and XANES bonding state measurements on a mineral by mineral basis in the IDPs.

Chemical analysis of the IDPs is performed using the X-Ray Microprobe at Beamline X26A. The X26A Beamline uses two Kirkpatrick-Baez microfocusing mirrors to produce a beamspot ~15 μm in size, ideally matched to the size of an individual IDP. When used as an X-Ray Microprobe the fall-off in x-ray intensity with increasing energy limits analysis to ~17 keV, accessing the K-lines of elements up to Sr, with a practical sensitivity for the elements from Cr to Sr of ~1 ppm. This includes the moderately volatile elements Cu, Zn, Ga, Ge and Se, whose contents can be used to associate IDPs with the various types of chondritic meteorites because the contents of these elements differ significantly between the different types of chondritic meteorites. A major sub-group of IDPs are the more fragile, porous IDPs which are vola-

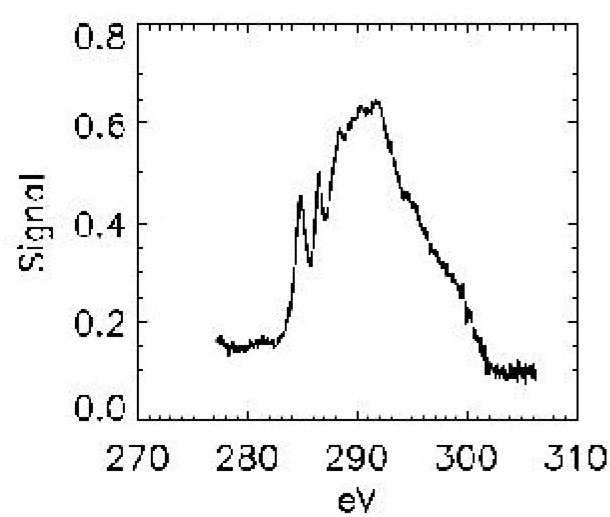


Figure 2. A carbon XANES spectrum showing the fine structure associated with the carbonaceous material in certain IDPs obtained with the scanning transmission X-ray microscope (STXM).

tile rich compared to the primitive chondritic meteorites, the most volatile rich type of meteorites. These fragile, porous IDPs have, on average, Cu/Fe, Zn/Fe, Ga/Fe, Ge/Fe and Se/Fe ratios that are 2 to 3 times the primitive chondrite values, and they appear to constitute a new chemical class of extraterrestrial material, never before available for laboratory study. Some of these fragile, porous IDPs are likely to be samples of comets, and the high volatile content of these particles is consistent with a spacecraft measurement of K/Fe, measured *in situ* in Comet Halley dust, that is also 3 times the value in the primitive chondritic meteorites.

Many IDPs are fine-grained aggregates of sub-micron grains, making them especially well-suited for mineralogical characterization by x-ray powder diffraction. As part of our ongoing effort to characterize the IDPs, we recently performed x-ray powder diffraction of individual IDPs, some with masses as small as ~1 nanogram, using a Brucker SMART 1000 CCD system, provided by SUNY-Stony Brook, installed on Beamline X26A. **Figure 3** shows the x-ray diffraction pattern obtained from IDP L2005J24. We anticipate that further development of this technique will allow non-destructive mineralogical characterization of the IDPs, preserving the particles for other measurements requiring whole, intact IDPs.

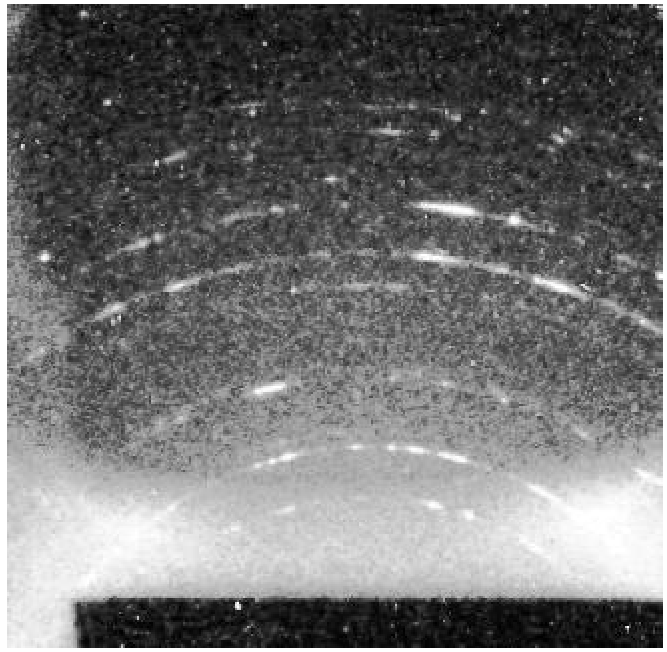


Figure 3. An X-ray powder diffraction pattern from IDP L2005J24 showing strong diffraction lines of pyrrhotite (an Fe-sulfide mineral common in IDPs).

Acknowledgements

The measurements made at the NSLS would not have been possible without the assistance of Janos Kirz, Chris Jacobsen and Sue Wirick at X1A, Lisa Miller and Larry Carr at U10B, John Sutherland and John Trunk at U9B, and A. Lanzirotti and W. Rao at X26A. This work was supported in part by grants from the NASA Cosmo Chemistry Program.

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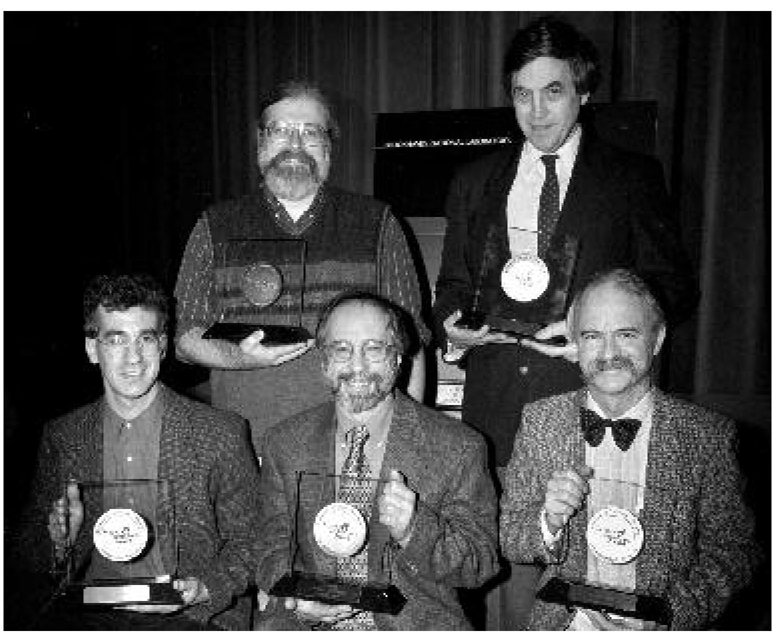
[2] Anders, E., “Pre-biotic Organic Matter from Comets and Asteroids”, *Nature*, 342, 255-257, (1989).



(Top left to right): Malcolm Capel, Marshall Newton. (Bottom left to right): Lonny Berman, Laurence Littenberg and Robert Sweet. Missing from photo: David Cox. Photo by Roger Stoutenburgh.

BNL Science & Technology Award

The first formal Employee Recognition Award Conferral Ceremony was held at Berkner Hall on February 2.

Congratulations to **Lonny Berman** (NSLS), **Malcolm Capel** and **Robert Sweet** (Biology), who share an award for their formation of a very successful team in the creation and operation of the structural biology consortium at NSLS. Together with other PRT-run structural biology beamlines on X-9 and X-4, the expansion and improvement of the facilities at BNL has been achieved at a rate commensurate with demand.

The three recipients of the BNL Science and Technology Award successfully bid for a NIH Research Resource grant a year ago which more than doubled the support for the consortium.

Marshall Newton (Chemistry), Laurence Littenberg (Physics), and David Cox (retired), also received awards.

X-Ray Ring Status

Jeff Rothman, X-Ray Ring Manager

Substantial progress has been made towards establishing low emittance operations at 2.8GeV. The old defocusing sextupole power supply has been connected to the focusing sextupole magnet, and the new higher power supply has been connected to the defocusing sextupole magnet. This is necessary since we require more current for defocusing than focusing. Both supplies have been commissioned and are operational. During studies, 275mA have been successfully ramped to 2.8GeV using the low emittance lattice. Further studies are required to reduce the beam size and correct the orbit. Once low emittance 2.8GeV operations are established, all operations will be at 2.8GeV. We estimate that 2.8GeV operations will begin in mid-July.

Work continues on the digital feedback system. The code has been ported from the old CPU and has run successfully on the new Power PC CPU. During studies, this prototype system ran at a 550Hz update rate and substantially reduced beam motion in the X-Ray ring resulting from booster operations. Hardware for the operational system is being tested in the UV ring. This includes new cabling, differential receiver boards to reduce noise pickup, and fast parallel conversion ADC boards to eliminate timing skew. The new system will use all PUEs and all trims to stabilize the orbit rather than the subset of trims and PUEs that is used by the current analog system. The operational system will update at a 1KHz rate. The bandwidth of the system will be limited only by the frequency response of the trim magnets.

The installation of the X-17 wiggler has been delayed and will not be installed during the winter shutdown. A problem was discovered in the main power lead during acceptance testing, and the unit has been shipped back to the manufacturer. Oxford Instruments is still evaluating the problem.

Initial measurements have been made with vacuum chamber motion detectors. These devices will measure horizontal vacuum chamber motion due to changes in heat loading as the beam current decays. This information will be used to improve orbit correction and orbit stabilization.

VUV Ring Status

Stephen Kramer, VUV Ring Manager

The ring came back from the spring shutdown on schedule and with most of the work completed. The major effort during this shutdown was replacing the U16 GP vacuum valve with a new VAT valve. This required bleeding up half the ring to nitrogen boil-off. Despite this cause for poor vacuum, beam was injected to over 1 Ampere within 2 hours after the start of injection. Lifetime has continued to improve as the integrated current increased. A record value of over 60 Ampere-hours was accumulated by Saturday May 20 at 8:00 a.m., when the ring was declared operational.

During the shutdown a major effort was extended at solving a long-standing safety issue of overloading of the electrical cable trays in the ring. It is estimated that more than 600 pounds of unused signal cables was removed from the overhead cable trays. These are the result of over 15 years of adding cabling to monitor and control the ring and user's systems. The amazing thing is that the ring came back into operations without any operational cables missing. This shows the care and planning that went into this potentially troublesome operation. There remains about an equal amount of cabling to be removed during a future shutdown. Once this is completed, it is planned to provide an upgrade of the ring monitor and control signals to the user beamlines. This will give better current, timing and injection signals to the users, as well as provide the ability to monitor user signals with the NSLS control system. The injection signals will allow users to gate out the injection period from their experiments, when the Top-Off Mode of Injection becomes operational.

The other major effort started during the shutdown was the installation of the prototype of a new front-end interlock system for the U16 Beamline. This system, once perfected, will replace the older system that required running a large number of signal cables between the front-end controller and the interlock control system in the center of the ring. The new system uses a single dedicated LAN cable and distributed PLC controllers to monitor and control the front-end components. The old cabling was a major component of the cable problem of the VUV Ring and limited the flexibility of the system when new functions were required.

Work was also done on the new digital feedback system, which will be tested on the VUV Ring. New buffer boards have been provided to give lower noise levels on the signals into the feedback system, and control of the trim power supplies has been added for the new system. This system should allow greater orbit stability than the older Global Feedback System, which could not be easily expanded to the additional trims. The final installation of the diagnostic Beamline U3B was also completed and the beamline has since been conditioned for operation to the full beam current of the VUV ring. This beam will provide measurements of the energy oscillations and distribution of the electron beam in the ring.

Safety and Compliance

Bob Casey - Assoc. Chair for Environment, Safety & Health

Generation of Hazardous Wastes

About 25% of the research conducted at NSLS produces waste materials either classified as industrial (e.g. oils, oily rags) or hazardous (e.g. solvents, acids). The total amount of waste generated by all experiments in a typical year ranges from 500 - 1000 pounds. Both industrial and hazardous wastes are subject to strict County, State and Federal regulations regarding handling and disposal. Training hazardous waste generators is an important part of these regulations.

As a part of the NSLS response to the Lab's efforts to become registered as compliant with ISO 14001 Environmental Management criteria, new "read & sign" training has become necessary for all members of an experiment that generates either hazardous or industrial waste. This training is provided during the ESH Orientation arranged by the User Administration Office, and is also available on the web at **http://www.nsls.bnl.gov/Safety/P&RMan/training-experiment-eva.pdf**. Users can review this material prior to arrival at NSLS and turn in the signed form upon arrival at NSLS.

In addition, one person from an experiment generating hazardous waste must assume overall responsibility for the waste which is generated and also complete an additional training program covering federal regulations for hazardous waste. This training is available on the web and can be accessed at **http://training.bnl.gov/cbt/hazwaste/** and takes about 30 minutes to complete. The course can also be taken prior to arrival.

Visitor Log in Requirements

The Laboratory has established new requirements for untrained personnel who enter radiological areas. At NSLS, this requirement resulted in a log-in sheet which is found at all access doors into the NSLS Controlled Areas. As previous, a user who has not received NSLS specific training and BNL General Employee Radiological Training (GERT) must be escorted while in areas posted as "Controlled Areas" at NSLS. Now, the untrained visitor and his/her escort must log-in prior to entry acknowledging that certain information on the form has been conveyed to the guest.

BLOSA: Beam Line Operations and Safety Awareness

Eva Rothman - Training Coordinator

Beam Line Operations and Safety Awareness Training (BLOSA) was initiated several years ago to reduce operational problems that sometimes occur with new or infrequent users. It also provides awareness of specific environment, safety, and health issues in the local environment where a user would be working, and which would not be covered in the general NSLS Facility Orientation. This awareness program was to be distinct from any training given which teaches the operation of the experimental hardware. Although many users and beamline staff are already aware of the BLOSA program, this article will serve both as a reminder and an update.

The NSLS policy as identified in the Users' Guide is as follows: "Each user must be trained on the beamline on which they will be conducting experiments. It is the responsibility of the cognizant beamline personnel and the experimenters to ensure that training is obtained."

BLOSA is provided by the staff responsible for the management of the beamline. Each beamline may choose how it wishes to provide the BLOSA training. Some users may begin experiments during off-hours or on weekends, when beamline staff may not be present. Advance planning and coordination between the user and the beamline staff is important to ensure that BLOSA training can be provided when needed so that experiments can begin when scheduled.

The NSLS BLOSA program has always been regarded as an excellent idea by any reviewers and auditors who have evaluated it. However, a recent review of the program shows that it is still languishing at about a 39% compliance level - even though users who are trained and beamline personnel who do actually train users agree that it is valuable to them.

Now that the NSLS has implemented the tools necessary to track compliance, it will be easier for NSLS staff to enforce the existing policy: **As a condition for beam authorization, effective June 1, 2000, a beamline will not be enabled by Operations Coordinators unless all personnel present at the beamline have received BLOSA training. All users arriving after the start of the experiment will be expected to receive BLOSA training at the time of arrival.**

BLOSA training does not take a lot of time to complete – anywhere from 5 to 30 minutes, depending on the beamline – but it conveys important information every user should know about their specific equipment and location. The experimenters and the beamline staff are jointly responsible for making sure all experimenters are BLOSA-trained for that beamline. Overall compliance of a beamline with the BLOSA program will remain the responsibility of the beamline staff. Information regarding BLOSA requirements is available at **http://www.nsls.bnl.gov/Training/BLOSA/blosahome.htm**.

Facility Update

Frank Terrano, Assistant to the Chairman

New General User Lab:

In response to the growing demand for laboratory facilities on the experimental floor at the NSLS, authorization has been given to proceed with the conversion of Room 110-D into a new General User laboratory. The new laboratory will be equipped with standard lab furnishings, including fume hood, sinks and deionized water. Room 110D is located in the northeast corner of the experimental floor, adjacent to the NSLS Library/User Lounge. We expect to have the conversion completed by the end of fiscal year 2000. This will bring the total up to five General User labs available to our research community. Anyone interested in becoming steward for the new lab should contact Building Manager, Mike Kelly at extension 3476.

Credit Cards for Users:

The electronic mall was established at BNL to provide an on-line vendor to carry stationery items previously (but no longer) available in the central stockroom. On-line vendors for electronics are slated to be following shortly. In response to User requests, BNL will now issue credit cards to Users, to allow for ordering stationery via on-line catalogs as well as other materials directly from vendors. It should generally take only a few days to get a credit card after completing the mandatory training that all credit card holders are required to have. Users wishing to obtain a BNL credit card must have an established account at BNL, before a card can be issued. Those interested should contact Rosalie Piccione at extension 3160.

It should be noted that BNL credit cards are required to use the on-line catalogs. However, Users with credit cards from their home institutions may still continue to make direct purchases with outside vendors, on their own cards, as before.

If you have further questions, call Jim Desmond at extension 4837 or me at extension 3963.

Lobby Upgrades:

Plans are underway for the replacement of the video wall in the main lobby of Building 725. The present matrix of nine 25" video screens, used for displaying highlights of the facility, machine parameters for the X-ray & VUV rings, video presentations and events telecast from Berkner Hall, will be replaced with larger screens using the new flat screen technology. Not only will the screens be replaced, but the whole system will be upgraded to be PC driven, which will also enable us to display Web based images and information, as well as CD-Roms. The lobby touch screen directory located to the left of the front entrance will also be upgraded. Is it time to say farewell to the old NSLS candle flame logo on the directory screen? Send us your thoughts.

Available Office Space for Users:

A limited number of offices have become available resulting from a consolidation of the ATF project staff into a building more conveniently located adjacent to the ATF facility. The offices are in modular Building 728, located on the east side of Railroad Street across from Building 725. Users wishing to occupy one or more of these spaces should contact Building Manager, Mike Kelly at extension 3476. Regular BNL space charging will be applied according to square footage.

NSLS Stockroom Inventory

At this point in time, the role of the NSLS Stockroom must now be redefined, due to Procurement and Property Management Division's (PPM) commitment to stocking fewer items onsite and the labwide use of credit cards & online vendor catalogs. The NSLS Stockroom Committee has been meeting to discuss the NSLS Stockroom inventory. We have recently received a list from the PPM Dept. of what the BNL Stockroom plans to stock.

In order to redefine the role of the NSLS Stockroom, we need feedback from the NSLS Staff and Users. The request form for additional NSLS Stockroom inventory is located in the NSLS Stockroom. Please take the time to fill out this form with a list of what you believe the NSLS Stockroom should have on hand and return it to Donna Buckley, Mailstop 725D or dbuckley@bnl.gov as soon as possible. Please keep in mind that these requests should be for wide range usage and not specific to only one person or group, and the current NSLS Stockroom is the only space we have to work with. However, the NSLS Stockroom Committee will be sensitive to all your needs.

The responses that are received will be discussed at our next NSLS Stockroom Committee Meeting. Our NSLS Stockroom Committee Members are: Randy Abramowitz, Steve Bennett, Bob Best, Donna Buckley, Scott Buda, Bill Cahill, Walter deBoer, Steve Ehrlich, Larry Fareria, Ken Koebel, Charlie Nielson, Gary Nintzel, and Bob Scheuerer.

Donna Buckley, Stockroom Manager

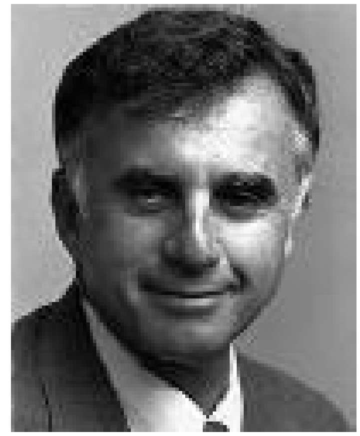
In Memoriam – Jerome B. Cohen

by Paul Zschack, University of Illinois

It is with great sadness that I learned of the passing of Jerry Cohen of Northwestern University in November. Jerry was a founding member of the X18A MATRIX PRT which was formed at the inception of the NSLS. He steered Northwestern's development efforts on behalf of the PRT, and served the entire synchrotron user community as a member of the NSLS Users' Executive Committee in 1985-6.

The bulk of his research work at NSLS was related to diffuse x-ray scattering from binary and ternary alloys and compounds, including Al-Cu-Zn, Al-Cu, Cu-Be, Cu-Au, Fe-based alloys and others. Having developed these experimental techniques years earlier in his laboratory, it was natural to exploit the high flux and tunability of the synchrotron for these demanding studies. He also directed the development of the first UHV chamber for surface diffraction studies to be used on this beamline; a portable unit which could be mounted directly on the diffractometer. With this instrument, surface reconstruction in oxides, particularly TiO_2, was studied. He also enthusiastically pursued surface small angle x-ray scattering work. From the PRT's beginning until the time he left it in the mid-1990s, Jerry advised a succession of Ph.D. students whose work was primarily done on X18A. He had a remarkable ability to motivate and inspire. He permitted those of us who worked with him just enough freedom to explore without going too far down the wrong path.

In a career spanning several decades, Jerry was well known in the materials science community for the study of many topics including his work in residual stresses. He was a past President of the American Crystallographic Association, former Dean of the School of Engineering and Applied Science at Northwestern University (for 13 years), and a member of the National Academy of Engineering. He placed considerable attention on education, and spearheaded the revamping of the undergraduate engineering curriculum at Northwestern during his tenure as Dean. One of his initiatives was to set up virtual teaching laboratories in which experimental equipment could be operated by students through a Web link. Such a capability was in preparation for implementation at the Advanced Photon Source with DND-CAT (of which he was also a founding member) at the time of his death. He had just stepped down as Dean in September, and was looking forward to returning to the classroom and ramping up a research program with the DND-CAT. He will long be remembered by collaborators and friends as an excellent scientist, an enthusiastic administrator, and an extraordinary mentor and friend. He will be sadly missed.



Jerry Cohen

In Memoriam - Laurent Fabrice Seve

by Boris Sinkovic, University of Connecticut

Laurent Seve

Laurent Fabrice Seve died suddenly of brain aneurysm on February 21, 2000 at his home in Grenoble, France. Born in Valence, France on June 23, 1970 Laurent earned his Diploma degree in Physics at the Ecole Nationale Superieure de Physique de Grenoble in 1993 and DEA Science et Structure des Materiaux at the Universite Joseph Fourier. His doctoral work in Physics was on "X-Ray Resonant Magnetic Diffraction Studies of Metallic Multilayers" working at the CNRS Laboratoire de Cristallographie in Grenoble which he completed in 1997.

In December 1997 he moved to the NSLS, where as a postdoctoral fellow he led a joint effort of the U. of Connecticut and BNL to image magnetic materials with the PhotoEmission Electron Microscopy (PEEM). During two years in the US he also performed experiments at the ALS/LBL and at APS/Argonne. In November 1999, he returned to France as a permanent member of scientific staff of the CNRS Laboratoire de Cristallographie in Grenoble and was embarked on development of UHV X-ray reflectometer and the PEEM project.

During his short career, Laurent showed talent and enthusiasm for research that was rarely matched, and was destined for a bright scientific career. He was exceptionally generous and personal, and was loved by his friends. His tragic and sudden death has been a shock to all the people who met him and observed his energetic ways in research and life in general. He will be greatly missed by his family, friends and acquaintances alike.

In Memoriam - Paul Sigler

by Lonny Berman - National Synchrotron Light Source

It is with sadness that I learned of the passing of Paul Sigler of Yale University in January. Paul was a member of the Howard Hughes Medical Institute (HHMI) structural biology PRT at X4 and an active user of several macromolecular crystallography beamlines at NSLS and elsewhere. After obtaining an M.D. and completing a medical residency in 1961, he switched gears and chose to pursue a research career in structural biology, a field which was then in its infancy. He worked first at the National Institutes of Health (NIH) before pursuing and completing graduate studies at the MRC Laboratory of Molecular Biology in Cambridge in the mid-1960s. There he assumed a faculty position at the University of Chicago, then moved to Yale University in 1989 where he remained until his death. It was during this latter period that he became an active synchrotron radiation user and made his most notable accomplishments, with support provided by the HHMI.

Paul Sigler (photo courtesy of Yale U.)

The structures which he determined included protein-DNA complexes involved in transcription and gene expression, G proteins and others involved in intra- and extra-cellular signal transduction, and perhaps most spectacularly, a large chaperonin complex GroEL/GroES which is involved in the folding of proteins (and was featured on the cover of Nature in 1997).

Aside from being an avid user of NSLS, Paul was a strong advocate of the macromolecular crystallography programs here. Not shy to express his views and opinions, he lobbied strenuously for crystallography infrastructure enhancements at NSLS, using his memberships on AUI, BNL, and NSLS oversight and review committees (most recently the NSLS SAC) to advantage as platforms. That structural biology at NSLS is in the strong condition that exists today owes some measure of gratitude to Paul's direct and indirect efforts; most of the research accomplishments cited above were based on crystallography data collected at NSLS, including my beamline, X25. His group was the most prepared and productive of all the structural biology groups which used X25.

Paul was the recipient of several honors and fellowships during his distinguished career, which included Fellow of the American Academy of Arts and Sciences and Member of the National Academy of Sciences.

I will most remember Paul as a friend of structural biology at NSLS, and for his "give 'em hell" approach for getting things done. But my most endearing memory is his kind offer, expressed to me last year, to take a leave of absence from my activities at NSLS to join him at Yale to learn structural biology. Who better than to reincarnate under as a structural biologist?

BNL Onsite Shuttle

A morning (7:30 to 8:30 a.m.) onsite shuttle service is available for guests, users and staff between the apartment area and the lab's facilities (see schedule at right).

An on-call, door-to-door service is available between the hours of 8:45 a.m. and 4:15 p.m.

Please call Ext. 2714 for pickup. Requests are accepted on a first-come, first-served basis. To be able to serve as many customers as possible, please be ready to board the van at the main entrance of your building immediately after making the call for pickup.

Please note: Radioactive and other hazardous materials are prohibited. Smoking is prohibited. An adult must accompany persons under the age of 16. If you have any questions, please e-mail transportation@bnl.gov.

STOP	TIME (a.m.)	LOCATION
1	07:30	Yale Road in front of Efficiency #43
2	07:34	Lollipop House
3	07:36	Yale Road (Cottages, Summer Only)
4	07:39	Fleming House Parking Lot
5	07:43	Cafeteria
6	07:46	Physics (Bldg 510)
7	07:49	NSLS
8	07:54	CAD (Bldg. 911)
9	07:59	CAD (Bldg. 1005)
10	08:04	Wide Angle Hall (6:00 Hall)
11	08:07	PHENIX/Pump House (8:00 Hall)
12	08:10	PHOBOS Experiment (10:00 Hall)
13	08:16	BRAHMS Experiment (2:00 Hall)
14	08:21	Brookhaven Av/Center St. Parking Lot

1999 Activity Report Available

The 1999 Activity Report is now available in printed format and on CD-Rom. You may obtain a copy either by stopping by our office or you can request it on-line at http://www.nsls.bnl.gov, then choose request copy of 1999 Activity Report. Also available is the revised Community Directory and Users' Guide. Please note that all beamlines will receive a copy of the Activity Report, Community Directory and Users' Guide in their mailslot soon.

Experimental Summaries (Abstracts) for the 2000 NSLS Activity Report

Start preparing your Experimental Summaries (Abstracts) for the 2000 NSLS Activity Report! The system will open earlier then September. The date will be announced soon!

Call for Publication References for October 1, 1999 through September 30, 2000

Our publication references are an important element in how funding agencies judge the productivity of the NSLS. All NSLS users are obligated to send the NSLS a complete publication reference for any paper based in whole or in part on research done at the NSLS. Each beamline PRT submits a list of their own papers as part of their Annual Beamline Progress Report, but the NSLS must also collect references by General Users and other collaborators in order to present the complete picture of the work being done here.

Please take a few moments to prepare your publication references for the year. An online submission system will open mid-summer.

Do your part to support the NSLS!

Identification and Tagging of Equipment

The Department of Energy requires that all capital equipment 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 at right).

Tags are available at the NSLS stockroom 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 & Materiel Division will be conducting periodic inspections to ensure proper identification of all equipment. If, during the inspection, untagged equipment is found, a tag will be applied.

If you need assistance or have any questions, please call Donna Buckley at X3599.

Focus On . .

NSLS Machine Operators

by Gary Weiner - Accelerator Operator

For the experimental user, the stable and bright synchrotron light available at the NSLS might be taken for granted. But for the Light Source's accelerator operators, making sure that light stays on 24 hours a day, seven days a week is their primary mission.

In the NSLS control room, the nerve center of the Light Source, the operators monitor the performance, correct the orbits, adjust the insertion devices and diagnose problems with the X-Ray and VUV synchrotrons as well as the injection systems, including the linear accelerator and the booster synchrotron.

The main task of the accelerator operator is to maintain the required amount of current in the X-Ray and VUV rings. At predetermined intervals, the beamline shutters are disabled, the injection systems are turned on and the X-Ray and VUV rings are filled to the desired amount of current. During the fill, the operator will tune the performance of the injection system to obtain the maximum amount of current in the shortest possible time. They must also be aware of the amounts and locations of radiation produced during the injection process and ensure that NSLS radiation guidelines are not exceeded.

The accelerator systems at the NSLS are made up of numerous subsystems, from magnets and RF cavities to feedbacks and interlocks, each of which can contain hundreds of devices. In all, there are thousands of device parameters in the NSLS control matrix, any one of which can cause the accelerator not to function. The operators must be familiar with all the subsystems, devices and machine control parameters and how each of them might cause the accelerator to function improperly or not to function at all. They must be familiar with the NSLS scientific, engineering and technical support staff so that, in the event that repairs are required, the right people are contacted to deal with it.

There are five accelerator operators at the NSLS, four operators: George Jahnes, Michael Santana, Gary Weiner and Edward Zeitler and their supervisor, Randolph Church. The NSLS control room must be staffed by a qualified operator at all times except during long maintenance periods and the Fourth of July holiday. The operators work 12-hour shifts with a schedule of two days on and two days off.

The job of NSLS accelerator operator is a multi-disciplinary one and requires knowledge in a wide variety of fields. The job is unique and the process of becoming an operator involves as much as two months of intensive, hands-on training with a senior operator until the trainee is ready to stand a shift on their own.

The accelerator operator also functions as the local emergency coordinator in the event of fire or other emergency. Such an emergency involves coordinating response activities with BNL emergency services, keeping the NSLS informed about what is taking place and ordering an evacuation if required.

NSLS Machine Operators. Top row (left to right): Gary Weiner and George Jahnes. Bottom row (left to right): Michael Santana, Edward Zeitler and Randy Church (Control Room Supervisor). Photo by Roger Stoutenburgh.

The operators at the NSLS perform a wide variety of tasks. They keep current in the ring. They interact with the user community, answering their questions about operating conditions, machine status, schedules and changes in orbit. They help the machine physicists and ring managers characterize and improve the performance of the synchrotrons. They keep the machine running.

Flik at BNL now provides users, visitors and staff with the ability to purchase certain groceries on site. Orders may be placed, paid for, and picked up at Berkner Hall Cafeteria. Below is an order form.

BNL Market

Name ____________________ Fax ____________________

Phone ____________________ Date ____________________

Building ____________________ Room ____________________

Order

Fax orders to 345-6475 by 10:00 a.m. or Drop off the order to the Berkner Hall Cafeteria by 10:00 a.m. Monday to Friday Pick up order by 4:00 p.m. Or with prior arrangements orders can be picked up at the Brookhaven Center after 5:00 p.m. Mondat through Friday. Sorry no weekend service at this time.

Payment

Please pay for orders at drop off, sorry cash only

Cold Cuts by the Pound

Chicken Salad	4.00	___
Ham Hormel	3.25	___
Roast Beef	6.00	___
Tuna Salad	3.00	___
Turkey Breast fresh Roasted	5.00	___
Bologna	3.25	___
Corned Beef	4.50	___
Liverwurst	3.25	___
Salami	3.50	___

Cheese by the Pound

Alpine Lace	3.99	___
American	3.00	___
Havarti Dill	4.99	___
Havarti Pepper	4.99	___
Muenster	3.00	___
Swiss	4.00	___

Produce

By the Head

Green Leaf Lettuce	1.00	___
Iceberg Lettuce	1.00	___
Red Leaf Lettuce	1.00	___
Romaine	1.00	___

Each

Apples	.60	___
Bananas	.40	___
Cucumbers	.50	___
Oranges	.50	___
Peppers Green	.65	___
Peppers Red	1.00	___
Tomato	.70	___

Each

Carrots Large each	.15	___
Onions Large each	.30	___

Meats

Bacon pound	3.99	___
Hamburgers 4/1 pound	2.99	___

Butter and Dry Goods

Butter pound	2.95	___
Basmati Rice pound	1.75	___
Converted Rice pound	.70	___
Flour pound	.45	___
Pasta by the pound	.99	___
Sugar pound	1.50	___

Beverages

2 Liter Diet Pepsi or 7u	2.00	___
2 Liter Soda Pepsi, 7up,	2.00	___
Bottled Water Liter	1.75	___
Coffee Pound	4.99	___
Eggs Dz.	1.25	___
Half & Half Quart each	.95	___
Milk Gallon each	3.25	___
Milk Quart each	.95	___
Skim Quart each	.95	___

Breads

Rolls **	.45	___
Sliced Bread loaf **	2.50	___
Baguette (extra long) **	1.75	___

MISC.

Paper Cups 12 oz 25 each	2.50	___
Paper Plate each	.10	___
Packaged Dressing Italian, Ranch, Russian	.45	___

*** Our bread is ordered fresh daily, and there may be limited quantities available, to best assure availability please order breads the afternoon prior to pick up

The Berkner Hall Cafeteria is open daily from 7:30 a.m. till 2:30 p.m.

If you don't see an item on the list please ask, we may have it.

Call for NSLS General User Proposals

For Beam Time in Cycle January - April 2001	Deadline is: Monday, October 2, 2000

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 beam

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 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 received on time have been allocated. Late 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 E. Pinkston or L. Rogers in the NSLS User Administration Office. 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.

Safety Approval Form

Safety Approval Forms (SAFs) are required for every experiment. Your SAF must be submitted online **at least one week before** your scheduled beam time. Do not send in SAFs with your proposal. Be sure to include the birthdates of each experimenter so that the final SAF will provide accurate training information. Go to URL:

http://130.199.76.52/safety

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Important Upcoming Dates

Aug. 7, 2000	1:00-3:00 NSLS Town Meeting UEC Meeting
Sept. 1, 2000	Deadline for submissions for November Newsletter
Sept. 30, 2000	Deadline for General User Proposals (Jan-Apr 2001 cycle)
Oct. 1, 2000	Deadline for Beamline Progress Reports
Oct. 1, 2000	Deadline for publication reference lists from staff and users
Oct. 1, 2000	Deadline to submit title for Activity Report science highlights
Oct. 15, 2000	Deadline for Abstracts

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

Mary Anne Corwin, Editor
Nancye Wright, Production Assistant

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

www.nsls.bnl.gov

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SUNY X3B1 Powder Diffraction Group

Powder Diffraction Beamline X3B1 at the National Synchrotron Light Source

X-ray powder diffraction is a widely used technique for materials characterization in fields as diverse as solid-state physics, geology, and medicine. An overwhelming majority of this work is carried out using laboratory x-ray tubes as sources, but there are distinct advantages to the use of synchrotron radiation: intensity, an intrinsically parallel beam, and tunability. We have set up a powder diffraction station at the X3B1 beamline of the National Synchrotron Light Source with the intention of making available the advantages of synchrotron powder diffraction on a reasonably routine basis.

Overview	***This page includes a brief overview of the experimental setup at X3B1 (NSLS, BNL).***	***Publication***	***Check out the list of publication from experiments that were carried out at the beamline. You can also see the abstracts submitted to NSLS Activity reports.***
Access	***Do you think that synchrotron powder diffraction might be just the ticket for your problem? We are very interested to talk to you and see if we can help. There are several ways this might work.***	***People***	***Find out about the people in the group. This also includes pictures of some of our users.***
Software and data	***This page has links to information about software frequently used to analyze powder diffraction data, and to some raw data available to test your own software.*** ***Powder Structure Solution Program*** **NEW!**	***Other Information***	***This page has links to pages with information about other Synchrotron sources, Powder Diffraction, The University and Long Island.***

This page is never entirely finished. Please send questions and comments to Webmistress.