BNL/SBU Internal Workshop on Future of NSLS-II
May 18, 2011, 1-6 p.m.
Hamilton Seminar Room, Chemistry Building (555)

Introduction:

About 125 Brookhaven Laboratory and Stony Brook University scientists and staff participated in an internal workshop to learn about the status and plans for the National Synchrotron Light Source II (NSLS-II) on Wednesday, May 18, 2011, at BNL. The workshop's purpose was to help us identify strategies for developing and enhancing research programs in the different areas of science at BNL and SBU that will benefit from NSLS-II's capabilities.

Attendees heard overview talks on the Laboratory's general vision and strategy, including the role of NSLS-II, a summary of NSLS-II status and plans, and a summary of the current state of the Lab's and SBU's science and technology (S&T) research interests (and collaborations) in using NSLS-II. During subsequent breakout sessions, workshop leaders solicited input for inclusion in the emerging strategies for developing, evolving, and positioning research programs to take maximum advantage of NSLS-II. Development of these strategies is being facilitated by a working group drawn from across BNL and SBU, including Allen Orville (ELS), Lisa Miller (PSD), Ron Pindak (PSD), Qun Shen (PSD), John Hill (BES), Jason Graetz (ST), Jose Rodriguez (BES), Lynne Ecker (GARS), Jeff Fitts (ELS), Ben Hsiao (SBU), Bob Haltiwanger (SBU), John Parise (SBU) and Doon Gibbs. The working group subsequently gathered the input from the breakout sessions and developed strategies for the further refinement of the developing NSLS-II based research programs as a part of the Laboratory's strategy for achieving its S&T missions. The results are presented here.

An executive summary describing the workshops main conclusions can be found at: http://www.bnl.gov/nsls2/workshops/05182011.asp. It is divided in 3 parts, including overarching observations, selected concerns (with actions) and additional strategies (and actions). The workshop agenda follows the executive summary. The individual reports from each breakout session follow the agenda. All slides may also be found at: http://www.bnl.gov/nsls2/workshops/05182011.asp

Executive Summary

Particular actions in bold are being followed up by us.

Observations

- Perhaps the largest benefit of the workshop, besides the information exchange, was the chance to engage SBU and BNL scientists with common interests. There was a lot of enthusiasm around these connections, and motivation for continuing the interactions. There was also a general benefit in a meeting that pulled such a diverse group together.
- The BNL/SBU community, at least as represented by those participating in the workshop, seem largely engaged in the NSLS II planning. There may be a few exceptions, but most

research areas seem to be represented and participating in the process--a very encouraging and positive result.

- The collective BNL/SBU science themes seem to be captured by the following list: correlated and magnetic systems, energy storage, extreme environment materials, soft matter and nanomaterials, catalysis/chemistry, earth and environmental sciences, structural biology, and biological imaging. However, more work may be needed to develop interests in systems biology--a DOE theme.
- Assuming all the approved beam lines are built, these would provide most of the capabilities needed by the BNL/SBU community. Nonetheless, there were capabilities missing from the NSLS-II suite of beam-lines, for example,

    - STXM imaging, which will be proposed in this year's BDP call. (now proposed)
    - Wide-field medical imaging and therapy, which will be proposed in this year's BDP call. (now proposed)
    - Ultrafast, time-resolved experiments (sub 50 ps resolution), neither as a dedicated beam-line nor in the exploration of timing modes for operations.
    - Polychromatic X-ray beams focused to a diameter of several microns create the opportunity to develop generalized time-resolved crystallography. This will require a new beamline, and a new specialized detector with large active surface area, high resolution energy discrimination, very fast speed and small pixel size.
    - Further coordination of efforts between the NSLS (NSLS-II) and CFN User Facilities would be mutually beneficial to both facilities.
    - It is worth following up the workshop with further meetings, but these might be smaller and centered on the breakout sessions. The next set of meetings could be held at SBU.

Concerns/Actions

A number of general concerns were expressed, including:

- Whether there will be sufficient capacity (or beam time available) at NSLS II to accommodate all existing and planned research programs. This is felt particularly strongly for "routine" experiments, e.g., macromolecular crystallography, powder diffraction or absorption spectroscopy, which attract many users during full operations.
- Lack of beam time during the transition period.
- The possibility that not all approved beam lines will be funded, leaving gaps in needed capability.
- Lack of lab space that will be available in the initial build out of the LOBs, including associated infrastructure and hardware. (Progress made: All LOBs have to be built out; to be fit out by BNL.)
- Limited or loss of access to workhorse beam-lines (e.g., fast powder x-ray diffraction) due to constricted funding.
    - **Actions**

        - With regard to the Concerns listed above, the Working Group recognizes that the Laboratory and NSLS II management are actively seeking to mitigate their possible impacts directly, or by working with the DOE. In addition to that activity, we encourage outreach by the Lab/NSLS II to other synchrotron sources to formalize, if possible, the shared use of these facilities the transition period (as was done, eg, at NSLS during the upgrade of SSRL). It might be possible to broker arrangements with overseas laboratories as well. (Erik Johnson in touch with other SR directors)
        - We also suggest that the Laboratory, both the core programs and the facilities, consider the possibility of miniature sabbaticals for affected staff, or other arrangements, involving several week to multi-month visits at other Labs with appropriate sources. These might be funded internally using Lab funds, but it also might be possible to interest DOE programs in collaborative arrangements provided they are set up in a way that mutually benefits all. (Still to be acted on)
        - Finally, the working group offers its own expertise, either in an advisory capacity, or in other ways to help if the Lab management sees ways in which we could be of use in any of these areas.
    - These recommendations have been made to the Science ALDs at BNL responsible for the PS, BES, ELS and GARs directorates.

Additional Strategies/Actions

We propose consideration and refinement of a number of additional strategies, involving actions, both on the part of BNL/SBU management as well as ourselves. We're interested in iterating with BNL/SBU management on these ideas.

- BNL/SBU should consider forming an energy storage consortium, similar to the synchrotron catalysis consortium that would develop common instrumentation, e.g., sample holder/cells, software and detectors that could be shared at the relevant beamlines. A similar proposal was brought forward by the Extreme Environment Materials session.
    - **Actions**
        - On energy storage and extreme environment materials, Jason Graetz and Lynne Ecker will, respectively,
            - Identify possible consortium members
            - Identify key workhorse beam-lines and techniques
            - Solicit feedback for shared instrumentation (sample holders/electrochemical cells, software, detectors, ...) and prioritize.
            - Create consortium white paper
            - Iterate with ALD on path forward
    - **Status** – A second energy storage workshop being planned; extreme environment consortium is at organization stage.
- NSLS II should enhance its efforts for remote access to beam-lines by biological crystallographers, industrial users, and participants in educational outreach programs.

- **Action**
    - We will invite Qun Shen, or designee, to speak to the working group – either describing what NSLS-II is already doing in this regard, or by opening a discussion about a path forward.
- **Status** – Still to be done.

- If not already underway, NSLS II or BNL/SBU should consider forming separate consortia for NSLS II advanced detectors, computing and data handling transfer needs.
    - **Actions**
        - Computing - Razvan Popescu is already working with a Laboratory wide working group developing a high level perspective of computing and data handling needed for NSLS-II. We suggest further that a similar Laboratory wide working group be formed by Bob Dalesio (NSLS-II) for data visualization and analysis needs to ensure coordinated and cohesive efforts among the different scientific focus areas.
            - **Status** – Underway.
        - Detectors - Pete Siddons is already working with the instrumentation division to develop novel detectors for NSLS-II.
            - **Status** – Underway
        - Another suggestion is that Popescu, Dalesio and Siddons meet with Walt Copan and the GARS directorate to explore possible commercialization efforts involving computing or detectors.
            - **Status** – Initial meeting.
- The Laboratory should consider taking the lead on arranging access to NSLS II for proprietary
    - **Action -** Qun Shen, Walt Copan, or designees
    - **Status** – Initial discussions on access underway with pharma
- Funding for biological beam-lines will require involvement from non-BES agencies, most notably NIH and DOE-BER. The Laboratory, including both the ELS and PSD directorates, and SBU, including Arts & Sciences, Engineering, and the Medical School, should work together to develop strategies for programmatic funding that includes NSLS-II beam-line capabilities.
    - **Action -** Together with NIH and BER, BNL and SBU should hold a workshop on biological imaging to explore the various options for biological imaging that will take advantage of NSLS-II characteristics while serving the largest user community and executing the highest impact science.
    - **Status** - Underway
- The Laboratory should consider spearheading a consortium or group centered on the production and complementary (and non-synchrotron) characterization of biological samples for NSLS II users. Similar comments are possible for the synthesis and characterization of samples for soft and hard condensed matter experiments, possibly taking advantage of expected calls for proposals from DOE/BES expected this year and/or outreach to universities.
    - **Action –** An LDRD for a "protein factory" for biological samples has been submitted to the Laboratory by ELS.

        - **Status** – LDRD proposed
    - **Action** – The Working Group will get input from respective ALDs of the BES, GARS, and PSD directorates on how best to proceed on "hard" condensed matter.
        - **Status** – Under discussion
- BNL/SBU should jointly develop educational programs for learning how to use synchrotron beam-lines, including summer schools.
    - **Action -** Working Group will iterate with Kathy Nasta and Gary Halada on possible paths forward.
    - **Status** – Initial proposal submitted; more to be done, eg. Working with APS, SSRC, etc.
- A centralized laser set-up and improved distributed timing signals of appropriate resolution would significantly improve the capability for time-resolved experiments.
    - **Action** - NSLS II should consider a concrete proposal for timing modes, including early, close coordination with users. NSLS II should also consider a strategic hire to coordinate between the experimental and accelerator divisions to address these questions and ensure that there are appropriate time-resolved facilities. John Hill and Qun Shen, or designees, will meet with respective ALDs and propose a path forward.
    - **Status** - Underway
- A working group should be formed to continue to explore ways in which the CFN and NSLS-II could work together more effectively. Possible participants: Ron Pindak, Chuck Black, Eric Stach and Oleg Gang. Ron Pindak will coordinate first steps.
    - **Status** – Underway
- The current Working Group should determine how it can foster the concept of 'Science Villages'. This concept has been enthusiastically welcomed by the NSLS-II user community but has only been implemented at the level of co-locating beam-lines with LOBs. There are a number of open questions concerning how to take the 'Science Village' concept to a higher level to enhance productivity of the different NSLS-II scientific user communities. In particular, what role should the BNL/SBU departments play in the process?
    - **Status** – Qun, or designee
- JPSI could play a role in many of the proposed strategies noted above.
    - **Action -** Doon Gibbs/Ben Hsiao will follow up with a proposal for JPSI
    - **Status** – Underway

Agenda
Laboratory Overview (Doon Gibbs, 30 minutes)

- Laboratory Vision/Strategy
- Priority Initiatives, including NSLS-II
- How NSLS-II Fits In Larger Laboratory Agenda
- Emergent BNL/SBU Research Themes
- Role of NSLS-II Working Group

NSLS II Overview (Qun Shen, 45 minutes)

- Project Status
- NSLS-II Capabilities
- Planned Beam-lines, End-stations, Schedules
- Connection of Planned Beam-lines to Emergent BNL/SBU Research Themes
- Access Policy
- Beamline Advisory Teams
- Early Science Experiments

Hsiao, Parise, Haltiwanger on SBU Interests (Ben Hsiao, Chair, SBU Chemistry; John Parise, Geoscience; Laszlo Mihaly, Chair, SBU Physics; Michael Dudley, Chair, SBU Materials Science and Engineering, Robert Haltiwanger, Chair, SBU Biochemistry; and Clint Rubin, Chair, SBU Biomedical Engineering, 20 minutes)

- Overview
- Status/Path Forward
- Physical Science Themes
- Life Science Themes

BNL Research Interests (5 minutes each): These talks will summarize Laboratory interests, capabilities, and connections to NSLS-II plans and needs in the indicated theme areas. More detailed discussion will follow in the break-out sessions.

- Structural Biology (Allen Orville)
- Biological Imaging (Lisa Miller)
- Soft Matter/Nanoscience (Ron Pindak)
- Condensed Matter Physics, Materials Science—correlated systems (John Hill)
- Condensed Matter Physics, Materials Science and Engineering/ Chemistry—Energy Storage (Jason Graetz)
- Chemistry/Catalysis (Jose Rodriguez)
- Materials Science and Engineering—Extreme Environment Materials (Lynne Ecker)
- Earth and Environmental Science (Jeff Fitts)

Examples of the kinds of questions discussed in the breakout sessions include:

- What is the expected usage of the currently planned beamlines by the existing research programs and personnel at SBU and BNL?
- Are there opportunities to enhance BNL/SBU representation in the areas of interest among the existing six NSLS-II beam-line advisory teams?
- Is there a need to propose additional beam-lines (beyond those already approved) to provide additional capabilities needed to meet the current and emerging challenges identified by the BNL and SBU community?
- What other infrastructure is needed at either BNL or SBU (besides NSLS-II) to attract and support the S&T communities that will utilize NSLS-II.
- What are the areas of strength for personnel in the existing research communities at BNL/SBU and what are the most pressing needs for additional expertise or personnel in order to mount leading research initiatives utilizing NSLS-II?
- What are the most effective strategies for strengthening the BNL/SBU research community (eg, strategic hires, partnerships, etc.), including leveraging industrial collaborations, especially in NYS?
- What are the funding opportunities to foster and support innovative, high-risk-high-reward R&D that benefits from utilization of NSLS-II at BNL/SBU? How do we nurture new communities and/or new investments by these communities in research at NSLS-II?

Comments on new aspects of the User Access Policy

Breakout Session Reports

Soft Matter / Nano-materials - Ron Pindak

Advancing Soft Matter & Biological Physics Science at NSLS-II

- **Participation** -- workshop attendance indicated that the community both at BNL and SBU were engaged in planning for NSLS-II. The workshop participants included: *from BNL* - Alessandro Cunsolo, Oleg Gang, Dmytro Nykypanchuk, Kevin Yager, Elaine DiMasi, Andrei Fluerasu, Ron Pindak, David Shapiro, Vesna Stanic, Masa Fukuto, Ben Ocko and *from SBU* - Christian Burger, Barney Grubbs (joint appt), Juliet Hahn, Ben Hsiao, Tadanori Koga, Miriam Rafailovich, Helmut Strey.
- **Missing beamlines** -- the soft matter and biological physics research communities are weak on *imaging* beamline facilities
  - It was recommended that as a near-term solution NSLS-II should instrument CSX and CHX to do soft and hard x-ray CDI imaging in the early phase of beamline operations**.**
  - The community backed promoting the establishment of a STXM facility at NSLS-II (the undulator-based facility has advantages for pushing frontiers in imaging but a work-horse bend magnet facility was equally valued – community supports both).
  - It was recognized that there is an additional need for a high-energy scattering beamline for studying buried interfaces and device structures, the SMB community should participate in a BDP led by another research community for a high-energy beamline (superconducting wiggler best) that could accommodate this facility.
- **Beamline capacity --** especially for work-horse techniques, was a concern.
  - It was recommended that a working group be established for developing an NSF Instrumentation proposal to fund the development of automated high-throughput sample handlers so users can make more effective use of limited beam time.
  - It was also recommended that the community should explore opportunities for funding the split of SMI into two independent branch beamlines thereby doubling the available beam time.
- **Infrastructure - lab and endstation hardware** -- there was a clear need identified for laboratory space adjacent to the beamlines. This is particularly important to facilitate sample preparations for the high-throughput facilities, for safe nanoparticle handling, and for handling environmentally sensitive samples. For the NSLS-II beamlines to meet their scientific potential it is also crucial to have advanced endstation instrumentation. Some of the specific needed instrumentation included:
  - Instrumentation to enable CDI on NSLS-II Project beamlines (cyro-sample cooling station and fast detector for soft x-ray CDI). Note: not only is the ability to prepare frozen samples needed but also the ability to transfer them to and maintain them in the experimental chamber.
  - Piezo driven diamond anvil cells (dDACs) & pulsed laser heating synchronized with x-ray pulses to study soft matter material dynamics at IXS.
  - Cell culture laboratory, i.e. CO2 incubator, BSL-2 hood near the soft matter and biological physics beamlines for sample prep

- Chamber for in-beam studies of living cells and surface adsorbed proteins with temperature and CO2 control. This chamber would be most useful on a beamline for studying buried interfaces, i.e. water/cell membrane interface.
- A Brewster Angle Microscope setup for the liquid surface scattering community

- **Infrastructure - support staff --** there was also a need identified for an accessible programmer, working full time solely for the soft matter and biological physics communities. The goal is intelligent, customizable visualization and analysis software.
- **Strategic hires** -- SBU/BNL currently lacks local research expertise in several key areas. This deficiency requires the use of external collaborators for proposals addressing grand science challenges. External collaborators do not always have BNL/SBU needs as a first priority so can impede progress.
  - SBU lost 2 research leaders in imaging (Jacobsen & Kirz) – there is an obvious need to rebuild this expertise since the brightness of NSLS-II enables world-class imaging facilities.
  - There is a surprising lack of faculty with a soft matter and/or biological physics research interest in the SBU *physics* department. This is a lost opportunity given strength in this expertise at BNL that provides potential collaborators and mentors.
  - Both BNL and SBU are weak in organic material synthesis - with the only exception being the recent addition of Barney Grubbs. The weakness in synthesis would be fatal for a soft matter and biological physics research center, since the interest in soft matter as materials of the future arises largely from the ability to precisely control the chemical structure of soft matter, which is essential to both directing assembly (structure) and imparting functionality (property). A major problem here is in identifying what area to focus on, in view of the diversity of soft matter and biomaterials. It may be a good idea to take a survey to identify what type of synthetic capability the local soft matter and biological physics community could benefit most from.
  - Soft matter and biological physics theory is another weakness with only Alexei Tkachenko (CFN), doing phenomenological theories for DNA-nanoparticle and hierarchical assembly. The local soft matter and biological physics community is likely to benefit from an additional theorist possibly at SBU.
- **Strengthening industrial collaborations** -- it was recommended that workshops focused on applied topics (like batteries or organic photovoltaics) be continued to engage industry and EFRC or NSF applications-oriented center researchers in collaborative projects – *but this requires seed funding to involve students or postdocs in the collaborative projects with industry*.
- **Funding opportunities** - - Ben Hsiao is heading an effort to prepare a proposal for an NSF Advanced Photon Sciences and Technology Center for Materials. The center would fund professional staff and students to develop the advanced endstation instrumentation and data visualization and analysis software needed for the NSLS-II programs in the physical sciences. This is the first major science proposal leveraging the world-leading capabilities of NSLS-II so will 'test the waters' regarding what engages the NSF program managers.
- **Next step in establishing a Soft Matter and Biological Physics Village** -- the local scientists need to interact more, so that everyone is aware of the others' activities. This may be accomplished by establishing a BNL-SBU soft matter and biological physics forum in which local researchers (or visitors) can present their recent work. It could be a seminar series or a regular but informal workshop. The latter can be just a few hours in one afternoon

per workshop, 3-4 times a year. (Doon Gibbs' workshop last week shows that local researchers can get together on relatively short notice if there is enough interest.) The challenge will be to do this effectively and keep up people's involvement without requiring a lot of preparation on the part of participants. Whatever the format, it would be hard to justify something like this unless the local soft matter and biological physics community is serious about developing into a center/hub/village.

CFN as an NSLS-II Partner User Facility

- **Opportunity for coordination** -- better coordination between the two user facilities would benefit the nanoscience community. The concept of the CFN as a *Partner User Facility* was proposed and it was recommended that a working group be formed to explore avenues for coordinated activities.
- **General User proposal systems --** since the facilities engage users in somewhat different ways (a high percentage of the CFN users are collaborators), it was decided that the format of the CFN and NSLS-II GU proposals needed to be different. At the same time, it was also recommended that the facilities share a common user data base to facilitate collection of accurate user statistics. Finally, it was recognized that rapid access of both facilities was crucial to the nanoscience community and better coordination would help so both facilities could be used during a single visit..
- **CFN ancillary NSLS-II laboratory --** since there was a general need expressed by the soft matter and biological physics community for non-x-ray characterization and fabrication facilities adjacent to the experimental floor, the CFN proposed constructing and operating a ancillary CFN laboratory adjacent to the NSLS-II experimental floor with mid-range instrumentation like SEMs.
  - The ancillary laboratory would be staffed by experienced operators under CFN supervision
  - The operators would be knowledgeable in the advanced instrumentation within the CFN so could direct NSLS users this instrumentation.
- **CFN endstations** -- the existing NSLS CFN endstations (with upgrades) have transition routes to NSLS-II approved and funded beamlines. A new operando-XAS aberration-corrected TEM facility was proposed
- **NSLS-II beamline selection process** -- it was recognized that some proposals, like the TEM facility, are for endstations that don't warrant a full beamline so need to be partnered with another endstation. Choosing the correct partner endstation is an important part of getting a highly rated BDP. It was questioned whether this was the most effective mechanism for attracting the best endstation concepts. It was proposed to have a selection process for endstations as well as beamlines.
- **CFN as NSLS-II Partner User Facility -- s**upport 30% beam time for Partner Users and stressed the importance of PUs having a voice in NSLS-II executive decisions perhaps through a Partner User Committee that meets regularly with the Photon Sciences ALD.

Condensed Matter Physics and Materials Science—Correlated Systems: John Hill

1) There are two key infrastructure areas that need additional resources NOW, since they are both very long lead items. These could be “super themes” to the white paper since they

cut across all disciplines and extend beyond the facility in scope. For that reason, I would elevate them above the bullets under beamline instrumentation n Jeff's summary.

They are also lab strategy questions since they tie into the future of the Instrumentation Division, to collaborations with other national labs and to lab computing infrastructure.

They are

- Detector development. We identified two in particular. There are certainly more, even from our group, let alone the other groups. These are
    i. Fast pixilated detectors for soft x-ray
    ii. Pixilated, low noise, large dynamic range for soft x-rays

  A lab strategy would identify important detectors required, and the key technologies associated with them, and then either partner with other institutions (LBL is active for soft x-ray CCDs for example), or develop them in house. The individual beamlines do NOT have the money to fund this development (though they can buy the detector once it exists). Development money would need to come from other sources – Instrumentation Division funds for example.
- Data handling and analysis software. There is an LDRD proposal to begin to develop data handling code. This is currently being pushed through the life sciences directorate. That is fine, but it should be clear, from the start that there are many different data types and requirements and these should be kept into account right from the very beginning, so that we don't end up with a system that is optimized for – say – biological data and then adding other data types would be a kludge after the fact. If we are going to have centralized data handling it needs to work equally smoothly for everyone (a tall order)

  Along these same lines, there is a second LDRD, through the BES directorate this time, to fund software development for data analysis. At a minimum, these two efforts should be talking to each other and ensuring smooth data flow between the two. At a maximum, the lab could force these two efforts into a single group as part of a grand strategy on software development.

The other bullets were more specific to the strongly correlated session:

2) The first priority was to identify funding for the remaining approved beamlines relevant to this community, specifically:
   HIX, SSS, MET, MPP
3) Ultrafast time-resolved experiments (defined as sub 50 ps time resolution) are not currently well served at NSLS-II, neither in dedicated beamlines (there are none), nor in the exploration of timing modes for operations. This is a small community now at NSLS and hence has had little attention. However, it is growing rapidly world-wide and will only increase in growth as the FELs come online. NSLS-II cannot compete at those time resolutions, but there are other time windows where it could be highly competitive. Recommendations:

- PSD should make a strategic hire in this area to coordinate between experimental and accelerator divisions to address these questions and ensure there is appropriate time-resolved facilities for the users.
- Work out concrete proposals for timing modes for NSLS-II ops
- Centralized laser and improved distributed timing signals of appropriate resolution (not currently supplied) would significantly improve the capability for time-resolved experiments at NSLS-II.

4) Soft X-ray Absorption Spectroscopy is a technique that is currently missing. An LOI has been submitted for such a beamline in this current round. A BDP is being developed.

Structural Biology - Allen Orville

More than two-dozen people participated in the breakout session. Many of attendees also participated in the Imaging breakout session immediately afterward. It appeared that participation by SBU personnel was better than BNL; obviously absent were BNL Biology members that are NSLS users (with the exception of several members of the PXRR group).

Attendees of the structural biology breakout heard brief descriptions about the eight approved beamlines (funded LiX, NYX, FMX, and AMX; not funded XFP, XAS, ABS, and SM3). This includes macromolecular crystallography (MX), X-ray absorption spectroscopy, X-ray footprinting, and solution X-ray scattering. The breakout group expressed concern that all eight beamlines should be completed; therefore, support must be identified for the four beamlines without funding lines.

The SBU faculty members from the Biology, Biochemistry and Pharmacology departments were interested in promoting educational capabilities at the NSLS-II. They highlighted success with NSF and HHMI funding programs directed at undergraduate research and training opportunities. For example, the SBU Biology Department has a grant to enhance the research experience in structural biology within the context of the introductory biology class (approximately 2000 students). Some members of the BNL MX community currently participate in this outreach and support expanding its scope. Some discussion focused on the difficulties with obtaining experimental –*vs*– observational access to the NSLS experiment floor by the diverse student body of such a class. This led to talk about remote data collection as an emerging trend, which could be an effective way to accommodate students in the biology class. Thus, remote data collection, user access policies and BNL firewall issues intersect.

Many of the people in attendance were concerned that access to beamtime would become more difficult, especially since fewer beamlines will likely be available in the early years than is currently available at the NSLS. There was interest in creating a beamline devoted to educational outreach. There was interest in creating a beamline with a primary mission of novel methods development. SBU personnel asked about the potential for biosafety level 3 capabilities at NSLS-II. It was pointed out that BNL is currently only approved for biosafety level 2 facilities. It was also noted that time-resolved crystallography was not currently in the scope of any of the proposed beamlines for NSLS-II. There was a general pessimistic perception that funding strategies for all of these types of beamlines were not clear and likely to be challenging.

Nevertheless, many believe that a very high priority should be given to completing all the NSLS-II LOBs. The SBU and BNL participants anticipate that shared instrument grants could be an important strategy to fill the labs with equipment appropriate for the user base. There was enthusiasm for a BNL initiative to support a large-scale facility for gene to protein production to biophysical characterization.

The philosophy of multidisciplinary research was popular. Should there be cooperation between beamlines to promote the concept of a "universal" sample holder? Remote data collection will certainly require standardization of sample holder and automation, both of which are well accepted in the MX field, but much less so in other complementary disciplines.

Materials Science and Engineering—Extreme Environment Materials – Lynne Ecker

Overview: Dr. John Parise gave a short description of the Center for Advanced Photon Science and Technology (CAPST), each beamline spokesperson introduced their beamline using the Beamline Development Proposal slide and each attendee briefly stated their interests.
Dr. Parise mentioned that it is a unique opportunity to have the NSLS II in such close proximity to SBU and that it is a golden opportunity to plan for extreme environment experiments before the beamlines have been finalized. He is not aware of a facility participating in this type of up-front planning with the scientific community, but thinks it can be very beneficial.
Dr. Michael Dudley mentioned after the discussion session that he has filed a LOI for a new beamline entitled "Monochromatic/White Beam X-ray Topography and High Resolution Diffraction Beamline at NSLS-II (HXT)"

It was also generally agreed that the discussion questions were "big" questions and that we were only able to begin the discussion in the allotted time.

What is the expected usage of the currently planned beamlines by the existing research programs and personnel at SBU and BNL?

The community expects to use the project beamlines.
The high pressure community is planning to install some additional equipment, including flow cells, in a hutch at XPD. However, XPD is expected to be heavily oversubscribed and users are concerned about having a very highly competitive proposal process that will discourage new users and experiments and short beamtime allocations.

In addition, HXN can be utilized for post mortem examination of material after exposure to extreme environments and will be capable of imaging tens of atoms of high Z materials.

Are there opportunities to enhance BNL/SBU representation in the areas of interest among the existing six NSLS-II beam-line advisory teams?

This community felt adequately represented on the BATs.

Is there a need to propose additional beam-lines (beyond those already approved) to provide additional capabilities needed to meet the current and emerging challenges identified by the BNL and SBU community?

The community has four LOI[1] for this round of proposals and the National Security Department at BNL is actively looking for a beamline willing to give them a fraction of a high energy beam for their own endstation and hutch.

There was a call for more 3D high resolution diffraction capability. There was general agreement that being able to look at microstructures in 3D with 1 µm resolution and get the complete strain tensor and the phase and grain orientation would be very valuable.
In addition, an integrated capability for high Q-space (>30 A^{-1}), high angular (<0.1^{o}) and high spatial (nm-µm) resolution measurements with diffraction imaging at extreme conditions was called for.

What other infrastructure is needed at either BNL or SBU (besides NSLS-II) to attract and support the S&T communities that will utilize NSLS-II.

This discussion focused primarily on sample chambers to provide extreme environments. It was generally agreed that BNL should provide a basic set of sample environments that can be accommodated at many NSLS II beamlines. The difficulty of designing, building and using the cells was mentioned. The cells must meet NSLS II safety standards and are also considered pressure vessels and must meet the ASME pressure vessel code.

It was suggested that NSLS II should provide sample environments and support to users for these experiments at a facility level rather than at the individual beamlines, perhaps through a dedicated group or individual. The environmental chambers can be expensive, but are a good investment because they can accommodate various experiments over many years.

It was also generally agreed that NSLS II should accommodate users who bring their own sample environments. It was suggested that it may be possible to engage the science community and generate funds for sample environments that are expensive. The benefit to NSLS II of this approach is that the sample environment would remain at NSLS II rather than returning to the home institution of the user. This will allow NSLS II to grow new capabilities rather than perform one time experiments.

Comments from slides:

- Satellite building for easier transportation and handling of active samples
- Radioactive Materials Storage Area in another building to avoid exceeding activity limits at NSLS II
- Sample preparation area in another building for loading low level samples into containment (glove box)

[1] Two LOI were described using slides and another is mentioned in this document. The forth has been submitted by Trevor Tyson, New Jersey Institute of Technology, for "NSLS-II Beamline for Combined High Magnetic Field and High Pressure"

- Ability to accommodate different sample environments at the beamline

- Satellite building for easier transportation and accommodation of engineering scale experiments and components
- Common indexing capability between beamlines

What are the areas of strength for personnel in the existing research communities at BNL/SBU and what are the most pressing needs for additional expertise or personnel in order to mount leading research initiatives utilizing NSLS-II?

This was interpreted in several ways:

- In terms of expertise needed to mount leading research initiatives, BNL is lacking mechanical engineering expertise in areas of fatigue, fracture mechanics, corrosion and aging and degradation of materials.
- There was generally a request for more expertise in detector development, particularly high resolution detectors.
- There was also a request for improved software, particularly for the ability to access the data quickly and for on-line analysis capability so that results can be viewed rapidly enough for adjustments to experiments to be made during one beamtime. On-line analysis is also a priority for users that are traveling so that they are able to return to their home institutions with the results in-hand.
- In terms of facility support, technical support for the beamlines and facilities, such as the machine shop, is considered important especially in times of decreasing budgets.
- It was also recognized that the current beamline staff is pressed to provide support to users at the NSLS. For the more sophisticated sample environments and some of the increasingly complex experiments that are anticipated at NSLS II, more demands on the beamline staff are expected. More resources will be required to provide the additional support to users.

Comments from slides:

- Material scientist with extensive experience working in a facility that handles active samples

What are the most effective strategies for strengthening the BNL/SBU research community (e.g., strategic hires, partnerships, etc.), including leveraging industrial collaborations, especially in NYS?

The most straight-forward way to get new industrial users is “give them beamtime.” The difficulties industrial users have in accessing synchrotrons are that they need longer beamtime and beamtime guaranteed through multiple cycles. The new user access policy should better accommodate this. In addition, industrial users need to be able to collect proprietary data and on-line analysis of data. It was suggested that it may be easier for an industrial user to partner with SBU to use the NSLS II rather than using the NSLS II directly because the SBU researcher can better accommodate these requirements.

It was also suggested to run a summer school for industrial users to introduce them to the type of experiments that can be performed and to train them as users.

It was generally agreed that industrial users require additional support relative to academic users. Perhaps the industries currently using the NSLS would be willing to form a consortium to fund an "Industrial Users Support Office" staffed with someone with experience in interfacing with industrial users that could provide guidance from the proposal process to the data analysis, ensuring that industrial users were getting the access and results they need. (Does this already exist at NSLS?) Perhaps NY state or JPSI would be willing to fund this type of effort.

What are the funding opportunities to foster and support innovative, high-risk-high-reward R&D that benefits from utilization of NSLS-II at BNL/SBU? How do we nurture new communities and/or new investments by these communities in research at NSLS-II?
ARRPA–E

Comments on new aspects of the User Access Policy
The new user access policy is widely considered an improvement.

Catalysis/Chemistry - Jose Rodriguez

Chemical transformations and catalysis Breakout session:

Beamlines for doing experiments at the NSLS-II

- The number of beamlines available at the NSLS-II for doing experiments of X-ray powder diffraction, X-ray absorption spectroscopy and photoemission seems to be substantially smaller than the number of beamlines currently available at the NSLS. Where the so-called "routine" experiments will be done? Most (~ 70%) of the attendants to this Breakout session mentioned that they were mainly interested in doing "routine" characterization of samples.

Access and easy operation of the new facilities

- People was concerned of how difficult will be to get beamtime at the NSLS-II, the lack of a well-defined user policy and the possible lack of technical support for the operation of the beamlines.

Outreach programs to the universities and industry.

- Many potential users at universities and the industry are not well informed of the characterization facilities that will be available at the NSLS-II or how this will operate. Furthermore, there is a need to overcome the activation barrier that usually exist to come and do work at a synchrotron facility. Training of new users is a big issue.

Integration of synchrotron and in-lab work, standardization of instrumentation

- Participants mentioned the need to integrate standard in-lab instrumentation to the synchrotron beamlines. This will make the studies more meaningful and simplify the correlation of experimental data obtained at the beamlines with work done outside the synchrotron. For example, incorporate an infrared or Rahman spectrometer to a beamline for XRD or XAFS. Also there is a need to create a pool of standard reaction cells and detection devices for the general users of the beamlines.

Technical support in the development of beamline optics and detectors

- A big challenge will be the optimization of the beamline optics and the development of new detectors to take advantage of the capabilities of the NSLS-II. The NSLS-II should have enough technical support to deal with these issues because most users are not experts in these areas.

Condensed Matter Physics and Materials Science--Energy Storage - Jason Graetz

The Energy Storage group is in general agreement that the suite of project and approved beamlines will meet their needs. There were some concerns regarding facilities and access:

- Currently there is a dedicated lab space in NSLS I equipped with cyclers, glove boxes, battery assembly equipment, etc. for the energy storage user community. It is unclear if this type of space will be available at NSLS II and how the transfer will work from NSLS I to II.
- There were also concerns about general beamtime access. BNL has established a strong reputation for characterization studies of new electrode materials. Although important, many of these studies are routine and do not require state-of-the-are facilities. Since beamtime at NSLS II will likely be very competitive, it will be important to figure out how to keep these types of studies going (e.g., high throughput capabilities).

A number of ideas were discussed for early high impact experiments:
- Probing single particle lithiation in real time.
- In operando imaging experiments of electrochemical alloying or conversion reactions to image real-time structural and morphological changes.
- Tracking and characterizing the formation of surface layers (e.g., SEI) that form at the electrode-electrolyte interface during electrochemical cycling.

Users in the energy storage community are interested in *in insitu* and *in operando* studies and there is a clear need for new, more robust sample environments. A few ideas include:
- A general electrochemical cell for studying battery electrodes in operando – ideally these cells could be used on multiple beamlines. Specialized holders to allow parallel experiments on multiple cells would help reduce beam time.
- Electrochemical cells designed to probe the cell cross section – important for measuring surfaces and electrode-electrolyte interface.
- TEM sealed sample cells that can be easily transferred to the synchrotron.

It may be useful to establish a battery consortium, similar to the catalyst consortium, that would provide a suite of tools and sample environments available to the battery community. This

consortium could be regarded as a partner user and allocated a certain amount of beam time each cycle. Strategic question: Will lab support a battery consortium?

Earth and Environmental Sciences - Jeff Fitts

Earth and Environmental Sciences

Breakout Summary

Earth and Environmental Sciences (EES) community members from SBU and BNL primarily attended two breakout sessions, "Extreme Environment Materials" and the combined "Environmental Sciences/Bio Imaging" sessions. In general, the EES community is very engaged in NSLS II development, where community members represent 20% of the Beamline Advisory Teams for the six project beamlines, are spokespersons of three approved beamlines (4DE, TES, XFM), and are leading at least one proposal in the second round (STX). Community members in both sessions raised concerns about beamtime capacity at NSLS II beamlines for high pressure experiments and x-ray imaging. Most of the discussion, however, focused on what instrumentation and resources are needed, but are not currently funded and do not have a clear champion in the SBU/BNL community. The EES community identified three critical areas in need of immediate institution-level support that cut across scientific disciplines/themes. The EES community recommends that BNL/SBU institute strategies to:

1) ***Develop sample environments for in situ, in operando, extreme conditions and sample preservation***. Many, if not most, of the next generation experiments enabled by the world leading capabilities of NSLS II will not be realized without beamline-compatible sample environment cells. Institutional support for BNL/SBU scientists to work with NSLS II beamline scientists to develop the necessary sample environments will serve as the foundation for competitive research programs.

2) ***Develop data management procedures and beamline software for real-time data analysis***. Large data sets will be the norm at NSLS II, especially for imaging, tomography and time-dependent studies. Many experiments will be severely compromised if the data cannot be analyzed at the beamline during an experimental run, a.k.a., running blind.

3) ***Instrument and support LOBs at NSLS II for sample preparation, offline characterization and in situ experiment setup.*** Sample preparation is critical for 2-D high-resolution imaging of spatially heterogeneous environmental and biological samples, which will typically need a cryo-microtome to section biologic samples and cryo-stages at the beamline. Offline optical and electron microscopes are needed to pre-screen samples and identify regions of interest in order to ensure efficient use of beamtime. Sample holders with fiduciary markings must be developed to go from LOB lab to different imaging beamlines.

Biological Imaging - Lisa Miller

The participants in the Biological Imaging breakout session represented a broad range of scientific disciplines including structural biology, earth and environmental sciences, bioengineering, and medicine. This community has participated in funded Beamline Development Proposals (BDPs) for NSLS-II including the NSLS-II Project beamline: Sub-micron Resolution X-ray spectroscopy (SRX); the NIH beamlines: Frontier Macromolecular Crystallography (FMX), Automated Macromolecular Crystallography (AMX), and Life Science Small-Angle X-Ray Scattering (LIX); and the NEXT beamlines: Inner Shell Spectroscopy (ISS) and Full-Field X-ray Imaging (FXI). They have also participated in other BDPs that have not yet received funding including infrared imaging beamlines (AIM, IRI), combined macromolecular crystallography and spectroscopy (AM3), X-ray Footprinting (XFP), X-ray spectroscopy (XAS), X-ray Fluorescence Microscopy (XFM), and Medical Imaging and Therapy (MIT).
The unifying theme expressed by the community is the need for biological imaging to cover multiple length scales from nanometers to millimeters and these imaging efforts should be coordinated across beamlines. Beamlines must be staffed sufficiently to accommodate novice biological users, remote users, and high-throughput experiments. Related to these points, the participants made the following observations:

- A suite of beamlines is needed to cover length scales from nanometers to millimeters and these imaging efforts should be coordinated across beamlines.
  - **Concerns:** There is currently no concerted effort to coordinate efforts among approved beamlines, including synergy with non-biological imaging.
  - **Possible Strategy/Actions:** A grass-roots "biology village" meeting is now being held weekly at BNL to discuss unifying strategies across beamlines. These efforts should be expanded to SBU (and beyond).

- Funding for biological imaging beamlines will require involvement from non-BES agencies, most notably NIH and DOE-BER.
  - **Concerns:** While NIH has agreed to fund two MX and one SAXS beamline, they have decided to postpone their decision whether to fund a biological imaging beamline at NSLS-II.
  - **Possible Strategy/Actions:** Together with NIH and BER, NSLS-II should hold a workshop on biological imaging to explore the various options for biological imaging that will take advantage of NSLS-II characteristics while serving the largest user community and executing the highest impact science.

- For large, intact samples, synchrotron techniques should be complementary to other conventional imaging methods, such as ultrasound, MRI, CT, and PET.
  - **Concerns:** Approved NSLS-II imaging beamlines focus on small length scales (micro- to nanometer). Additional attention needs to be paid to full-field techniques that can examine large samples (e.g. plants, small animals) at modest resolution quickly and preferably with low x-ray dose (e.g. diffraction-enhanced imaging).

- **Possible Strategy/Actions**: This concern can be addressed partially with the approved FXI beamline, but the proposed medical imaging beamline would add additional capability and capacity. Funding this beamline will require engagement from BNL Medical Department and SBU Medical School (among others).

- For high resolution imaging to be successful, careful sample preparation and complementary characterization (e.g. AFM, EM) are imperative.
    - **Concerns**: NSLS-II does not have a budget to outfit LOBs with offline sample preparation and characterization tools. Adequate staff are also necessary to maintain these facilities.
    - **Possibly Strategy/Actions**: BNL can facilitate improved coordination with CFN for access to their characterization tools. Also, SBU faculty have access to funding mechanisms that can help provide necessary offline characterization tools (e.g. NSF Major Research Instrumentation grants, NIH Shared and High-End Instrumentation grants). Industry engagement may also provide resources. Collaborative efforts can begin now.

- The education pipeline needs to be strengthened.
    - **Concerns**: There will be insufficient staff at NSLS-II to accommodate novice biology users. Scientists that speak the language of the biologist and have expertise in physics and instrumentation are few and far between.
    - **Possibly Strategy/Actions**: Together with Stony Brook, build that education pipeline with courses in synchrotron techniques and instrumentation that will benefit all science majors. SBU professors are eager to participate.