

## Short Course Participants Learn the Value of Synchrotron Light for Powder Diffraction

January 25-27, 2005

Fifteen participants recently attended the High Resolution Powder Diffraction Data Collection and Analysis Short Course, which was held at the NSLS from January 25-27, 2005. The 3-day course consisted of lectures, guest talks, hands-on data collection, and data analysis, and was co-organized by Peter Stephens (Stony Brook), Christie Nelson (NSLS), and Chi-Chang Kao (NSLS), with administrative support provided by Corinne Messana (NSLS).



Participants of the 2005 High Resolution Powder Diffraction Data Collection and Analysis Short Course

The 15 participants included graduate students, post-docs, and scientists from national labs and universities. While most of the students were familiar with lab-based powder diffraction techniques, very few had synchrotron experience. The participants were all quite eager to learn about the impact that synchrotron-based powder diffraction could have on their own research.

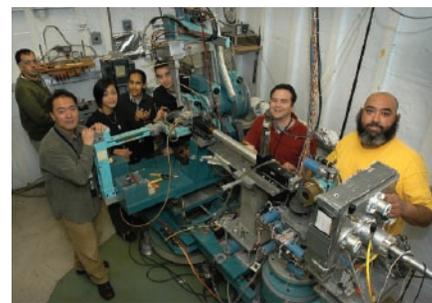
The lectures were presented by Peter Stephens, Pat Woodward (Ohio State), and John Parise (Stony Brook), and covered the basic physics of powder diffraction, experimental aspects of data collection, Rietveld refinement, and indexing. In addition, specialized talks on cutting edge research on high-pressure, high-temperature, and time-resolved powder diffraction were given by guest speakers Yongjae Lee (BNL-CMP), Cam Hubbard (ORNL), and Jonathon Hanson (BNL-Chemistry), respectively.

The hands-on data collection component of the course was carried out on NSLS beamlines X3B1, X7A, and X14A, with beamline instructors Peter Stephens, Yongjae Lee, and Jianming Bai (ORNL), respectively. The participants first learned about beamline operation and sample preparation,



Data collection at beamline X3B1

and then collected data from a corundum standard. Next, the participants collected high-resolution data from samples of interest in their own research projects.



Setting up at beamline X7A

In addition to the lectures and data collection, the participants also spent time learning about data analysis techniques. "Homework" assignments included refining the corundum standard data as well as additional data sets, and then students tackled the data obtained from their own samples. The participants were greatly aided in the completion of these tasks by their three lecturers.

At the end of the intensive three-day course, the participants left with a foundation of knowledge about applying high-resolution powder diffraction to their own research projects. Many expressed interest in becoming NSLS general users, and we look forward to seeing them back here soon.

The organizers would like to thank the lecturers, guest speakers, beamline instructors, Elaine Dimasi (NSLS), Jae-Hyuk Her (Stony Brook), Corinne Messana, and the NSLS User Administration Office and safety staff for all of their help in making the short course such a success.

— Christie Nelson

## NSLS Engineer John Skaritka Wins BNL's Engineering Award

January 26, 2005

At the BNL Employee Recognition Award Ceremony held on January 26, 2005, NSLS engineer, John Skaritka was presented with a 2005 Engineering Award by BNL's Deputy Director for Operations, Michael Bebon. The award, consisting of a plaque and \$5,000, was also presented to BNL employees Ove Dyling, Joseph Harder, and Alan Raphael.



John Skaritka

The award recognizes distinguished contributions to BNL's engineering and computing objectives over one or more years. Contributions may be in any engineering or computing discipline. Nominees are evaluated on the exceptional nature and level of difficulty of the contributions as well as their benefit to the Lab.

John Skaritka was cited for a body of work that contains semi-

nal as well as sustained contributions. His many achievements speak collectively to outstanding breadth, creativity, drive, and dedication in support of BNL missions.

Skaritka was the sole mechanical engineer for BNL's Accelerator Test Facility (ATF) for many years, making key contributions to the design of elements of the accelerator and experiments that were essential to the success of those projects. He contributed to the design of ATF Gun III and Gun IV, regarded now as standard in the world and running at many other facilities.

He was also the mechanical engineer in charge of coordinating all mechanical design, fabrication, and installation activities at the Source Development Laboratory, resulting in a state-of-the-art facility that produced both a self-amplified spontaneous emission free electron laser and a high gain harmonic generation free electron laser.

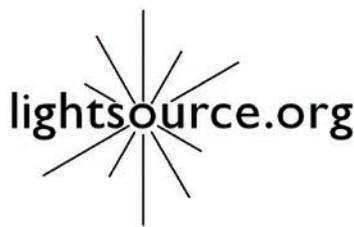
Skaritka is also known for his considerable talent in supporting the NSLS User Science programs, recently, for example, in the construction of a unique instrument pivotal in research on three-dimensional strain mapping to study crack propagation and fatigue failure in alloys.

— Liz Seubert

## Unique Global Light Source Website Launched

February 17, 2005

On February 17, 2005, the international light source community launched the first website dedicated to providing the media, general public, and scientific community with the latest news and information on the world's accelerator-driven light sources (synchrotrons and free-electron lasers) and the science they produce.



The web site — [www.lightsources.org](http://www.lightsources.org) — was developed and is jointly maintained by the Light Source Communicators Group, whose members represent the world's light source facilities in

Europe, North America and Asia. Funding for the project is provided by science funding agencies of many nations.

Accelerator-driven light sources can be large, roughly circular machines or linear machines (usually about the size of a football field to much larger) that accelerate electrons to almost the speed of light. They act like gigantic microscopes that generate intense beams of brilliant light to view the microstructure of materials.

Light sources around the world are advancing research and development in fields as diverse as medicine, drug design,

environmental science, agriculture, minerals explorations, advanced materials, forensics, engineering, and materials fabrication.

Visit [www.lightsources.org](http://www.lightsources.org) for the latest news releases on cutting-edge areas of advanced light source applications for science and technology from facilities around the world.

Anyone can subscribe free of charge to "News Flash," which will email subscribers when news releases and other light source information are posted to the website. Also available on the website are an image bank of light source-related photos and graphics, clippings of news stories, links to light source facility websites, and relevant articles and presentations.

Educators will find links to websites relating to light sources and the science conducted at these facilities. Researchers can find specific information regarding each light source facility, including job opportunities and events related to science outreach activities.

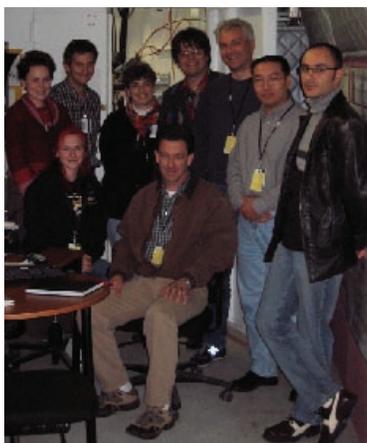
### Sponsors of this collaborative project include:

- Advanced Light Source (ALS)
- Advanced Photon Source (APS)
- Canadian Light Source (CLS)
- ELETTRA (Sincrotrone Trieste)
- European Synchrotron Radiation Facility (ESRF)
- Hamburger Synchrotronstrahlungs Labor (HASYLAB)
- National Synchrotron Radiation Research Center (NSRRC)
- National Synchrotron Light Source (NSLS)
- Photon Factory (KEK Laboratory)
- Pohang Light Source (PLS)
- Stanford Synchrotron Radiation Laboratory (SSRL)
- SPring-8
- Synchrotron Radiation Center (SRC)
- Synchrotron Ultraviolet Radiation Facility (SURF III)
- Swiss Light Source (SLS)
- The Free-Electron Laser at the Thomas Jefferson National Accelerator Facility (JLab)

## X6A Workbench Provides Hands-On Training in Synchrotron Crystallography

March 1-4, 2005

Beamline X6A, the National Institute of General Medical Sciences facility at the National Synchrotron Light Source, offers comprehensive hands-on training in synchrotron data collection and analysis for biophysicists, biochemists, and molecular biologists.



X6A Workbench: Advanced Structural Biology Tools workshop participants

The first “The X6A Workbench: Advanced Structural Biology Tools” workshop took place this year from March 1-4. Participants practiced cryogenic protection of their samples and learned how to load sample cassettes for the X6A automounter. The program followed with hands-on crystallography data collection and analysis. Molecular replacement and multiwavelength anomalous diffraction

(MAD) software suites were discussed. Participants screened their own samples and applied the new data-analysis concepts introduced during the workshop.

The X6A workbench is regularly offered throughout the year. The other three workshops were held on April 26-29, July 12-15, and October 25-28. For more details and registration information, go to: <http://protein.nsls.bnl.gov/news/workbench.php>.

— Vivian Stojanoff

## BNLers Help Promote Community Interest in Science

March 4, 2005

Two BNL “Peters” — Peter Wanderer of the Superconducting Magnet Division and Peter Takacs of the Instrumentation Division — are not only passionate about doing their own science



Three BNLers who volunteer time with the Long Island Sciencenter are (from left) Peter Takacs, Marty Woodle, and Peter Wanderer, who are examining model bridges used for demonstration during a recent bridge-building program at the Sciencenter. The bridges are loaned by BNL’s Office of Educational Programs (OEP), examples of previous years’ bridges made for BNL’s annual high-school model bridge-building contest. Woodle, a founder technical advisor in the organization of the contest, helped OEP in this past year’s event that was held on March 12.

but also about spreading the fascination of science to others in the community. That’s how they came to join a group of people who formed a board and set up the Long Island Sciencenter, a new science museum in Riverhead.

“It’s been a busy time,” says Wanderer. “We are still working on the museum and getting more exhibits.” Through the BNL Science Museum, some key current exhibits have been lent to the Sciencenter by the Lab, for example, the Videosphere.

“The BNL Science Museum staff and directors, first Janet Tempel, then Dolores O’Connor, and now, Gail Donoghue, have been very helpful,” Wanderer says.

Another BNLer, retiree Marty Woodle, now a National Synchrotron Light Source Department guest scientist, is a keen Sciencenter supporter. Woodle most recently volunteered his help with a bridge-building program held in late February.

“This March, the Sciencenter is presenting an adult lecture series open to the public, with three interesting talks,” says Takacs. “I believe people at BNL would enjoy them.”

Three LI Sciencenter Lectures, March 4, 11, and 18 were:

- March 4: “Wine: Science or Magic,” Louisa Thomas Hargrave, founder of the first winery on Long Island.

- March 11: “The History and Destiny of Fisheries near Long Island and in the World,” Carl Safina, President, Blue Ocean Institute, Cold Spring Harbor.

- March 18: “The Adventure of Wildlife Photography,” George Loweth, professional photographer.

— Liz Seubert

## Scientists Create, Study Methane Hydrates in “Ocean Floor” Lab

Data may help develop strategies for mining natural gas locked up in seafloor sediments

March 13, 2005

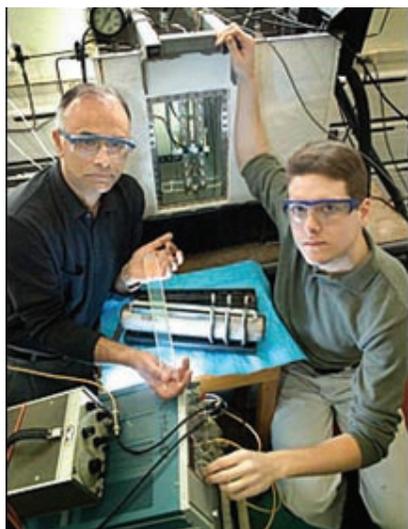
Scientists at BNL have recreated the high-pressure, low-temperature conditions of the seafloor in a tabletop apparatus for the study of methane-hydrates, an abundant but currently out-of-reach source of natural gas trapped within sediments below the ocean floor. Michael Eaton, a Stony Brook University graduate student working for Brookhaven chemist Devinder Mahajan, presented a talk outlining the use of the apparatus for the creation and study of methane hydrates during a special two-day symposium co-organized by Mahajan at the 229th National Meeting of the American Chemical Society in San Diego, California. The talk took place on Sunday, March 13, at 3:05 p.m. in room Madeleine C-D of the Hyatt Regency.

“The amount of natural gas that is tied up in methane hydrates beneath the seafloor and in permafrost on Earth is several orders of magnitude higher than all other known conventional

sources of natural gas — enough to meet our energy needs for several decades,” Mahajan says. But extracting this resource poses several challenges.

For one thing, methane hydrates — which are ice-like cages made of water molecules surrounding individual methane molecules — are only stable at the very low temperatures and high pressures present at the ocean floor. “If you try to bring it up, these things fizzle and decompose, releasing the trapped methane,” Mahajan says.

So a multi-agency team led by the Department of Energy — as part of its mission to secure America’s future energy needs — is trying to learn about the conditions necessary for keeping hydrates locked up so they can be extracted safely and tapped for fuel.



Devinder Mahajan (left) and Michael Eaton

Mahajan’s group has built a vessel that mimics the seafloor temperature and pressure conditions, where they can study the kinetics of methane hydrate formation and decomposition. Unlike other high-pressure research vessels, the Brookhaven apparatus allows scientists to interchange vessels of different volumes, study even fine sediments, and visualize and record the entire hydrate-forming event

through a 12-inch window along the vessel. In addition, mass-balance instrumentation allows the Brookhaven group to collect reproducible data in the bench-top unit. Even better, Mahajan says, they can study the kinetics in actual samples of sediment that once contained hydrates — as close to the natural conditions as you can get in a lab.

“You fill the vessel with water and sediment, put in methane gas, and cool it down under high pressure. After a few hours, the hydrates form. You can actually see it. They look like ice, but they are not. They are stable at 4 degrees Celsius,” he explains.

One further advantage of doing this work at Brookhaven Lab is that the scientists can use the NSLS — a source of intense x-rays, ultraviolet, and infrared light — to measure physical characteristics of the sediments under study. Using x-ray computed microtomography, the scientists gain information about the porosity and other physical characteristics that may affect the availability of nucleation sites where hydrates can form.

Such data about hydrate formation in natural host sediment samples are scarce. By studying different samples and learn-

ing what combinations of pressure and temperature keep the methane locked up, the scientists hope to identify ways to compensate for the changes the hydrates experience as they are brought to the ocean’s surface so they can be extracted with a minimum loss. The comparisons of different sediment samples might also help pinpoint the most abundant sources of locked-up methane.

“It may be at least a decade before we can even think about mining these deposits, but answering these fundamental questions is certainly the place to start,” says Mahajan, who holds a joint appointment as a Stony Brook University professor. “This is a very important issue tied to our future national energy security.”

This research was initially funded by Brookhaven’s Laboratory Directed Research and Development program and is now funded by the Department of Energy’s Office of Fossil Energy. The symposium on Gas Hydrates and Clathrates was co-sponsored by the Petroleum and Fuel Divisions of the American Chemical Society.

— Karen McNulty Walsh

## Ceria Nanoparticle Experiments at NSLS Promise Cleaner Fuel Future

March 15, 2005

Experiments on ceria (cerium oxide) nanoparticles carried out at BNL may lead to catalytic converters that are better at cleaning up auto exhaust, and/or to more-efficient ways of generating hydrogen — a promising zero-emission fuel for the future. Jose Rodriguez of the Chemistry Department presented results from two studies exploring the composition, structure, and reactivity of these versatile nanoparticles during the 229th National Meeting of the American Chemical Society on March 15 in San Diego, California. This research was funded by the Office of Basic Energy Sciences within DOE’s Office of Science.

After using a novel technique to synthesize the ceria nanoparticles, Rodriguez and coworkers Xianqin Wang and Jonathan Hanson, also both of Chemistry, used beams of x-rays at the NSLS to study how their composition, structure, and reactivity changed in response to doping with zirconium in one case, and impregnation with gold in another.

“In a catalytic converter, ceria acts as a buffer, absorbing or releasing oxygen depending on the conditions of the engine to maintain the catalyst in its optimum operating condition for converting harmful emissions such as carbon monoxide and nitrogen oxide to carbon dioxide and nitrogen gas,” Rodriguez said. Others have found that adding zirconium improves ceria’s ability to store and release oxygen.

The studies at the NSLS explain why zirconium changes



Jonathan Hanson

the ceria's structure to increase the number of oxygen "vacancies" — or places for oxygen uptake and release.

Furthermore, Rodriguez said, "The ceria nanoparticles we studied have much better performance, higher chemical reactivity, than the bulk form of ceria currently used in catalytic converters."

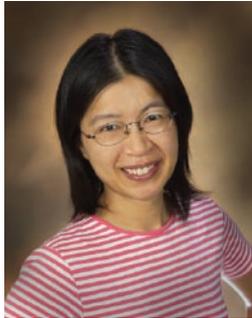
Thus, this research holds promise for more efficient catalytic converters — and cleaner air.

In the second study, Wang, Hanson, and Rodriguez deposited gold on the surface of ceria nanoparticles and used x-rays at the NSLS to determine the catalyst's "active phase" — the conformation responsible for the catalytic activity — in the conversion of water and carbon monoxide to hydrogen gas and carbon dioxide.

This "water-gas shift" reaction is important for generating hydrogen, which can be used for chemical transformations and as a fuel in a hydrogen-based economy. Hydrogen is one of the leading energy sources being investigated by scientists sponsored by DOE as part of its mission to ensure the nation's future energy needs.

"In both cases, we are learning about the fundamental conditions necessary for optimal operation of the catalysts," Rodriguez said. "This kind of knowledge eventually will lead to a rational design of even more effective catalysts."

— Karen McNulty Walsh



Xianqin Wang



Jose Rodriguez



Tom Seda

supplies the initial high energy electrons for the NSLS.

While Seda has not yet worked on plumbing on the job, he has constructed and programmed a single-chip programmable logic device (PLD) to handle the timing that controls the Linac's electron gun. The PLD replaces three logic chassis that control the release of electrons from the electron gun, the origin of electron bunches for x-rays, infrared light and ultraviolet light for experiments at the NSLS.

Seda is now a senior technical specialist assigned to the Operations Group at the NSLS and his primary task is to work on a new design for the extraction magnets of the NSLS Booster Ring. The current magnets — which kick electron bunches at an energy of 800 MeV into the NSLS storage rings, where the energy is ramped up to 2.8 billion eV — are encased in a vacuum chamber.

"The problem with the current design is the short power pulse has to be fed through long conductors to get into the vacuum-encased pulse magnet, known as a kicker. That's not an efficient way to bump the beam," Seda said. "I'm going to try to redesign the system with the pulse magnet outside the vacuum chamber. That would make storing the beam much less troublesome."

The kicker magnets date back to 1983, when the Booster was built, and they are constructed with the standard ferrites that were available at the time. Seda is now investigating newer ferrites for these magnets — specific ferrite alloys currently manufactured for the next generation high-energy accelerators. "We may be able to reconfigure our current bunch patterns with the faster kicker magnets," he said.

"I'm researching the current papers on kicker designs as well as speaking with the scientist and design engineers at other national laboratories," said Seda. "They have been very helpful in identifying vendors who may have the materials and manufacturing skills needed for the new design."

In the past, Seda had constructed and tested a new modulator for the Deep Ultraviolet Free Electron Laser energy upgrade, and he worked on two klystron units in the accelerator Test Facility, which supply RF power to a linear accelerator for advanced laser experiments. Among his suggestions was to replace the PCB-contaminated oil in the klystrons with biodegradable oil.

## What Do You Do At Work?

### Tom Seda: Bringing Bright Ideas to the Light Source

March 18, 2005

*This story was the first in a series entitled "What Do You Do at Work?" featuring BNL employees and their jobs at the Lab.*

When I first came to BNL in 1992, I was told that I'd be working on everything from plumbing to programming," said Tom Seda, then a principal technician for the Power Systems Group at NSLS, specializing in the Linac, the linear accelerator that

Seda also helped to test the Marx generator section of the Sandia Pulser Terra Watt Laser, which BNL tested for DOE's Sandia National Laboratory. For his exceptional job performance on this project coupled with helping recover the NSLS after only one week of downtime due to an equipment fire, he is a two-time winner of the BNL Spotlight Award.

"Working as a technician at the NSLS brings opportunities to be involved in all aspects of electronics, with the added benefit of being involved in interesting and ever-changing projects," Seda commented. "I love working firsthand with these amazing machines along with dedicated, talented employees who often go beyond what is expected of them on the job."

Born in the Philippines, Seda, who is of Puerto Rican and Filipino descent, immigrated to the Bronx, NY, with his family when he was an infant. The first in his family to earn a college degree, he received a B.S. in electronic engineering technology from the DeVry Institute of Technology, Chicago, Illinois, in 1988. He then worked as a technician at Magneto of Holtsville, NY, where his responsibilities included designing custom military-grade transformers and inductors, before he joined BNL in February, 1992.

Seda is married to Anna Seda, an administrative assistant in the Energy Sciences & Technology Department. The couple has an 8-year-old son and a 2-year-old daughter. Tom Seda is the president of the BERA Camping Club, and both Anna and Tom Seda are participants in the BERA kickboxing class offered on site. In addition, he and his wife enjoy traveling abroad and going on cruises.

— Diane Greenberg

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## Brookhaven Town Honors Two BNL Scientists

March 22, 2005

Two BNL scientists — Rita Goldstein and Lisa Miller — were among 11 women honored for their accomplishments at the Brookhaven Town-sponsored Women's Recognition Night at Brookhaven Town Hall on March 22. Goldstein and Miller were recognized for their contributions to science in the Town ceremony, which celebrates National Women's History Month.

Lisa Miller, a biophysicist at the NSLS, uses infrared light and x-rays at the NSLS to study the chemical composition of bone tissue in diseases such as osteoarthritis and osteoporosis. She also investigates protein-folding diseases, such as Alzheimer's disease and scrapie, the sheep form of mad cow disease, in which specific proteins in the brain fold into incorrect shapes and cause damage to brain cells.

Miller also plays an important role in science education and the public understanding of science. She often mentors students from high school to the postgraduate level. In addition, Miller

is responsible for outreach activities on behalf of the NSLS, including publications, the website and tours. For example, she organizes an annual open house at the NSLS for BNL's Summer Sundays, when the Lab's facilities are open to the public.

"I am very pleased to receive this honor from Brookhaven Town," Miller said. "I'm glad that my research is recognized, and I am happy that many of the students I've mentored have chosen to pursue scientific careers."

Miller earned a B.S. in chemistry from John Carroll University in 1989, an M.S. in chemistry from Georgetown University in 1992, and a Ph.D. in biophysics from the Albert Einstein College of Medicine in 1995. After serving as a postdoctoral fellow at Lawrence Berkeley National Laboratory and BNL, she joined BNL in 1999 as an assistant biophysicist, and she was promoted to biophysicist in 2003. Since 2002, she also has been an adjunct assistant professor in Stony Brook University's Department of Biomedical Engineering.

This year, Miller was invited to serve on the scientific advisory committee of the Canadian Light Source, a role served only by world-class scientists. For her work with students, Miller received DOE's Outstanding Mentor Award in 2002.

— Diane Greenberg



Lisa Miller

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## EnviroSuite: Environmental Science at the NSLS

March 30, 2005

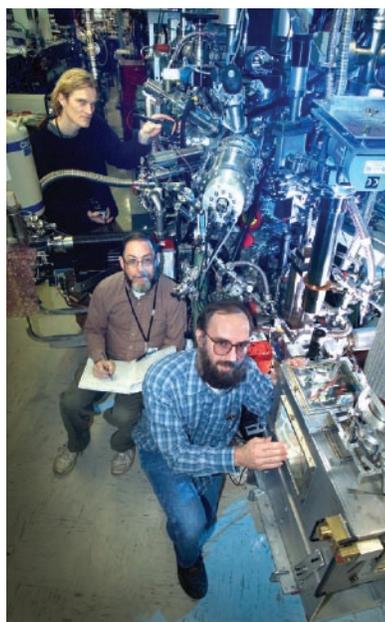
Created in response to rapidly growing interest in environmental synchrotron science, the EnviroSuite Strategic Initiative is designed to support and develop a suite of state-of-the-art resources at the NSLS for molecular environmental science research. Its mission is to optimize and expand synchrotron-based techniques for exploring environmental questions, to establish substantial involvement in several beamlines to bring a multifaceted approach to complex environmental processes, and to introduce new users to these capabilities at the NSLS. EnviroSuite now provides a unified voice for the diverse community of environmental science users.

EnviroSuite is coordinated by the Environmental Research and Technology Division of BNL's Environmental Sciences Department, and is funded by the DOE Office of Biological & Environmental Research, Environmental Remediation Sciences Division (BER:ERSD). Similar programs have been initiated

at all four DOE synchrotron facilities. Its BNL core consists of a number of environmental scientists, who work closely with the NSLS and with CEMS, the NSF/DOE-funded Center for Environmental Molecular Science based at Stony Brook ([www.cems.stonybrook.edu](http://www.cems.stonybrook.edu)).

EnviroSuite is taking an active role in both PRT and NSLS facility beamlines, in order to direct the course of beamline development and harness the resources to conduct leading research. As a result, both capital funding and scientific staff have been brought to the NSLS. Some of these are described in more detail below. In addition, a key goal of the EnviroSuite program is to establish the framework for multi-beamline studies, such as combining bulk EXAFS with microspectroscopy and imaging of elemental and species distributions.

NSLS facility beamline X27A, a new hard X-ray microprobe beamline, was highlighted in the December 2004 NSLS Newsletter. It has a  $5 \times 15 \mu\text{m}$  spot size at 3.5 - 32 keV, a 13-element solid state detector, and control software modeled after the beamline X26A system. EnviroSuite collaborated with the NSLS, X26A, and CEMS for the design and commissioning of X27A, and provided the detector. This beamline will greatly increase available microbeam resources at the NSLS. Environmental applications include X-ray fluorescence microanalysis of trace elements, mapping of their distribution, and microspectroscopy.



Environmental scientists (from left) Jeff Fitts (EnviroSuite Coordinator), Mark Fuhrmann (X11 Spokesperson), and Paul Northrup (X15B Spokesperson) at the X15B end station.

Beamline X11 is one of the most scientifically productive and historically important beamlines at the NSLS, being used primarily for bulk EXAFS experiments. It has an unfocused beam ( $0.5 \times 10 \text{ mm}$ ), and operates in the energy range from 4.5 - 35 keV. It is versatile, and can accommodate a variety of sample types as well as in-situ studies. EnviroSuite is adding a new 13-element Ge detector to X11A, to enhance its capabilities for low-concentration and otherwise challenging environmental samples. Detector capability at X11B will also be upgraded.

Beamline X15B is designed for low- to medium-energy bulk and surface XAS (optimized for 1.7 - 5 keV). It has a 1 mm focused spot size, and can address samples in ultra-high vacuum or air/He atmosphere. Current research includes phosphorus, sulfur,

and silicon K-edge, cadmium L-edge, and uranium and lead M-edge spectroscopy.

Beamline X1A is a soft X-ray beamline used for scanning transmission x-ray spectromicroscopy. Its primary emphasis is on organic materials at the carbon and oxygen absorption edges. With a resolution of  $\sim 30 \text{ nm}$ , X1A is well-suited for imaging molecular chemical features on a sub-cellular scale, such as for research exploring mechanisms of biotransformation of radioactive and toxic species. Recent upgrades include a BER: ERSD-funded laser interferometer.

EnviroSuite provides guidance for new and experienced general users with environmental science research at these and other beamlines. BNL Environmental Science Department resources include laboratory facilities for handling radioactive and hazardous materials and wastes, and for sample preparation. Experimental protocols are being developed to facilitate safe handling and analysis of samples containing radionuclides. For further information, see the EnviroSuite web page ([www.bnl.gov/envirosuite](http://www.bnl.gov/envirosuite)) or contact Jeff Fitts ([fitts@bnl.gov](mailto:fitts@bnl.gov)).

— Paul Northrup

## Crystallographers Bloom at RapiData 2005

April 5-11, 2005

Once again in the spring, nearly 50 budding crystallographers from around the world gathered at Brookhaven National Laboratory for RapiData 2005, a week-long course designed to introduce students to the best people, newest equipment, and latest techniques in the field of macromolecular x-ray crystallography.

The course is offered annually by Brookhaven's Biology and NSLS departments, and is always a successful event for participants and instructors alike. In 2005, it ran from April 5 to 11.

The course began with two days of lectures and tutorials taught by scientists from Brookhaven, industry, academia, and other national labs. Then, the instructors and other participants guided the students through a marathon, 60-hour data-collection session on eight NSLS beamlines. Half of the 48 students came with their own specimens to analyze, while the other half learned as observers. Six students left with solved structures that may be publishable in scientific journals.

The course was organized primarily by Bob Sweet and Denise Robertson of Biology. However, they emphasize that its success absolutely depended on enthusiastic help from most of the 24 members of the PXRR (the Biology and NSLS Macromolecular Crystallography Research Resource), NSLS staff members, and several outside teachers.

The majority of the funding for the course comes from the National Institutes of Health's National Center for Research Resources and the Office of Biological & Environmental



Participants in the RapiData 2005 Macromolecular Crystallography course

Research within the U.S. Department of Energy's Office of Science. Additional support is provided by the NSLS and several equipment vendors and drug companies. For more information, go to: [www.px.nsls.bnl.gov/RapiData2005/](http://www.px.nsls.bnl.gov/RapiData2005/)

— Laura Mgrdichian

## CFN Site Dedication Draws Special Guests to the NSLS

April 15, 2005

Several distinguished guests visited the NSLS on April 15 as part of activities for the Center for Functional Nanomaterials (CFN) site dedication ceremony. The guests included Congressman David Hobson, Chairman of the Energy and Water Development Appropriations Subcommittee in the House of Representatives; Congressman Tim Bishop; DOE Office of Science Director Raymond Orbach; and Patricia Dehmer, Associate Director of the Office of Basic Energy Sciences within the Office of Science.

After a welcome by NSLS Chairman Steve Dierker, the group gathered in front of the lobby viewing window, which gives an impressive view of the VUV experimental floor. Dierker then gave an overview of the NSLS and its research. He also discussed the bright, new light source proposed at Brookhaven Lab, NSLS-II, and how the new synchrotron would act as a sister facility to the CFN, complementing and enhancing the nanoscience research to be done there.

On this key theme, Hobson mentioned the cutting-edge, third-generation synchrotrons that exist or are under construction in several other countries. "Nanoscience is a whole new era," he said, that requires advanced machinery. In response, Dierker discussed how NSLS-II would take the U.S. to the forefront of synchrotron science and nanoscience. For example, NSLS-II would use CFN instrumentation to focus its beams down to

very small sizes, enabling studies of nanowires, which are the basis for a new class of electronic circuits.

"NSLS x-rays can't get down to the nanoscale," said Dierker. "We need a powerful new photon microscope, a new technology for a whole new industry."

He continued, "It is the remarkable behavior of materials at the nanoscale that is thought to hold the key to the future of United States energy problems. NSLS-II will give us the tools we need to regain world leadership in this area."

Later, at the site dedication ceremony, the CFN site sign was unveiled by several of the invited dignitaries and BNL leaders. A crowd of BNL employees came out to participate in the event and, after a welcome by Lab Director Praveen Chaudhari, heard remarks by Hobson, Bishop, and Orbach.

In his talk, Orbach touched on NSLS-II and its planned relationship to the CFN. "Think of the two as a team," he said. "Without both, we will be robbed of opportunities that they uniquely can bring. NSLS-II will give us a leg up on every other laboratory in the world."

He also had an important message: "We need to convey to the public what science can and will do, to convey to everyone the nature of scientific enterprise and scientific discovery," he said. "What we're doing here today is conveying that message in a whole new era of opportunity. No one knows the dimensions of discoveries that are present."

"Research into nanomaterials is one of the most exciting things since the microchip," said Hobson. "Right here at Brookhaven, you're getting to be in the middle of that."

Hobson also praised BNL for its status as a basic-energy research lab, stressing that basic research is an essential, but waning, component of U.S. science. "The [DOE] labs are the last areas of basic research in our country," he said. "You should all be very proud of what you're doing."



From left, NSLS Chairman Steve Dierker, Congressman Tim Bishop, Congressman David Hobson, DOE Office of Science Director Raymond Orbach, and BNL Director Praveen Chaudhari.

Bishop was equally supportive. “We have on this site some of the world’s best minds. The CFN will bring more of the best minds here, and Long Island will benefit from that.”

Among other distinguished guests invited to the Lab were Dennis Kovar, Associate Director for Nuclear Physics, who is also DOE landlord of the BNL site; Michael Holland, Manager of DOE’s Brookhaven Site Office; Vice Admiral Dennis McGinn, who is Vice President for Strategic Planning for Battelle; and Robert McGrath, SBU Provost and Executive Vice President for Academic Affairs, who also serves as SBU Vice President for Brookhaven Affairs.

Earlier in the day, the special guests also toured BNL’s Relativistic Heavy Ion Collider and the Positron Emission Tomography facility to learn about the research performed at each. The keynote speaker at the luncheon preceding the event was Shirley Strum Kenny, Stony Brook University (SBU) President and also Vice President of Brookhaven Science Associates, an institution formed of SBU and Battelle, which manages BNL for DOE.

— Laura Mgrdichian

## Strain-Mapping Workshop Marked by Enthusiasm and Idea-Sharing

April 18-19, 2005

Useful, lively discussions characterized the recent workshop on Strain Mapping in Engineering Materials with High-Energy Synchrotron X-Rays, held at the NSLS from April 18-19. The workshop brought together researchers in the field of strain mapping to discuss their work and talk about how to advance NSLS strain-mapping capabilities. Some of the talks are summarized below.

Asuri Vasudevan, from the U.S. Navy’s Office of Naval Research, discussed how he works to extend and predict the life of aircraft and helicopters by studying “residual stresses” — the stresses within a material left over after a single or repeated use, which are caused by temperature or the material’s chemical environment. Residual stresses can cause cracks on surfaces that may be stable or unstable. Vasudevan is interested in studying these cracks, but said that the tools available to him limit the size of the crack he can study as well as the sample’s thickness and particular composition.

Mel Roquemore and Ruth Sikorski from the Air Force Research Laboratory addressed the potential applications of strain mapping to evaluate jet engine components. Their aims include using the determined stresses that occur within the engine components to predict and model how complicated engine systems will respond to duty-cycle loading. This information will help them determine how to increase the life of engine components.

Another key speaker was Roger Klaffky, who runs the X-Ray

and Neutron Scattering Facilities program within the U.S. Department of Energy’s Office of Science. He spoke about the DOE’s mission to advance nanoscience research for energy needs, and the advantages of x-ray diffraction in this respect. He also gave examples of current stress/strain research now being done at DOE national labs, such as studying why fractures occur over time in stents and how that process may be stunted.

Additionally, an overview of the NSLS beamlines and user community was presented by NSLS scientist Chi-Chang Kao. He laid out the NSLS three-to-five year plan, which aims to continue the growth of life and geo/environmental science user groups, and attempt to reverse the decline in materials and chemical science users. Other initiatives are to advance the biomedical imaging program here and develop a new nanoscience user base. But in the area of strain mapping using high-



Participants in the Strain-Mapping workshop

energy x-rays, Kao said the NSLS needs to win funding for a new end station dedicated solely to that field.

The scheduled discussion period at the end of the workshop, and the several smaller discussions in between, produced many ideas and ways to bolster the strain-mapping program at the NSLS. The participants compiled a “wishlist” of capabilities they would like to see at X17B1, which is where strain-mapping research is now performed, and described current limitations to their research. For example, they discussed how to decrease the time it takes to make a strain map, which is one limitation may now prevent industrial users from coming to the NSLS.

The group also talked about potential future beamline X17A, which could free up X17B1 to become a strain-mapping-only beamline. Currently, high-energy x-ray scattering and medical researchers share the limited beamtime at X17B1 with scientists in the strain-mapping program.

— Laura Mgrdichian