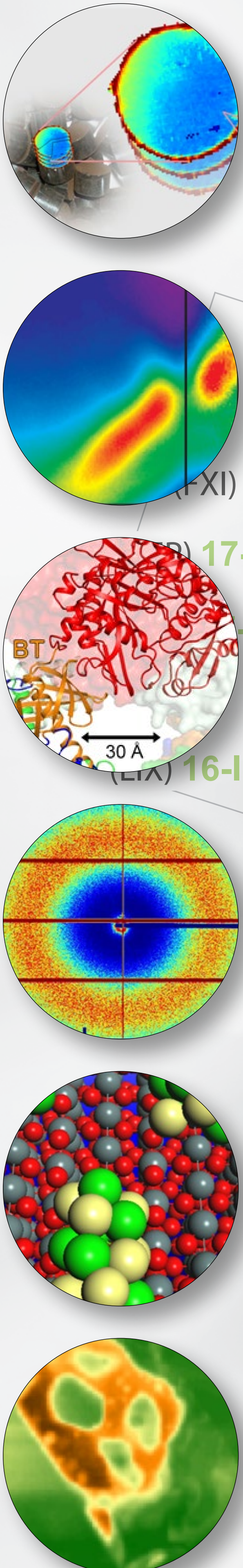

NSLS-II Five-Year Strategic Plan

May 2017

BROOKHAVEN NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

NSLS-II MISSION

To develop and operate a premier user facility that embraces diversity to safely and efficiently deliver high-impact and cutting-edge science and technology for the benefit of society.

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EXECUTIVE SUMMARY

Located at Brookhaven National Laboratory (BNL) on Long Island, New York, the National Synchrotron Light Source II (NSLS-II) is a US Department of Energy Office of Science Basic Energy Science scientific user facility. It is the most advanced synchrotron light source facility in the US and one of the newest low-emittance storage ring facilities in the world. As a result, it produces very bright beams of photons over a wide range of wavelengths from the far infra-red to the hard x-ray. These photons are used to carry out a hugely diverse set of experiments, many of which could not be carried out anywhere else. The photons are delivered to the experiments by beamlines, each of which is optimized to enable high-impact research in key science and technology areas. There is provision for around 60 such beamlines at NSLS-II. Experiments are carried out by users who gain access to the capabilities through a competitive peer-reviewed process. Users from academia, industry and National Laboratories from the US and around the world come to use the capabilities at NSLS-II. Access is free for all non-proprietary research. When fully built out, NSLS-II is expected to host over 4000 users per year. It began operations in October 2014, and is currently rapidly ramping up its science and user programs and continuing the development of new beamlines and associated scientific capabilities. This document summarizes the vision for the facility, the high level strategy for achieving that vision and a five year plan documenting the next steps. The short term goals are to operate the synchrotron and reach its design performance, complete and operate the first 28 beamlines and seek to develop the additional beamlines to grow the capabilities and user program further to realize the full potential of this remarkable machine.

The vision for NSLS-II is to develop world leading scientific capabilities and leverage them to enable and conduct a broad range of high-impact, discovery class science and technology programs to address the critical scientific grand challenges in energy security, advanced materials synthesis and manufacturing, environment, and human health. The strategy to achieve this vision is to integrate community interests, BNL research initiatives, and NSLS-II strengths and expertise to develop and conduct a suite of advanced science programs based on innovative technology and approaches to address the grand challenges facing society today as identified by the scientific communities.

The approach we have adopted is to: (a) create a vibrant environment that attracts world-class staff, partners, and users pioneering research areas aligned with NSLS-II strategic directions; (b) develop and operate world-class accelerator and beamline systems with innovative and breakthrough capabilities tailored to strategic research areas as identified by our stakeholders; (c) coordinate with other BES light source facilities to advance enabling technologies in accelerator systems, X-ray optics and detectors, software, and instrumentation and methods; (d) spearhead the development of new strategies in data acquisition, data management, and data-driven science by working with BNL and other National laboratories; and (e) leverage BNL strengths and community interests to facilitate university-industry-government cooperative partnerships that support the theme from discovery to deployment.

Based on our strategy and approach, we are currently operating and developing a suite of 28 cutting-edge beamlines, along with associated sample environments and support technologies (see side box). This set of current activities is informed by many years of strategic planning working, with the user community and other key stakeholders. These beamlines, with 19 of them already in operations, provide world-class scientific capabilities in such areas as nanoscale to mesoscale structural and chemical imaging, coherent scattering on complex materials and dynamics, photoelectron spectroscopy and imaging, advanced x-ray scattering for materials self-assembly and membrane science, inelastic scattering on complex nanoscale disorder and electronic excitations, science-driven high-throughput structural biology, in-situ and in-operando diffraction and, and advanced infrared spectroscopy. With phased completions in the 2014-2019 timeframe, these 28 beamlines collectively support a large, highly engaged, and productive user community to address scientific challenges in many scientific disciplines.

The current beamline suite represents only about half of the capacity of NSLS-II. This presents a tremendous opportunity to increase the impact of the facility and grow the user community. NSLS-II will therefore continue to work the scientific user community to identify and develop additional beamlines. A number of additional capabilities have been identified through a rigorous strategic planning process. Among them, six new beamlines, as shown in the Table at the right, have been selected as high-priority beamlines to build in the current planning period. These additional beamlines, along with a high-energy beamline already in design, would significantly expand the scientific capabilities of NSLS-II, advance our stakeholders' missions, and leverage the substantial capital investment that has been made in NSLS-II.

A critical part of our plan is to continue research and development in accelerator technology, advanced x-ray optics and detectors, coherent x-ray optics and optical metrology techniques, precision engineering and mechanical metrology, and new techniques and tools for multimodal and in-situ/operando studies. Advancing these enabling technologies and sample environments is an integral part of the DOE-BES scientific user facilities' mission and is essential to maintaining our leadership in driving the cutting-edge in synchrotron technologies and applications.

As the experimental activities ramp up at NSLS-II, advanced techniques and detectors will continue to drive higher data rates and data volumes and increase the complexity of experimental datasets. In order to achieve its full scientific potential, NSLS-II is working with BNL and other Laboratories to develop a high-performance data management infrastructure with a flexible architecture, as well as dedicated software tools for data analysis, data mining, and visualization to enable both real-time analysis during experiments as well as post-experiment analysis.

NSLS-II: 28 Beamlines in Operations or Under Development

AMX	Automated Macromolecular Crystallography
BMM	Beamline for Materials Measurements
CHX	Coherent Hard X-ray Scattering
CMS	Complex Materials Scattering
CSX-1	Coherent Soft X-ray Scattering
CSX-2	Soft X-ray Spectroscopy
ESM	Electron Spectro-Microscopy
FIS	Frontier Infrared Spectroscopy
FMX	Frontier Macromolecular Crystallography
FXI	Full-field X-ray Imaging
HXN	Hard X-ray Nanoprobe
ISR	In-situ and Resonant Scattering
ISS	Inner-Shell Spectroscopy
IXS	Inelastic X-ray Scattering
LIX	X-ray Scattering for Life Science
MET	Magneto, Ellipsometric and Time-resolved IR Spectroscopy
NYX	New York State Structural Biology Center
QAS	Quick X-ray Absorption and Scattering
SIX	Soft Inelastic X-ray Scattering
SMI	Soft Matter Interface
SRX	Sub-um Resolution X-ray Spectroscopy
SST-1	Spectroscopy Soft and Tender 1
SST-2	Spectroscopy Soft and Tender 2
TES	Tender Energy Spectroscopy
XFM	X-ray Fluorescence Microscope
XFP	X-ray Foot-Printing
XPD	X-ray Powder Diffraction
PDF	Pair Distribution Function

New Beamlines in the Development Plan

HEX	High-energy Engineering X-ray Scattering and Imaging
CDI	Bragg Coherent Diffraction Imaging
ARI	ARPES & RIXS nano-Imaging
SMF	Spectro-Microscope Facility
QIX	Quick Resonant Inelastic X-ray Scattering
PLS	Processing & Liquid Scattering
INF	Infrared Near-Field Nano-spectroscopy

Another key ingredient for achieving our vision is to create a vibrant environment at NSLS-II that attracts world-class scientists pioneering new research areas. Building upon the over thirty-years of success at NSLS, we are developing a world-class scientific and technical workforce and integrating community interests and participation into lasting partnerships. We are exploring forming cross-cutting science groupings to integrate science across beamlines, provide specialized instrumentation, and expand the user community through outreach. The beamline development process, the open designs of the Laboratory and Office Buildings, the initiatives for integrated centers and partnerships, and physical colocation of science-oriented beamlines are just a few examples of ways in which we are working to encourage and promote community interactions, communications, and engagement.

Looking further ahead, we are working to develop concepts for future NSLS-II accelerator and insertion device upgrades to maintain NSLS-II's competitive advantage in the coming years. We will also work with the scientific community and contribute to the development of future light sources through the development of novel accelerator concepts and by identifying and developing the science drivers that define the performance requirements for future light sources.

The NSLS-II Five-Year Plan presented here summarizes our strategic science directions, our approach, and our development plans in key areas for the next five years in order to accomplish our mission. Our development plans in specific areas of NSLS-II operations take into account the current funding levels and assumes reasonable funding expectations in the respective areas. Our overall priorities for the next five years will be:

- Maintain reliable accelerator operations and ramp-up storage-ring performance,
- Efficiently operate the suite of beamlines currently in operations or under development, and ramp up user science programs at these beamlines,
- Continue to develop additional beamlines and additional scientific capabilities, and
- Pursue R&D, data science and computing, and strategic partnerships critical to NSLS-II mission.

This document will serve both as our high-level strategic plan and as our basis for budgetary priorities for all our major operations and development activities in the next five years. The execution of this plan will depend on the actual funding in the coming years and will reflect these priorities.

1

INTRODUCTION

This *NSLS-II Five-Year Strategic Plan* describes a comprehensive and realistic science and technology agenda for NSLS-II for the next five years. It serves both as a concise strategic plan that has evolved over the past two years since 2015, and as a high-level tactical plan that provides an actionable to-do-list and serves as the basis for budgetary priorities in fiscal years 2017-2021. It is expected that this document will be updated yearly to reflect changes in science and technology landscape and in expected funding realities.

Since the start of operations in October 2014, NSLS-II has rapidly ramped up its science capabilities and user programs, and has delivered 19 new beamlines into operations through an aggressive beamline construction program. This is truly an exciting time at NSLS-II. At the same time, since half of the facility's capacity will be built out in the next couple of years, the new facility faces two main challenges in this next five-year period – how to enable and deliver high-impact science with sustainable accelerator and beamline operations, and how to develop a strategy and attain additional resources to build out the remaining facility. This Plan attempts to address these questions through a comprehensive discussion of several key areas that NSLS-II plans to pursue in the next five years.

1.1 VISION, STRATEGY, AND APPROACH

NSLS-II vision is to be a world-leading scientific user facility with cutting-edge capabilities and expertise that enable a broad range of high-impact science and technology programs.

Our strategy to achieve this vision is to integrate community interests, BNL research initiatives, and NSLS-II strengths and expertise to develop and conduct a suite of advanced science programs based on innovative technology and approaches to address the grand challenges facing society today, as identified by the scientific communities.

Following this strategy, we have adopted the following approach:

- Creating a vibrant environment that attracts world-class staff, partners, and users pioneering research areas aligned with NSLS-II strategic directions;
- Developing and operating world-class beamlines with innovative and breakthrough capabilities tailored to strategic research areas;
- Coordinating with other BES light source facilities to advance enabling technologies in accelerator systems, X-ray optics and detectors, and instrumentation and methods;
- Spearheading the development of new strategies in data acquisition, data management, and data-driven science by working with BNL and other laboratories;
- Leveraging BNL strengths and community interests to facilitate university-industry-government cooperative partnerships that support the theme from discovery to deployment.

1.2 INTEGRATING COMMUNITY INTEREST

A key aspect of our strategy is the close engagement with the scientific community and the key stakeholders in a form of cooperative partnership in the development and the operations of NSLS-II beamline facilities and associated science programs. This strategy includes the following elements.

Beamline Development Process: All beamlines at NSLS-II are developed through calls for Beamline Development Proposals (BDPs) to solicit ideas and concepts from the scientific community concerning specific research needs and specific beamline facilities at NSLS-II. The expectation is that such BDPs will be encouraged following an initial short pre-proposal submitted to NSLS-II management. The full beamline development proposals are peer reviewed and then rated by the NSLS-II SAC. The NSLS-II management makes the final decision to approve or disapprove each proposal based on the input and with the concurrence of the SAC.

Beamline Advisory Teams: All NSLS-II beamlines under construction each utilize a Beamline Advisory Team (BAT) during their construction period. The role of the BAT is to represent a segment of the scientific user community and to advise the beamline development group on the scientific and technical scope of the beamline as well as on the beamline design to ensure that each beamline is developed to meet the community needs.

User-Assisted Science Commissioning of Beamlines: In order to efficiently commission NSLS-II beamlines and promote the community engagement in the commissioning process, NSLS-II has developed a *phased commissioning* strategy to commission each beamline after its construction is completed. Using this strategy, scientific capabilities are commissioned sequentially based on scientific priorities determined through interactions with the BAT and user community. Once a specific scientific capability is commissioned, general user operation will commence for that capability, interleaved with commissioning activities of other capabilities. This approach permits thorough technical commissioning of all planned science capabilities while achieving early high-impact scientific productivity at the beamline.

Commissioning of each science capability progresses naturally in two phases: *technical commissioning*, where the focus is on beam delivery through the main beamline optical system into the experimental endstation, and *science commissioning*, where the focus is to evaluate the endstation instrument and data acquisition system for the planned science experiments. NSLS-II welcomes direct participation of the user community during the science commissioning phase of each beamline. This is being done by soliciting science commissioning proposals through special announcements of newly available beamlines or beamline capabilities during regular calls for General User (GU) and Partner User (PU) proposals. These science commissioning proposals are peer-reviewed and rated by the NSLS-II Proposal Review Panel for allocation of science commissioning beam time at the beamline.

Partner Beamlines and Partner Users: NSLS-II encourages and welcomes community participation in co-developing new scientific capabilities and new scientific user communities at NSLS-II beamlines through the Partner User approach. The main objective of the Partner User program is to leverage the interest, the expertise, and the resources that may exist in the community in joint development of new scientific programs at NSLS-II. Through this approach, a partner user group may contribute cutting-edge instrumentation, new analysis software, and/or specialized staff expertise to NSLS-II beamlines to bring new capabilities that would otherwise not available at NSLS-II. This may include the construction and operation of a complete beamline. Typically, the partner user group submits a partner user (PU) proposal through the NSLS-II proposal system, outlining the science case, the new capability they would bring, and the beamtime required to develop the new capability and its user program. The PU proposal is peer-reviewed and rated by the same NSLS-II proposal review panel (PRP), and is additionally reviewed by NSLS-II management and the NSLS-II SAC. NSLS-II management makes the final decision with concurrence of the SAC.

Integrated Science Initiatives and Consortia: In order to enhance scientific impact, cultivate innovation, encourage collaboration, and ensure that NSLS-II stays at the scientific frontier in the always-evolving science and technology landscape, NSLS-II plans to work and partner with BNL core programs departments and the community at-large to develop and implement a number of focused programmatic initiatives in selected target areas. Each initiative will function as a cross-cutting integrated research team or consortium that will (a) engage the research community to discuss scientific challenges in a specific field of science through workgroups, workshops, seminars, journal clubs, and other activities that promote staff interactions and brainstorm new research directions, (b) define the strategies and approach to enhance and expand the research programs in the specific area in order to address the scientific challenges, (c) promote, identify, and pursue appropriate external funding to enhance NSLS-II operations in the specific science area, and (d) drive and coordinate the development of special equipment at NSLS-II beamlines and support laboratories such as sample environment, ancillary instruments, and analysis software.

Users' Executive Committee (UEC): NSLS-II UEC is an executive committee of the NSLS-II Users Association, elected by the user community at large. The UEC serves as the official voice of the user community in its interactions with NSLS-II management. The UEC elects its Chair and Vice-Chair from among its members, and the UEC Chair has an ex-officio seat on the NSLS-II SAC. The UEC meets four times per year. The primary purpose of the NSLS-II UEC is to:

- promote and encourage research at NSLS-II
- provide opportunities for the user community to exchange ideas and concerns
- communicate user needs to facility management, including the NSLS-II, Brookhaven National Laboratory, and the Department of Energy
- broadly advocate the role synchrotrons play in the greater scientific enterprise
- provide a channel for communicating with federal funding agencies, Congress, the White House, and other federal and state agencies.

The NSLS-II Users Association organizes the annual NSLS-II Users' Meeting in cooperation with NSLS-II, and jointly with the BNL Center for Functional Nanomaterials (CFN) Users Association. In addition, the UEC Chair and Vice Chair meet with the NSLS-II management monthly to communicate on various subjects that are of mutual interests to the users and the NSLS-II.

1.3 NSLS-II CURRENT STATUS

NSLS-II Storage Ring: The NSLS-II is a 3 GeV storage ring synchrotron facility designed and built based on an optimized storage ring lattice consisting of 30 double-bend achromat (DBA) cells, with straight sections alternating in length of 6.6 m and 9.3 m, with low and high values of horizontal beta functions, respectively. The performance goal of the 0.6 nm-rad horizontal emittance for the NSLS-II storage ring will be achieved when operating with a full complement of insertion devices, including damping and superconducting wigglers. As of May 2017, seventeen insertion devices, including three 7 m damping wigglers, are operating in the storage ring, resulting in ~0.9 nm-rad horizontal emittance during normal operations. The main design parameters of the NSLS-II storage ring and the current operating parameters are summarized to the right.

The NSLS-II accelerator systems were commissioned in 2014 and there has been steady progress toward achieving the design performance. Over the past two years the NSLS-II Accelerator Division has succeeded in:

- Increasing the circulating current in the storage ring to 300 mA, with >95% of reliability in FY17 to-date, in routine top-off operations,
- Demonstrating a maxi-mum circulating current of 400 mA,
- Installing, commissioning and integrating into routine operations 16 new insertion devices (IDs) and three 3-pole wigglers (3PWs) with their associated front-ends (FE), in addition to the 6 original project IDs / FEs,
- Installing, commissioning and conditioning the second RF cavity,
- Commissioning the fast orbit feedback system and demonstrating of required beam stability,
- Enabling a "sleeping mode" of injector operation for low power consumption and reduced orbit noise.

At present in FY17, the NSLS-II accelerator operations goals are several fold: (a) deliver 4500 hours of beam operations with an continued reliability >95%, (b) maintain routine user operations with stored beam current of 300 mA in top-off, (c) commission new IDs, new FEs, and new beamlines, and (d) develop and ready the accelerator systems for increasing beam current towards the design value of 500 mA in the coming two years..

NSLS-II Beamlines: Over the past decade, NSLS-II has worked with the scientific community and strategically identified twenty-eight beamlines to develop as the initial suite of scientific facilities. Among these twenty-eight beamlines, as of April 2017, nineteen of them have completed construction and are either in user operations or under commissioning while the remaining nine beamlines

Main Parameters of the NSLS-II Storage Ring	Design Value	Operating Parameters April 2017
Ring energy (GeV)	3.0	3.0
Ring current with top-off (mA)	500	300
Ring circumference (m)	792	792
Number of DBA cells	30	30
Number of 9.3 m straights	15	15
Number of 6.6 m straights	15	15
β_h in 9.3 m straights (m)	20.1	20.1
β_v in 9.3 m straights (m)	3.4	3.4
β_h in 6.6 m straights (m)	1.8	1.8
β_v in 6.6 m straights (m)	1.1	1.1
Vertical emittance (nm-rad)	0.008	0.025
Horizontal emittance (nm-rad)	0.6	0.9
RMS energy spread (%)	0.12	0.09
RMS pulse length (ps)	15-30	30
Time between bunches (ns)	2	2
Revolution period (μs)	2.64	2.64
RF frequency (MHz)	500	500
Number of RF buckets	1320	1320
Number of bunches	1056	1056
Average bunch current (mA)	0.47	0.28
Average bunch charge (nC)	1.25	0.75

continuing their construction. Based on their scientific capabilities themes, all beamlines are currently sub-grouped into six program areas that exploit synergies among the beamlines and enhance efficiencies in operations. These six program areas are: Soft X-Ray Scattering and Spectroscopy, Hard X-ray Spectroscopy, Complex Scattering, In-Situ Scattering and Diffraction, Imaging & Microscopy, and Structural Biology. The key scientific capabilities of these twenty-eight world-class beamlines are summarized below.

Soft X-Ray Scattering and Spectroscopy program develops and operates six beamlines that exploit the best source properties of the NSLS-II in the soft x-ray spectral region, with a scientific emphasis that includes characterization of electronic structures in correlated electron systems, ambient pressure chemistry studies, and understanding and control of low-energy excitations in real materials systems.

- Coherent Soft X-ray Scattering (CSX-1) – Coherent soft x-ray scattering and imaging with world-leading high-coherent flux and detector for probing electronic textures and dynamics.
- Coherent Soft X-ray Scattering and Spectroscopy (CSX-2) – allows studies of ambient pressure photoelectron spectroscopy (AP-PES) with world-leading soft x-ray beam size and flux enables chemical activity studies at realistic ambient conditions.
- Electron Spectro-Microscopy (ESM) – Combined LEEM /PEEM as well as μ-ARPES provide world-class spatially resolved photoelectron spectroscopy and imaging capabilities for electronic structures in crystals as well as in polycrystalline materials.
- Soft Inelastic X-ray Scattering (SIX) – a long beamline under development for inelastic soft X-ray scattering with a state-of-the-art spectrometer located in a satellite building providing world-leading ~14 meV energy resolution at 1 keV for probing low-energy correlated electronic excitations with high sensitivity.
- Frontier Synchrotron Infrared Spectroscopy (FIS) and Magneto, Ellipsometric and Time-Resolved Optical Spectroscopy (MET) are a pair of IR beamlines currently under development for in-situ optical studies of condensed matter and materials under high-pressure environment.

Hard X-ray Spectroscopy program develops and operates a suite of cutting-edge x-ray spectroscopy beamlines enable research on real systems in complex environments over extended duration of systems operations.

- Inner Shell Spectroscopy (ISS), Quick Absorption & Scattering (QAS), and Tender Energy Spectroscopy (TES) beamlines, offer an advanced suite of *in-situ* X-ray spectroscopy capabilities, including a state-of-the-art confocal X-ray spectrometer at ISS, with a set of specimen environments and a hazardous gas handling system for characterization of catalytic reactions and processes under industry relevant conditions.
- NIST Spectroscopy Soft and Tender (SST-1, SST-2) beamlines, under development in partnership with NIST, enable X-ray photoelectron spectroscopy and near edge X-ray absorption fine structure (NEXAFS) spectromicroscopy for materials science. The BMM beamline on a 3-pole wiggler port is also being developed in partnership with NIST and adds a diffraction/scattering capability.

Complex Scattering program operates four advanced beamlines that take full advantage of the NSLS-II high brightness and coherence for coherent scattering, inelastic scattering, and in-situ structural studies of mesoscale complexity and dynamics in heterogeneous and non-equilibrium systems.

- Coherent Hard X-ray Scattering (CHX) – X-ray photon correlation spectroscopy with world-leading hard x-ray coherent flux and detection system for fast dynamics into the μs regime.
- Soft Matter Interface Beamline (SMI) – Simultaneous small-angle and wide-angle x-ray scattering at grazing incidence, and specialized x-ray reflectometry for liquid interfaces, including a wide x-ray energy range of 2-24 keV to access element edges important to soft matter *e.g.* P, S, K, Ca.
- Complex Materials Scattering (CMS) – High-throughput small-angle and wide-angle x-ray scattering in transmission and reflection mode covering broad q-range from $4x10^{-4}$ to $7\ A^{-1}$, with an auto-sample-changer and versatile sample environment for stimuli-responsive *in-situ* experiments, and micro-beams for heterogeneous sample mapping of complex hierarchical materials.
- Inelastic X-ray Scattering (IXS) – Inelastic X-ray scattering with a goal of world-leading sub-meV energy resolution at 9.1 keV for studying low-energy excitations from nanoscale heterogeneity and disorder, particularly well-suited to the study of soft matter systems.

Diffraction and In-Situ Scattering program develops and operates four world-class scattering & diffraction beamlines that enable advanced in-situ and operando studies for a wide range of fundamental and applied materials research problems.

- X-ray Powder Diffraction (XPD) is a powder diffraction beamline that offers cutting-edge capabilities with a wide suite of in-situ sample cells under extreme conditions and real-world in-operando sample environments.

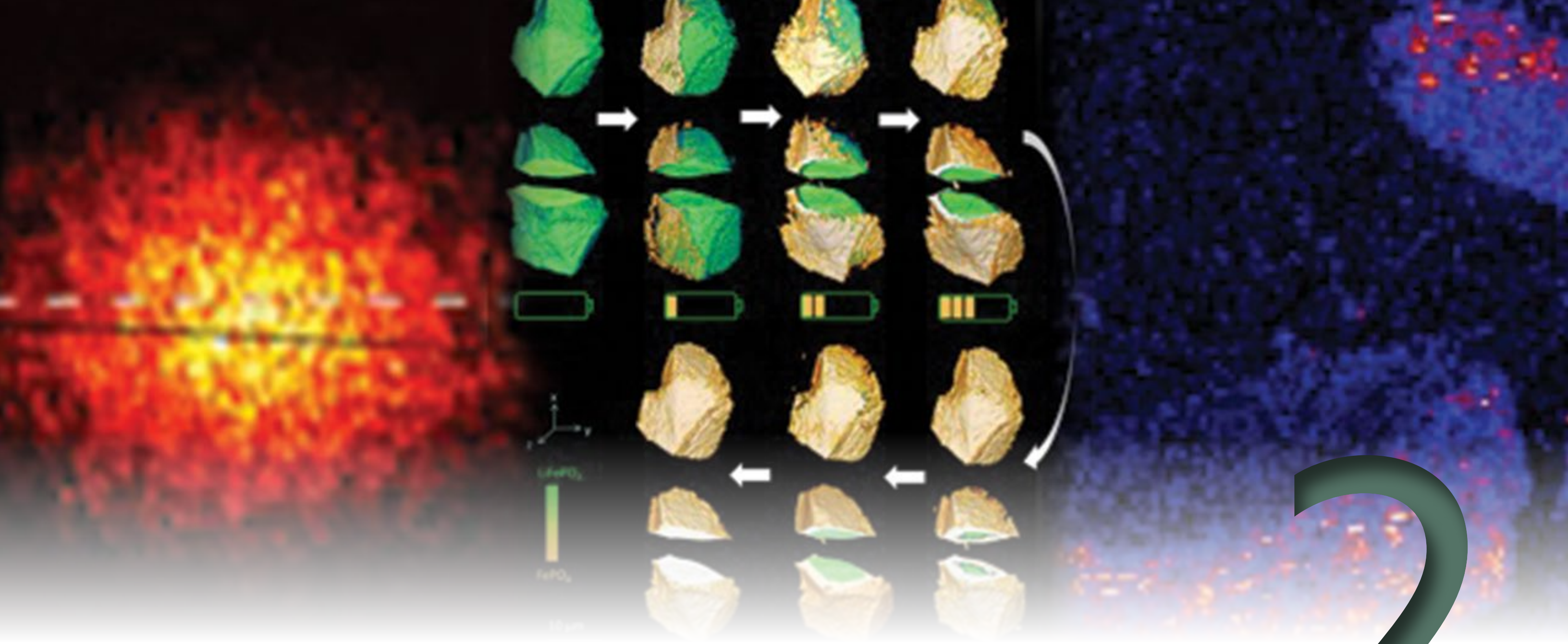
- X-ray Pair Distribution Function Scattering (PDF) beamline is currently under development and will provide dedicated PDF capability for in-situ studies of nanoscale deformations in many materials systems.
- In-situ and Resonant Scattering (ISR) beamline enables real-time studies of thin-film synthesis and growth that aims to control the nucleation kinetics during the growth process and allows polarization dependent diffraction studies of variety of materials under high magnetic field.

Imaging and Microscopy program operates and develops a suite of advanced imaging beamlines that take full advantage of the NSLS-II high brightness and small source size, and provide world-leading capabilities in in-situ multiscale imaging of heterogeneous structures and chemistries.

- Hard X-ray Nanoprobe (HXN) is a state-of-the-art 110m-long beamline for structural and fluorescence imaging and ptychography with world-leading 10 nm spatial resolution.
- Submicron Resolution X-ray Spectroscopy (SRX) beamline offers world-leading high-throughput chemical imaging capability with sub-100 nm and sub-µm spatial resolution.
- Full-field X-ray Imaging (FXI) is a state-of-the-art beamline under development for transmission hard X-ray microscopic imaging at 10-20 ms time-resolution and better than 30 nm spatial-resolution, with full 3D nano-tomography in <1 minute.
- X-ray Fluorescence Microscopy (XFM) is a beamline currently under development for high-throughput X-ray fluorescence imaging and tomography with ~um resolution.

Structural Biology program operates five state-of-the-art X-ray crystallography, X-ray scattering, and X-ray footprinting beamlines that provide microfocused X-ray beams with world-leading X-ray photon densities for a wide range of cutting-edge investigations in molecular structural biology and enzymology. This suite of world-class structural biology beamlines at NSLS-II brings structural biology at storage rings to a new level, enabling discovery-class as well as hypothesis-driven projects with potentially large numbers of samples in life science research.

- Frontier and Automated Macromolecular Crystallography (FMX/AMX) are a pair of micro biological crystallography beamlines on canted undulators with world-leading micron-sized x-ray flux densities in the 5-30 keV range, and a suite of automated novel crystal mounting and handling systems (Figure 4), including an acoustic-droplet ejected system and a dynamic slit system to adapt beam to crystal size, to enable high-throughput, and challenging projects using multi-crystal serial crystallography at cryo- or room temperatures.
- NYSBC Biological Microcrystallography (NYX) – Developed in partnership with New York State Structural Biology Consortium (NYSBC), the NYX beamline provides cutting-edge optimized single- and multiple-wavelength anomalous scattering (SAD and MAD) capabilities in the 6-17.5 keV range.
- X-ray Scattering for Life Science (LIX) – Time-resolved solution scattering for studying macromolecule conformational changes in solution and advanced grazing-incident scattering for structural studies of membrane complexes.
- X-ray Foot-printing (XFP) – Developed in partnership with Case Center for Synchrotron Biosciences, the XFP beamline provides a unique X-ray coupled mass spectroscopy capability for structural studies from non-crystalline macromolecule specimens, enabling investigations of more complex biological systems and allowing access to timescales in the micro-seconds range.



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STRATEGIC DEVELOPMENT DIRECTIONS

Given the current state of the NSLS-II and the needs to further develop this young scientific user facility, it is important to examine the evolving scientific landscape, analyze our competitive and risks, and identify our strategic development directions for the coming five years. In this Chapter, we first discuss the relevant national and global context, then evaluate our strengths, risks, and opportunities, and finally outline our guiding strategic directions for our research and development.

2.1 NATIONAL AND GLOBAL CONTEXT

NSLS-II facility is being developed and starting operations at a time when the world is entering a new era with a global economy fueled largely by scientific discoveries and technological innovations. Increasingly, the research and development activities are driven by the need to address the key grand scientific challenges that the society is facing today in energy security, in clean environment, and in human health. In a 2015 Department of Energy (DOE) Basic Energy Science (BES) advisory committee (BESAC) report *"Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science"* [1], the BESAC reviewed the progresses made since 2007 when five grand challenges were identified in a landmark report titled *"Directing Matter and Energy: Five Challenges for Science and the Imagination"* [2]:

- How do we control material processes at the level of electrons?
- How do we design and perfect atom- and energy efficient synthesis of revolutionary new forms of matter with tailored properties?
- •How do remarkable properties of matter emerge from complex correlations of the atomic or electronic constituents and how can we control these properties?
- How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?
- How do we characterize and control matter away - especially very far away - from equilibrium?

The committee confirmed that these Grand Challenges are still compelling and the landscape has changed as a result of the progress made in the past ten years. The progress included the development of the LINAC Coherent Light Source (LCLS) and the National Synchrotron Light Source II (NSLS-II) from a vision to a reality, and the increasing interests in research at the meso-scales [3]. As a result of this progress, the Committee further concluded that the following new transformative and crosscut opportunities have emerged that have their foundations in the Grand Challenges:

- Mastering hierarchical architectures and beyond-equilibrium matter
- Beyond ideal materials and systems: understanding the critical roles of heterogeneity, interfaces and disorder
- Harnessing coherence in light and matter
- Revolutionary advances in models, mathematics, algorithms, data, and computing
- Exploiting transformative advances in imaging capabilities across multiple scales.

In other scientific disciplines, similar discussions on grand scientific challenges have been conducted by panels led by the National Academies of Sciences [4], the National Science Foundation [5], the National Institutes of Health, and the DOE Office of Biological and Environmental Research (BER) [6]. In environment and biological sciences, the grand challenge questions focus on understanding and ultimately control of the complex geochemical, biogeochemical, and atmospheric processes in the environment, and on the fundamental understanding of how life functions at the molecular, cellular, systems, and evolution levels:

- How is the information stored in a genome translated into microbial, plant, and eco-system processes that influence biofuels, climate feedbacks, and the natural cycling of carbon?
- What are the biological, geochemical, and physical forces that govern the behavior Earth's subsurface environment?
- What is the physics and chemistry of life?
- How do cells work, how do they interface with the environment, and how do single cells develop into multi-cellular organisms?
- How do genomes generate organismal robustness and diversity, and what is the molecular basis of evolution?

The capabilities of NSLS-II and its mission are well-matched to addressing these high-level grand challenge questions and crosscutting themes in the various scientific disciplines, and thus these provide a foundation for developing a set of driving strategic directions for NSLS-II.

Synchrotron science worldwide is also entering an exciting phase of rapid development. Since the conceptual inception of NSLS-II – the first synchrotron designed to reach below 1 nm-rad (designed for 0.6 nm-rad) horizontal emittance – about a decade ago, there has been increased interest worldwide in pursuing ultimate low-emittance storage-ring synchrotron sources using the multi-bend achromat (MBA) lattice concept [7]. MAX-IV in Sweden is the first of the MBA kind, and several MBA storage rings are now in construction at other facilities, including the European Synchrotron Radiation Facility (ESRF) in Europe and the SIRIUS synchrotron in Brazil. In this country, the Advanced Photon Source (APS) is moving forward to upgrade to a MBA design with a horizontal-emittance goal to reach around 0.15 to 0.07 nm-rad range in the 2022-23 timeframe. The Advanced Light Source (ALS) is also developing a conceptual design on a MBA upgrade with a goal of <0.07 nm-rad round beam on a somewhat later schedule.

Such worldwide effort, benefited from the many pioneering discussions on the exciting science potentials for NSLS-II, is driven largely by the desire to reach fully or close to the diffraction limit for hard X-rays (i.e. an emittance ~0.01 nm-rad) in the horizontal plane. Such a facility would lead to high-degree transverse coherence applications in the hard X-ray regime while still retaining operational flexibility and efficiency, as compared to free electron lasers, and large beamline capability inherent in a storage-ring based synchrotron source.

In this context, being the first low-emittance synchrotron facility starting operations in the world, and the *only* one in the US in the next five years, NSLS-II plays a critical and transformative role in advancing high-brightness synchrotron technology and associated research and development, enabling pioneering science to address challenging problems in the society, and cultivating and developing the ever evolving scientific user community to maximize the scientific impact of the low-emittance synchrotron facilities. This is an excellent opportunity to work together with the synchrotron light source community at-large and develop leading-edge scientific capabilities and associated research programs at NSLS-II.

It has been widely recognized that a particular strength of a low-emittance synchrotron source is in nanoscale imaging and in high-coherence applications. At the time of this report, NSLS-II is the world-leading operating synchrotron in these areas. Thus NSLS-II is poised to seize the opportunities to lead the development of new science strategies to begin to tackle the grand scientific challenges that our society is facing today.

2.2 STRENGTHS, RISKS, AND OPPORTUNITIES

As part of the current status assessment, it is worth noting how NSLS-II stands at present and in the next 5-10 years in the global landscape of synchrotrons. This allows a careful evaluation of the strengths, the risks, and the opportunities for the NSLS-II facility.

As the newest synchrotron facility and possibly the only green-field synchrotron facility in the US in the foreseeable near future, NSLS-II was designed and constructed to be world leading, with many advanced characteristics:

- First synchrotron light source constructed to achieve 0.6 nm-rad horizontal e-beam emittance
- Largest medium-energy facility with world-leading circumference and beamline capacity (4^{th} largest circumference among all green-field synchrotrons, following Spring-8, APS, and ESRF)
- World-leading high brightness and coherence in the soft to 20 keV hard x-ray range
- Broad range of synchrotron spectrum from IR on soft-bending magnet to very hard x-rays using superconducting wigglers

- Operating current of 500 mA – matching all medium energy storage rings and typically a factor 2.5x to 5x greater than the higher-energy rings
- Advanced beamlines with cutting-edge X-ray optics, detectors, and instrumentation
- Excellent storage ring beam and experimental floor stabilities designed from ground up
- Special sunken bypass corridors and the green-field site to easily accommodate long beamlines with external buildings
- A dedicated, world-class staff with the skills sets required for the new NSLS-II facility.

Closely matching these world-leading characteristics is a world-class, devoted scientific community that is highly engaged and excited about doing world-class and high-impact science at NSLS-II. While this could be said for any new facility coming online, the NSLS-II community has several unique aspects including:

- There is already a large existing scientific user community based on former NSLS-I that has a tradition of being highly engaged and productive for the past three decades
- There are strong genuine interests in the scientific communities, both existing and new, in taking advantage of the unique NSLS-II properties to develop unique scientific capabilities and partnerships
- NSLS-II is ideally located in the greater northeast US, a region that is vibrant and dynamic with a high concentration of world-renowned academia and industrial institutions - home to 45% of the top fifty US national universities (including seven in the top ten) and to headquarters of over 130 Fortune 500 companies (including Pfizer, Merck, Bristol-Myers, Honeywell, Corning, DuPont, General Electric, and IBM)
- NSLS-II's home institution, Brookhaven National Laboratory, is a DOE multidisciplinary national laboratory that conducts basic and applied research in a broad-range of discovery-to-deployment disciplines. BNL science departments, including Center for Functional Nanomaterials (CFN), have strong interests in developing research programs at NSLS-II in the areas of condensed matter and materials physics, catalysis and energy storage, nanoscience, and environmental and biological sciences
- BNL is managed by Stony Brook University and Brookhaven Science Associates, consisting of six premier research universities - Columbia, Cornell, Harvard, MIT, Princeton, and Yale. Considerable interests exist among these institutions to form cooperative partnerships with NSLS-II to pursue research in energy and health
- BNL is in close partnerships with many science consortia and organizations in the region, with particular emphasis on research and development of tomorrow's energy technologies. This includes partnerships with New York Battery and Energy Storage Technology consortium (NY-BEST), as well as with several newly funded Energy Frontier Research Centers in the region, including the Center for Emergent Superconductivity led by BNL, the NorthEast Center for Chemical Energy Storage led by SUNY – Binghamton, and the Center for Mesoscale Transport Properties led by Stony Brook University.

As a brand new synchrotron facility entering into operations, NSLS-II also faces risks. First, on the operation side, the high-degree of complexities that exist at NSLS-II accelerator and beamlines present another risk area that needs to be addressed. In general, cutting-edge capabilities require more effort to commission, troubleshoot, and maintain. At the same time, these cutting-edge capabilities are often in high demand by the scientific user community, thus also requiring more effort for user support and user training. It is therefore a significant challenge to balance these two major aspects in NSLS-II accelerator and beamline operations.

A second major risk for NSLS-II is the prospect of availability of construction funding that has traditionally been the main source for construction of new beamlines at the BES scientific user facilities. The current federal funding climate makes it a considerable challenge to our plan to build out the remaining open beamline ports, leading to close to the full capacity of ~60 beamlines and the full suite of cutting-edge science programs for the NSLS-II facility in a timely fashion. Mitigation of this risk requires significant effort to develop a diversified portfolio of science programs and partnerships that can attract funding from nontraditional sources and agencies.

Finally, while NSLS-II enjoys world-leading characteristics at present among all operating facilities with users, the synchrotron landscape is changing significantly. As pioneered by MAX-IV facility in Sweden, a number of facilities based on multi-bend achromat (MBA) lattices are being constructed, or are planned, to achieve significantly lower horizontal emittances leading to higher degree of coherence towards a fully diffraction-limited source for hard x-rays (**Figure 1**). The risk to NSLS-II will be the increased competition for the best user groups that pursue high-brightness-based science in this highly competitive field, potentially affecting the NSLS-II impact to the community.

Identification and thorough understanding of these risks can lead to new opportunities for NSLS-II. In particular, as

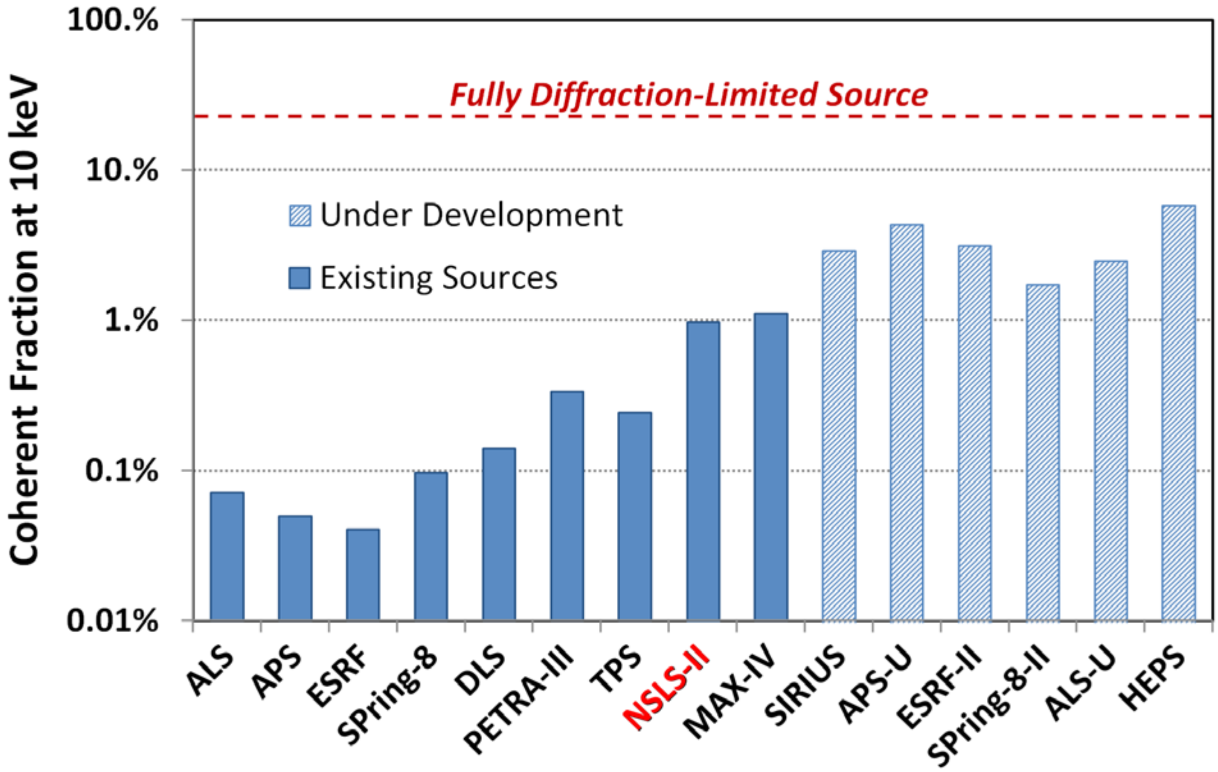


Figure 1. *Coherent fractions for photon beams of 10 keV of several representative synchrotron storage-ring based light sources around the world. Among them, Advanced Light Source (ALS) and Advanced Photon Source (APS) in the US, European Synchrotron Radiation Facility (ESRF) in France, Super storage ring 8 GeV (Spring-8) in Japan, Diamond Light Source (DLS) in UK, PETRA-III in Germany, Taiwan Photon Source (TPS) in Taiwan, MAX-IV facility are in operations, and SIRIUS in Brazil, APS-Upgrade (APS-U), ESRF upgrade (ESRF-II), Spring-8 upgrade (Spring-8-II), ALS upgrade (ALS-U), and Beijing high-energy photon source (HEPS) in China are under construction or being planned. Information are based on references described in Ref. 8*

the first low-emittance synchrotron facility in user operations in the world and the only one in the United States for at least another 5-6 years, we see that NSLS-II plays a critical and transformative role in advancing high-brightness synchrotron technology and associated R&D, in pioneering high-brightness science to address challenging problems in society, and in cultivating and developing the ever evolving scientific user community to maximize the scientific impact of the low-emittance synchrotron facilities. This represents an excellent opportunity to work together with the synchrotron light source community to develop leading-edge scientific capabilities and associated research programs at NSLS-II.

Our analysis of NSLS-II strengths and risks helps to clarify our role in the evolving landscape of synchrotron sources, to identify opportunities where we may focus our effort, and to develop new strategies to manage the risks. These are detailed in the following sections of this document. In short, the unique aspects of the NSLS-II facility on the national and world stage, its strongly engaged and interested communities, and its geographic location in the region of high-level scientific activities represent enormous opportunities for NSLS-II and lay the foundation for defining the NSLS-II strategic science directions for many years to come.

2.3 NSLS-II STRATEGIC DEVELOPMENT DIRECTIONS

To realize our vision and address the scientific grand challenges in the national and global context, we plan to develop and pursue research programs focused in three strategic scientific directions – complex materials and emergent behavior, *in-situ* and *operando* science, and multiscale structures and functions.

Emergent Behavior and Complexity: From simple material systems with self-organized interacting phases to intrinsically heterogeneous functional systems, complexity and its dynamics is increasingly one of the key themes in scientific studies in the 21st century. The high brightness of NSLS-II will enable world-leading coherence, nano-imaging, and inelastic scattering capabilities that will be ideally suited for fundamental understanding, and ultimately control, of intrinsic and emergent heterogeneities and associated naturally-occurring, unclocked, and irreversible processes in materials synthesis and processing, in strongly correlated quantum materials, and in complex hierarchical materials structures.

In-situ and Operando Science: In almost all scientific disciplines, one of the most challenging research goals is to understand how things work in real functional environment and under working conditions. This is often the key to connect the basic knowledge of materials properties to actual working devices and engineering systems. Therefore there is a clear need and demand in the scientific community for advanced characterization tools to allow in-situ and operando studies of real or realistic functional materials systems under working conditions that are relevant to natural or industrial processes. NSLS-II high brightness and flux in a broad range of synchrotron spectrum will enable correlated in-situ and operando capabilities in scattering and diffraction, spectroscopy, and imaging studies in a variety of functional systems critical to future energy needs, the environment, and human health.

Multiscale Structures and Functions: Building upon the enormous atomic-scale scientific knowledge acquired in the past century, it has become apparent that the structural, electronic, and chemical behavior on length and time scales between the atomic and the macroscopic world, hold the key to the control of emergent macroscopic properties and functions of materials, environmental, and biological systems. Taking advantages of high brightness and small source size, NSLS-II is in an ideal position to develop a suite of advanced structural, electronic, and chemical imaging programs that span multiple length and time scales, enabling cutting-edge correlative and multimodal studies in a variety of scientific disciplines.

As illustrated in **Figure 2**, these three strategic directions or themes are well aligned with the grand scientific challenges and the transformative opportunities that our stakeholders and the scientific community have identified.

In addition, we recognize four key crosscutting enabling technology areas that we plan to pursue in support of the strategic science themes –

- *Accelerator science and technology* that is the foundation for stable and reliable operations and for enhancing the performance of NSLS-II accelerator systems,
- *Advanced X-ray technology* in x-ray optics and detectors, and in nano-precision engineering that is required to the development of innovative world-leading programs,
- *Multimodal sample environments* playing an increasingly important role in modern science today from complex materials, operando chemistry, to geo-environmental and biosciences, and
- *Data-driven science* that is crucial to the productivity and the impact of all NSLS-II science programs, and in enabling new modes of experimentation involving advanced simulation, multi-modal experiments, and machine learning driven data analysis.

These four enabling areas will be discussed in more detail in later Chapters. They are critical in keeping the NSLS-II scientific capabilities at the cutting-edge and in enabling new and high-impact science at NSLS-II.

2.4 REALIZATION OF OUR STRATEGY

The process and the approach that NSLS-II has established will ensure that the strategic development directions are being realized and implemented as we develop scientific capabilities and conduct user science programs at NSLS-II. **Figure 3** illustrates how the current suite of NSLS-II beamlines are aligned with the NSLS-II scientific strategic

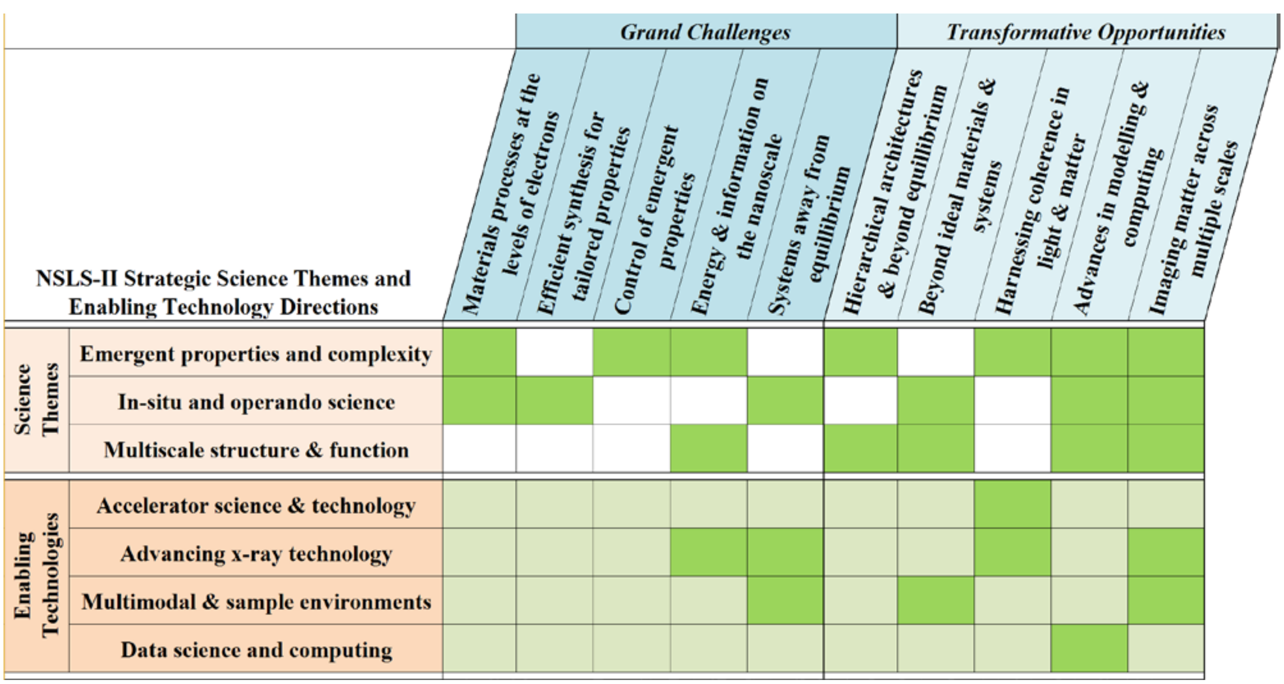


Figure 2. *NSLS-II strategic science themes and crosscutting enabling technology directions, and their alignments with DOE-BES grand challenges and transformative opportunities as identified by the scientific community.*

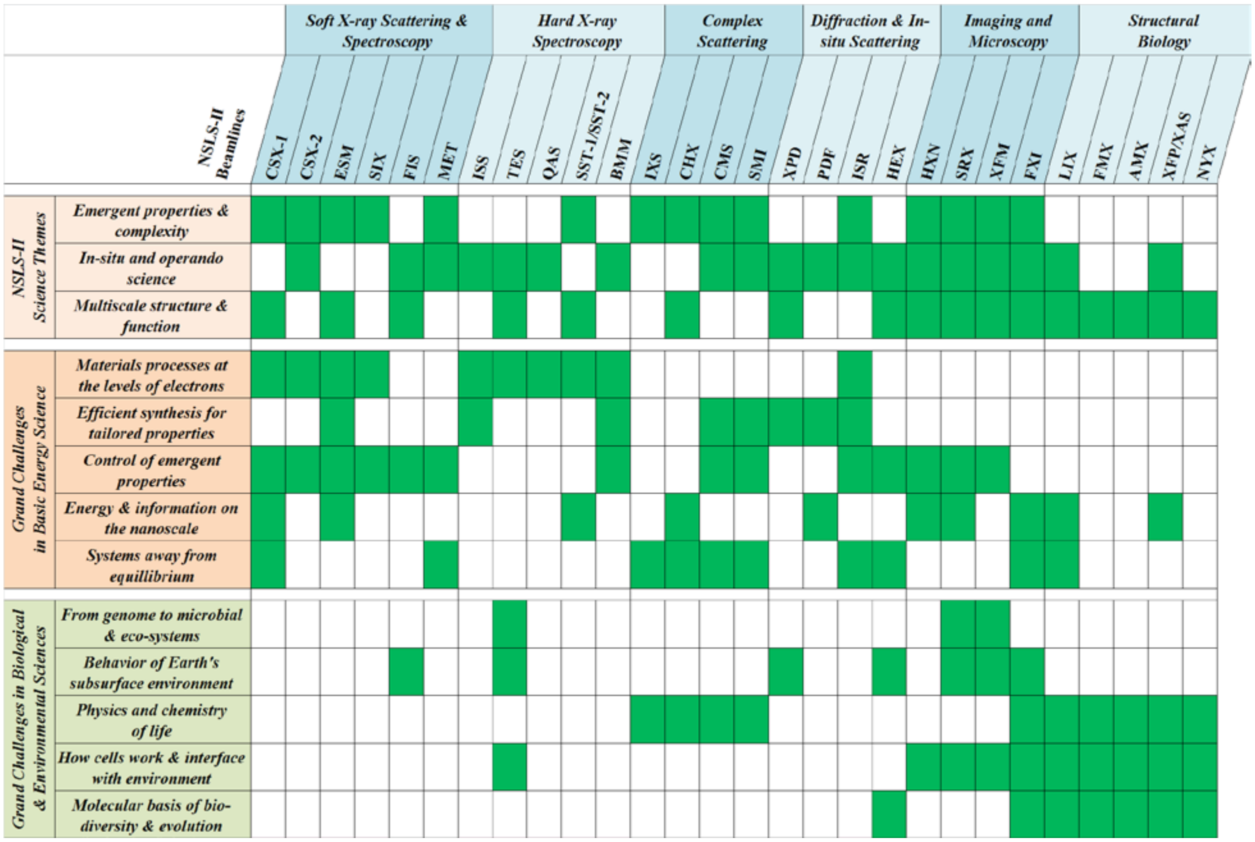


Figure 3. *Illustration of how the scientific capabilities being developed and operated are aligned with the NSLS-II science themes, and may help to address specific scientific grand challenge identified by the scientific community.*

directions and help address a number of scientific grand challenges in basic energy sciences as well as in biological and environmental research. In the next five years, NSLS-II will continue to use this approach to identify scientific needs and to develop, improve, and enhance our capabilities in key program areas on the NSLS-II facility.

In accelerator systems, NSLS-II plans to pursue accelerator development in the following areas: (i) developments that support reliable storage-ring operations for user programs, (ii) developments that are required to ramp up the storage-ring performance to its design values, and (iii) R&D that will lead to enhanced or upgraded NSLS-II source performance beyond design specifications, and to explore potential future high-brightness upgrade options in the longer-term.

In beamline programs, NSLS-II plans to pursue activities (i) to develop impactful user science programs at operating beamlines, (ii) to deliver new beamlines currently under construction, (iii) to improve beamline performance and efficiency to accommodate more users, (iv) to optimize and enhance capabilities to deliver more high-impact science, and (v) to start development of additional new beamlines at NSLS-II to meet the additional research needs of the scientific community.

In controls and data science, NSLS-II plans to meet the needs of accelerator and beamlines by (i) delivering a standardized yet versatile experimental controls and data acquisition system that can be tailored and optimized for different needs including remote and mail-in access, (ii) design and delivery of an efficient multi-tiered data management system that will grow with beamlines experimental data, in coordination with BNL's Computational Science Initiative (CSI), (iii) developing and implementing a functional library of data visualization and analysis routines and codes in close coordination with our sister facilities, and (iv) developing a post-experiment processing system and providing support to data visualization and analysis after completion of an experiment.

In enabling technologies R&D, NSLS-II plans to contribute to the overall DOE BES scientific user facilities mission by continuing our activities and leadership in the development of nanofocusing diffractive X-ray optics, nano-precision engineering, hard X-ray photon detectors, and optics metrology and modelling. In addition, NSLS-II recognizes the needs for, and plans to pursue, developments that will enable multi-modality and multi-technique investigations in a variety of scientific disciplines.

Finally, NSLS-II plans to continue to develop our talented workforce as the most important asset of the facility, to develop and implement effective partnerships that leverage the interest, expertise, and resources in the community, to develop and implement innovative user access modes for streamlined access to NSLS-II, and to improve user experience and overall facility infrastructure at NSLS-II.

These planned activities are described in more detail in the following chapters. Together our strategy and plan will impact how we conduct business and what we aim to accomplish in the coming years, and help us to achieve our vision.

3

ACCELERATOR DEVELOPMENT

The continued evolution of the NSLS-II accelerators is an essential part of the facility strategy. In the next five years, NSLS-II plans to pursue accelerator development in the following high-level categories:

- developments that support reliable storage-ring operations for user programs,
- developments that are required to ramp up the storage-ring performance to its design values,
- R&D that will lead to enhanced or upgraded NSLS-II source performance beyond design specifications.

Following these priority directions, NSLS-II plans to pursue a range of accelerator development activities with the following types of projects:

- Baseline projects to optimize performance of the components that are not operating properly or are required to reach design performance goals
- Improvements projects that significantly improve operations performance, increase beam stability and availability, and decrease downtime
- Enhancement projects that produce new capabilities of NSLS-II accelerator operations by adding new software or hardware tools
- R&D projects that are aimed at novel techniques needed for upgrades in the longer-term future.

In this Chapter we describe the first three categories of projects in more detail. The R&D projects will be discussed in Chapter 6 – Enabling R&D and Support, for research and development towards potential future upgrades of the NSLS-II accelerator systems.

3.1 BASELINE PROJECTS

Our path forward in increasing the operating ring current is presented in the next Figure below, where the current in mA is shown in blue and the radiated power from the X-ray sources is depicted in red. We note that two NSLS-II RF systems currently in operations will provide up to 200 kW of RF power.

In FY17, the priorities for machine development is to (a) increase the storage ring current, (b) gain control over the vertical beam size in operations, (c) improve the least reliable hardware, (d) continue creating sufficient redundancy and procuring spares for the least reliable components, and (e) continue establishing a required pool of accelerator spares.

Increase in circulating current (see **Figure 4**): As mentioned previously, we have achieved one of our major goals in FY17 for the NSLS-II accelerator performance - routinely operating at 300 mA for user operations. The increase in FY17 has been accomplished in two steps: from 250 to 275 mA in mid-February and to 300 mA in April. During the May 2017 shutdown, replacement of ceramic vacuum chambers with the newly developed spares is planned provided that coating the chamber in-house produces reliable results. After the machine restart we will test the chamber performance at high current during beam studies to assess the path towards 500 mA.

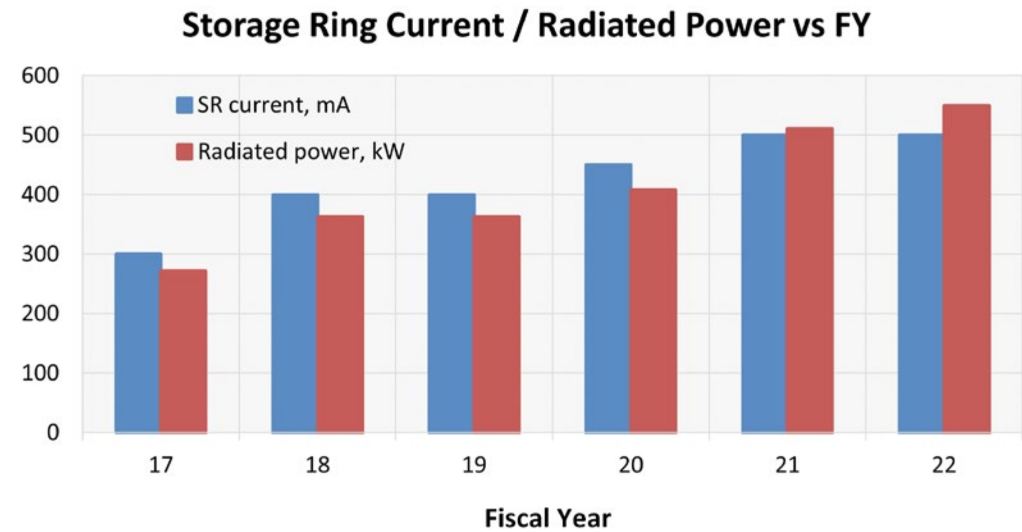


Figure 4: *Projections for NSLS-II operating current ramp-up (blue) and required RF power (red) to support the growing set of NSLS-II beamlines in FY17–FY22; It assumes the operations of all IVUs / EPUs and the three 7m damping wigglers in the current beamline suite, plus one superconducting wiggler (SCW) for a high-energy X-ray beamline.*

Insertion Devices: Another important goal for FY17 is to gain control over beam vertical emittance during regular operations. As demonstrated by recent studies, the beam lifetime varies with the average vertical beam size around the ring. The latter is caused by changes in the ring coupling, i.e. the ratio of vertical and horizontal beam emittances, and these variations are driven by uncompensated sources of skew quadrupole fields in the machine. Some of these skew multipoles originate in the fringe field of small gap insertion devices. We recently initiated a program of studies and simulations focused on analysis and compensation of the spurious skew quadrupole fields. We plan to systematically address the skew quad fields in FY17-18.

In addition, we plan in FY18 to align all installed IDs with respect to beam lines to maximize the brightness of X-ray beams on the detectors. We will use beam-based methods together with capabilities of the beam line instruments for high precision alignment. This program is focused on adjusting the positions of the ID jaws to increase the spectral brightness of the undulator radiation at the working harmonics.

Development of Third RF Cavity: A 3rd 500 MHz RF cavity is required to serve as a hot spare should either of other cavities fail to supply the needed voltage and RF power. This 3rd cavity is also necessary for operation at high current with a full suite of insertion devices, including superconducting wigglers. This 3rd cavity will be installed at the C22 straight section together with the transmitter and the associated cryogenic system. Procurement of the long lead components for the cryo-module was initiated in FY16 with the goal of establishing a spare cavity suitable for replacing either of the installed ones in FY18. Additional funds are required in FY17, FY18 and FY19 to complete the cryo-modules, purchase the transmitter, the cryogenic valve box and the transfer lines, and to deliver the 3rd RF system. According to the technically limited schedule, the 3rd RF cavity will be delivered in FY19 and will serve as a cold spare while the procurement of transmitter and cryo systems is in progress.

Development of 3rd harmonic cavity: The 3rd harmonic 1.5 GHz cavity, operated passively, will increase the beam lifetime by stretching the electron bunch length, thus reducing the frequency of top-off injections and the interruptions seen by the user experiments This cavity and the associated cryogenic system will be located at upstream of the two 500 MHz cavities in C24. A prototype 1.5 GHz cavity was constructed by NioWave and tested in 2012. The current scope includes design and modification of the cryomodule, improved cavity processing (650oC, Buffer Chemical Processing/high pressure rinse of the cavity), design and fabrication of the tuner, procurement of the HOM damper, and the fabrication of the cryogenic connections. The present plan has the harmonic cavity and its cryomodule completed and tested in FY19, and ready for operations in FY20.

Overcoming Heating Issues: Our ceramic chambers are used at the four out-of-vacuum injection kickers in the storage ring to allow the penetration of the fast pulsing kicker field into the beam path. A thin layer of conductive Ti coating is deposited onto the inner surface of the ceramics to allow the smooth passage of the beam image current. Excessive heating of the ceramic chambers was observed during high-current beam studies, which was caused by non-uniform coating. This excessive heating will hinder SR operation at high currents. Further, no spare ceramic chambers are available should one of the existing chambers fail. Bare ceramic chambers were ordered in FY16. An in-house magnetron sputtering coating system is being assembled to coat these spare chambers with Ti in FY17. If coating is deemed suitable, one will be installed in the May 2017 shutdown and high current tests will be carried out. A parallel effort of improved chamber design in collaboration with colleagues at other facilities is planned, and may be started this year.

Improving Injection System: Six cold cathode thyratron type pulse modulators are used in the Booster kickers for injecting linac beam into the Booster and extracting to the SR. These modulators have tripped frequently hindering SR injection and top-off operation. A conventional high voltage modulator has been undergone extensive tests in FY16. Upon successful evaluation, the vendor-built modulators will be replaced with these hot cathode, high voltage switch tubes.

Linac klystrons manufactured by Thales have shown frequent arcs within the vacuum envelope which trips the modulator. These arcs are due to poor design of the tube for operation at the specific cathode voltage. These Thales tubes will be replaced by klystrons from Toshiba. The first Toshiba tube and its associated high voltage modulator was purchased in FY16. The plan is to purchase an additional klystron and modify the associated modulator at the rate of one per year.

100 MeV injection into the booster: The booster synchrotron has been designed to operate in the energy range between 200 MeV at injection and 3 GeV at extraction. The first years of linac operation have demonstrated inadequate performance of the Thales 3 GHz klystrons with frequent trips and faults hindering continuity of top-off and reliability of the NSLS-II operations. While actively pursuing the linac klystron upgrade program, in parallel we initiated an R&D effort focused on enabling lower-energy injection into the booster-synchrotron. The goal of these beam studies is to enable operations with an injected energy of 100 MeV, which requires only a single klystron to power the linac, thereby permitting continued operation if a spare klystron is not available. The low booster dipole fields at 100 MeV present may make it difficult to control the orbit, tunes and matched injected beam envelopes around the machine, leading to excessive losses during injection process. The program will concentrate on studying these issues with low energy booster operation and will seek to develop reliable booster magnet ramps for 100 MeV injection.

New generation of BPM electronics: There are over 200 RF beam position monitors (BPM) in the storage ring, each with 4 BPM buttons. Currently it takes a very long time to get large waveform data from BPM to the Input-Output Controller (IOC). This work will develop new digital front end (DFE) hardware and software, utilizing latest FPGA processor. The new DFE module will be compatible with the existing DFE module. The new DFE will have the bandwidth to stream simultaneously and continuously turn-by-turn, fast acquisition) and slow acquisition data; and permits the use of a standard Linux operating system to drive the functionality of the BPM. The new DFE will be capable of resolution down to 10 nm with fast and large memory. The design and prototype work has started in FY16 and will continue in FY17.

Power Supplies, Utilities, and Instrumentation: There are three quadrupole power supplies delivered by the booster vendor and their charger units have many design and construction issues. Any failure will require extensive effort to trouble-shoot and repair, with spares available at the component level only. The improvement will replace the vendor built units with commercially available switch-mode bridge amplifiers and off-the-shelf commercial power converters, which are easily replaceable should a fault occur. This new design will use the standard NSLS-II power supply regulator chassis with existing PSIs (Power Supply Interfaces) and decouple the operation of these quad power supplies from each other. Design and testing of the prototype quadrupole power supply started in FY16. The fabrication and installation of all units will be completed in FY18.

Deionized (DI) water purification and bleed ports: The DI water needs to have extremely low air and oxygen levels to minimize any galvanic interaction in magnet coils and vacuum cooling channels. This upgrade will pretreat the DI water before it enters the secondary systems. Addition of bleed ports to the 15 secondary DI water pumps will remove the trapped air. Both purification system and the bleed ports can be installed in FY17 and FY18 during maintenance and shutdown periods.

We plan to increase efficiency and expand the capabilities of the controls interface to the Equipment Protection System (EPS) so that the nature of the fault that led to the beam dump is clearly identified. The interface will identify the machine subsystem responsible for the fault, the location of the faulty equipment, and provide diagnostics capable of describing the nature of the failure.

3.2 ACCELERATOR IMPROVEMENTS

The improvements will be required in the following areas: RF, pulsed magnets, diagnostics, controls, insertion devices, utilities and mechanical systems.

The pulsed magnets used for injection and extraction in the booster use thyratrons that have proven to be unreliable in operation and require frequent adjustment. Pulsed magnet development program will focus on producing pulsers with alternative switches to increase reliability and accuracy of the injection / extraction systems. The new units will be built and installed on the operating pulsed magnets as they are completed.

New tools are being developed to measure the vertical emittance with the goal of achieving 8 pm-rad in regular operation. The pinhole optics for the visible synchrotron radiation from the bending magnet in cell 22 has already been improved to increase the photon flux. A pinhole beamline to see synchrotron light from the three pole wiggler in cell 22 in a dispersion region is under development for energy spread measurements. A double slit interferometer using visible synchrotron light is being considered as a complementary way to measure the ultra-small vertical emittance.

A new front-end design has been developed for the x-ray beamlines. This new design has integral Conflat flanges which do not have to be brazed onto the vacuum chambers allowing for rapid production. They are made from a readily available material, CuCrZr, replacing the proprietary alloy, GlidCop, which simplifies the maintenance of a spares inventory. The new design can be manufactured in advance and be easily adapted for individual beamlines. The design has also been adopted at other facilities including at ESRF.

The current beam-cavity RF feedback system is sensitive to beam synchrotron oscillations. It uses a proportional-integral feedback loop on the cavity field error. A low-amplitude feedback on the beam phase error (<1°) will damp synchrotron oscillations. It requires a multiple input, multiple output feedback system and can be realized with state variable feedback resident in the existing RF controller FPGA logic. Possible improvements to the noise floor of beam phase monitor front end electronics may be needed.

The NSLS-II storage ring RF system is powered by conventional klystron amplifiers. Solid state amplifiers have become available and are now used at Soleil, ESRF, and the Swiss Light Source although at different frequencies and lower power than our 275 KW at 500 MHz RF system. The solid state amplifiers are built from many inexpensive parts, there is no HV supply, and consist of many parallel modules. A solid state system may therefore respond to a fault by switching off a single module and may not dump beam. Solid state RF would then benefit NSLS-II with regard to cost and reliability but, without a currently commercially available option, we need to work with vendors to build one for our requirements.

The discussion so far has been devoted to the storage ring RF system but improvements to the LINAC RF are also needed for reliable operation. The lifetime of an S-band klystron is about 30,000 hours. With three (two operational and one hot spare) in service a new klystron must be purchased every two years. They cost $250K and come with a limited warranty of 6 months or 1500 hours. It is a high risk to test them in the LINAC which requires bleeding up the entire waveguide network, removing a functioning klystron, and re-conditioning after installation. To mitigate this, a test stand should be built to evaluate newly purchased klystrons when they are received.

Improvements are being made to methods for correcting the magnetic field in insertion devices and aligning them in the storage ring. The IDBuilder software is being used to optimize magnetic fields for compensation of ID field integrals leading to the optimal radiation spectrum. After installation in the storage ring, final alignment of the beam through the insertion device is accomplished by optimizing the measured x-ray spectrum.

Supporting continuing development of the NSLS-II accelerators requires adequate laboratory space. Labs are needed to troubleshoot malfunctioning equipment, research the cause of system faults, assemble and test equipment prior to installation, and conduct accelerator research and development. The Accelerator Division needs an insertion device lab, an instrumentation and diagnostics lab, a front end assembly and testing area, a pulsed magnet lab, a gun test stand, and a linac test stand preferably all in Building 744. Currently there are nearly 900 sq. ft. of laboratories scattered in cages on the experimental floor and in other buildings on-site.

The existing Accelerator Division computing cluster is about ten years old. It is becoming obsolete and cannot be maintained. A powerful cluster is required for accelerator physics calculations, synchrotron radiation analysis, front-end ray tracing, and shielding calculations. Five nodes approximately 40 cores each were purchased recently and additional nodes may be purchased in the future. The division is also exploring the use of the new BNL computing cluster.

3.3 ACCELERATOR ENHANCEMENTS

Going beyond the NSLS-II design parameters, improvements can be made to the beam stability, the fill pattern, and by installing different types of insertion devices, to the x-ray beam properties.

Beam diagnostic systems. NSLS-II now relies on the RF beam position monitors (BPMs) in the storage ring to maintain beam stability. A more direct measure of the beam seen by the users comes from the x-ray BPMs in the beamlines. Feedback on the x-ray BPM signals can potentially improve the x-ray beam position stability but may cause a fast orbit beam instability. This will be a substantial project to implement but will be important to achieving the ultimate x-ray beam stability if the fundamental sources of drift between the storage ring and the beamlines cannot be located and corrected.

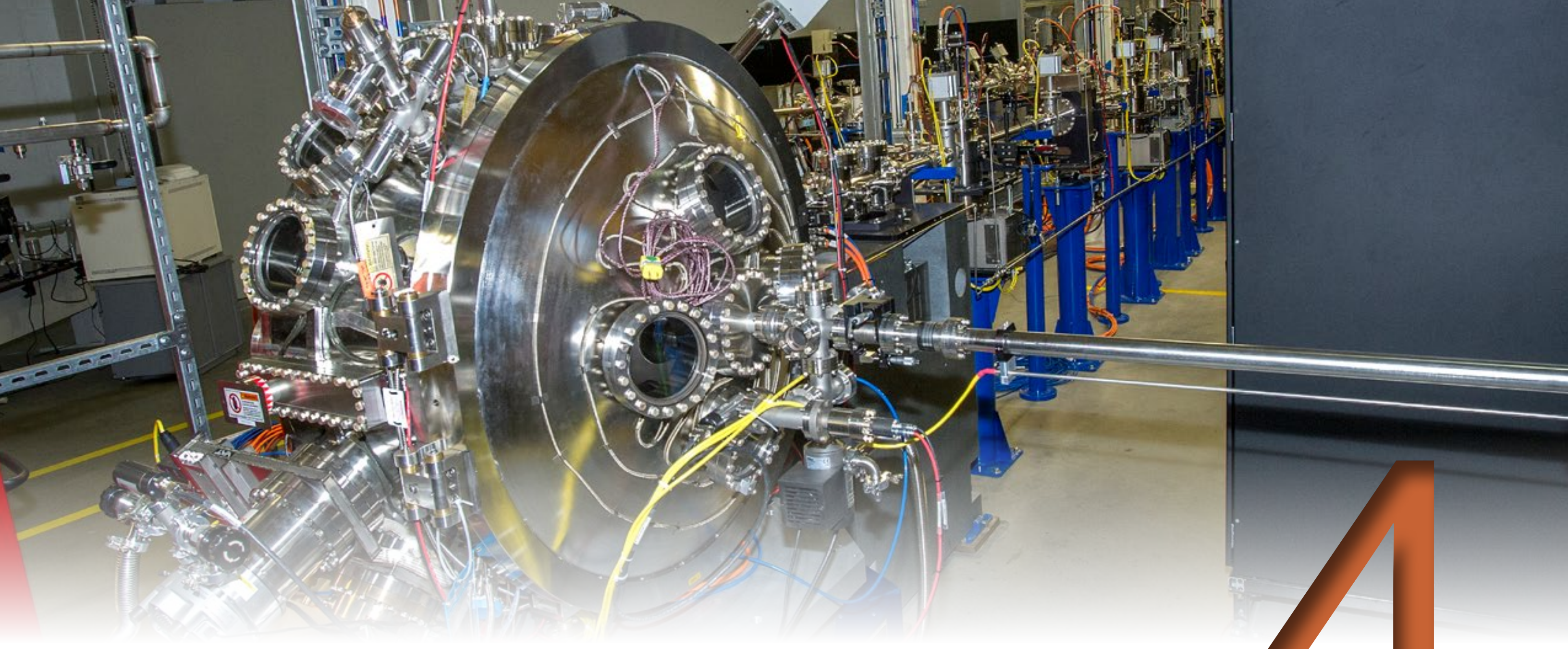
The existing x-ray BPMs rely on commercially supplied photoemission blades. NSLS-II is starting the development of a blade type X-ray BPM which will provide better cooling and closer blade positioning to the beam resulting in better sensitivity and position stability. The existing electronics will still be used.

Optimizing fill pattern. It has been observed at NSLS-II that fill patterns in the storage ring can affect spurious heating vacuum chambers and also the electron lifetime during routine operations. We plan to further explore the different fill patterns for the benefit of improved storage-ring operations. In addition, operation with higher current in a single bunch has been studied both to understand beam dynamics issues and for future operating modes. Measuring a small bunch adjacent to a big bunch requires higher dynamic range diagnostic system than our present system with a 105 dynamic range. An X-ray photodiode can be installed to achieve a 108 dynamic range. This can also be used with transverse multi-bunch feedback for bunch cleaning.

The storage ring is now filled using a pattern of 1056 bunches of electrons followed by 264-bunch gap. (One of the buckets in the gap is filled for use by a feedback system but that is not generally relevant for the users.) Other patterns can be produced to meet user requirements but the ability to produce different patterns is limited by the performance of the electron gun. The linac gun pulser can produce either single bunches or bunch trains. Bunch trains from the gun are not uniform due to the design of the gun pulser. More flexible patterns, such as bunches spaced by more than 2 ns require an upgrade to the gun pulser or another means to shape the bunch train. Adding a beam chopper after the gun will allow better uniformity of the bunch train in the storage ring when multiple short bunch trains are used.

High-Current Single Bunch Operations. The single-bunch beam intensity is limited by transverse mode coupling instability (TMCI) resulted from the single-bunch collective effects. Stabilizing effect of positive chromaticity and fast transverse feedback can effectively suppress this instability and significantly increase the single-bunch current. The longitudinal single-bunch microwave instability does not limit the beam intensity. For example, the operating single-bunch current of APS is 17mA, which is much higher than the microwave instability threshold current of 7mA. But the microwave instability can deteriorate the beam quality because it causes the current-dependent energy spread increase of the electron beam. Longitudinal feedback systems are not effective to suppress this instability and no stabilizing mechanism has been found yet. We will study a possibility to accumulate a high (>20mA) single bunch current in the NSLS-II storage ring in combination with various filling pattern configurations. An important part of these studies is optimization of the transverse feedback system working with a high-chromaticity lattice to determine a principal limit of the single-bunch beam current. We will also study mechanisms of the single-bunch longitudinal instability to analyze the energy spread growth above the instability threshold. The studies will determine conditions and beam parameters at which we can support the hybrid mode operation of NSLS-II.

Reducing β_x at High-β Straights. The NSLS-II lattice was designed with 15 identical, 6.6 m low-beta straights and 15 identical, 9.3 m high-beta straights. At present, the beta functions at the high-beta straights provide an electron phase-space that does match well with the desired phase-space of the X-ray photons produced by insertion devices. This current lattice can be modified to change the beta functions in the individual straights to fit the requirements of specific beamlines if required. The possibilities for the long straight include reducing β_x from 20 m to 6.5 m in the long straight while keeping β_y the same. It is also possible to add a defocusing quadrupole at the center of the long straight to create two 4m straights. We plan to conduct studies to further explore these options and will form a concrete plan to pursue the best path forward in the FY18-19 time frame.



4

EXPERIMENTAL PROGRAMS

In this Chapter, we describe in more detail our planned development activities at NSLS-II beamlines. These planned activities are grouped into two categories – those at the existing operating beamlines or beamlines under construction, and the activities associated with the new beamlines.

4.1 DEVELOPMENT AT CURRENT SUITE OF BEAMLINES

As described in Chapter 1, the NSLS-II beamlines are grouped into six beamline programs based on commonalities in beamline techniques and science applications. The planned development activities for all these programs follow our strategic development directions in Chapter 2, as well as our priorities in (i) developing impactful user science programs at operating beamlines, (ii) delivering new beamlines currently under construction, (iii) improve beamline performance and efficiency to accommodate more users, (iv) optimizing and enhancing capabilities to deliver more high-impact science, and (v) starting to develop additional new beamlines to meet the additional research needs of the scientific community

4.1.1 Soft X-ray Spectroscopy & Scattering

The soft x-ray scattering and spectroscopy program at NSLS-II centers around the following two science focus areas:

- *Understanding and controlling the physics of quantum materials and their emergent behavior on the nanoscale.* This area focuses on electronic properties of quantum materials using such techniques as infrared (IR) spectroscopy, resonant elastic X-ray scattering (REXS), resonant inelastic X-ray scattering (RIXS), and angle-resolved photoelectron spectroscopy (ARPES). Applications include understanding the role of nanoscale electronic textures, and the role of reduced dimensionality systems with a view to exploiting quantum materials in useful devices.
- *Studies of energy relevant catalysis in operating conditions using real catalyst materials.* This area focuses on transforming catalysis experiments from model systems to real materials under catalytic reactions, and from experimental environments e.g. high vacuum to realistic pressures such as near ambient pressure and above, based on ambient pressure photoelectron spectroscopy (AP-PES).

At present the Soft X-ray S&S program develops and operates six soft X-ray and IR beamlines. Our development plans at these six beamlines are described below.

Coherent Soft X-ray Scattering Beamline (CSX-1, 23-ID-1). CSX-1 is a soft x-ray scattering beamline optimized for coherent flux with full polarization control in the range 200-2000 eV. Aside from remarkable capabilities in "standard" resonant techniques, like reflectivity, scattering and diffraction experiments, the beamline has shown its potential in coherent scattering and diffraction imaging, XPCS and in imaging via zone plates on a series of strongly correlated materials, like high Tc superconductors (see **Figure 5**), colossal magneto-resistivity, and frustrated magnetic materials. The possibility of investigating electronic orders and their dynamics and inhomogeneities has already proved central in understanding some of the peculiar subtleties in the complex and intriguing phase diagrams of these materials, where forefront quantum behaviors and possible innovative device functionalities are to be searched.

The future plans of CSX-1 aim to consolidate the above capabilities and enhance them to include sample perturbations like electric field, currents, magnetic fields, and IR laser heating. These enhancements will broaden the investigation of electronic competing phases and interaction between electric and magnetic degrees of freedom, and in particular looking at interfaces. In parallel, new techniques aimed at understanding surfaces in terms of their structures, reconstructions and dynamics will be implemented, in order to provide the scientific community with innovative approaches for a complementary perspective to the fascinating world of matter facing vacuum. In summary, CSX-1 will investigate the electronic and structural properties of hard condensed matter by exploiting coherent soft x rays, in order to reveal the behavior of relevant electrons in relation to external stimuli, localization, chemical composition and thermodynamic characteristics of the samples.

During FY17, technique development for phase retrieval for coherent diffraction patterns will start with test samples to develop both ptychography and coherent diffraction imaging in partnership with the Condensed Matter Physics and Materials Science Division at BNL. The relevant hardware is currently installed at 23-ID-1 so commissioning will focus on starting with test samples and then moving to system of interest in the area of quantum materials. In parallel, development of IR laser heating will start. During FY18 first science commissioning experiments will be undertaken on both these developments. Once commissioned, the coherent diffraction imaging capability will be entered into the user program possibly in late FY18. In the period FY19 to 21, these techniques will be fully integrated into the user program with the CSX-1 team actively working with the user community.

Soft X-ray Spectroscopy Beamline (CSX-2, 23-ID-2).
CSX-2 is a soft x-ray spectroscopy beamline that currently includes two endstations. The ambient pressure photoelectron spectroscopy (AP-PES) endstation, operated in partnership with the CFN, can be operated with a maximum pressure of 5 Torr and sample temperature of up to 900°C (see **Figure 6**). The IO-XAS endstation is dedicated for ex-situ samples at present, and reactor cells are currently in development. The scientific focus of the beamline is in situ soft x-ray spectroscopy of energy processes and materials, specifically heterogeneous catalysis. Catalysis is an important process that contributes to ~35% of the world's GDP and accounts for ~85% of processes in the chemical industry. These include the production of fuels, polymers,

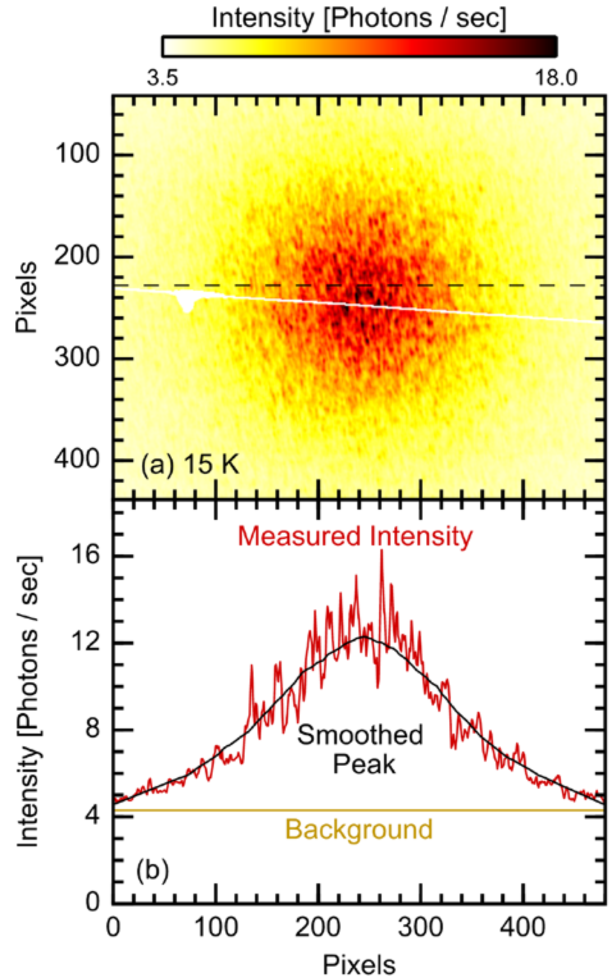


Figure 5: *a) Coherent scattering image from the La2-xBaxCuO4 1/8 CDW Bragg peak at 15 K. The white diagonal line is an artifact from the beamstop. (b) A line cut of the measured intensity taken on the dotted line in panel (a) is shown in red. Black and yellow lines indicate the smoothed peak envelope and the fluorescence-dominated background, respectively. The speckle modulations on top of the peak arise from coherent interference between different CDW domains [9].*

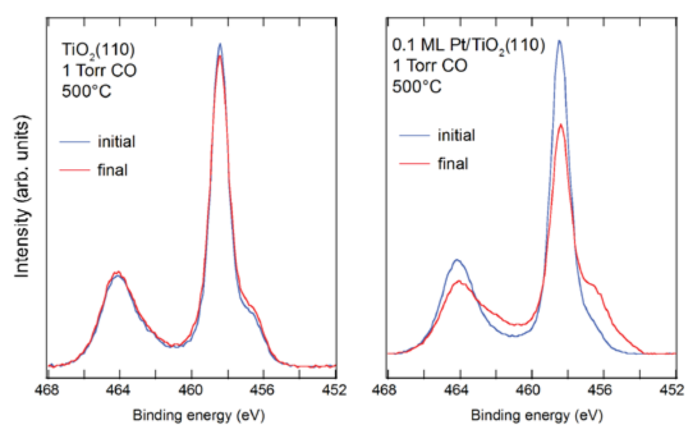


Figure 6: *(Left) Ti 2p AP-XPS spectra of bare TiO2(110) in 1 Torr of CO at 500°C, showing no change in the oxidation state of Ti. (Right) On the Pt-modified surface under the same experimental conditions, TiO2 is reduced by CO and Ti4+ is converted to Ti3+ and possibly Ti2+.*

medicine, and other chemical products. In addition, catalysis is crucial in the production of clean and renewable energy, for example through biomass conversion or the use of fuel cells, and thus is one of the key missions of BNL and DOE. Through in situ techniques such as AP-PES and XAS, we can observe changes in the oxidation and chemical state of the components of the catalyst and of the adsorbed chemical species, identifying surface intermediates, and determining reaction mechanisms under working reaction conditions. This information will lead to the improved design and synthesis of more efficient catalysts.

In FY17, in collaboration with the CFN, we will begin the technical development and construction of a new capability of adding simultaneous AP-XPS and IRRAS measurements using an IR source (globar/SiC). We will also install and start technical commissioning of the in situ reactor cell for the IO-XAS endstation. In FY18, we will commence technical commissioning of the combined AP-XPS/IRRAS endstation and science commissioning of the IO-XAS reactor cells. By the end of FY18, we expect to start science commissioning with users for the AP-XPS/IRRAS endstation and general user operation of the IO-XAS reactor cells.

In FY19-21, the AP-XPS/IRRAS endstation will be fully operational for general user operation. In addition, the potential development of the INF beamline would allow us to transition from the lab IR source to a synchrotron one, providing significantly higher brightness (up to 3 orders of magnitude) as well as an extended spectral range into the far-IR region (down to 300 cm-1) that cannot be achieved using a lab source. This would be a unique instrument in the world.

Electron Spectro-Miscroscopy Beamline (ESM, 21-ID). The Electron Spectro-Microscopy (ESM) beamline is a wide range (15 – 1500 eV), high resolution (ΔE/E =105, below 100 eV; 104 above), microscopy instrument dedicated to the study of the electronic structure of solids. The beamline features two microscopy end stations, an endstation for high-energy resolution angle-resolved photo-electron spectroscopy (ARPES) measurements, with the ability for scanning microscopy (lateral resolution 1μm) and, in partnership with the CFN, a full-field aberration-corrected X-ray photo-emission electron microscopy (AC-XPEEM) for high lateral resolution measurements (10 nm).

In terms of energy resolution, flux and sample handling, ESM has been conceived to play a forefront role in advancing our understanding of the fundamental physics and chemistry of correlated materials with a particular emphasis on two-dimensional systems. The combination of the two complementary microscopes (μ-ARPES: high energy/low lateral resolution and XPEEM: low energy/high lateral resolution) makes ESM an extremely versatile instrument, capable of high impact on practically any conceivable study of the electronic structure of materials.

The new science areas of ESM are closely coupled with its unique capabilities. The *1 meV energy resolution* will attempt to fill the gap between transport measurements (where meV resolution is routine but k-information is conspicuously absent) and ARPES data which directly display the anisotropic character of the electronic structure and, most crucially, of its low energy excitations.

By using the *1 μm spot size*, entirely new experiments become possible. First, most simply, smaller samples become measurable: this is highly relevant. Newly synthetized crystalline materials are often very small. Few microns are typical sizes. Additionally, poly-faceted surfaces resulting from cleaved samples are also a common occurrence even in larger samples. ESM, however, also aims at using the small spot for imaging. The development of high-resolution ARPES with 1 μm lateral resolution will allow the study of polycrystalline samples with grain sizes of a few microns or even demagnetized samples with magnetic domains of a few microns. The latter is particularly relevant in ferromagnetic materials where spin-resolved mapping of bands has been particularly hampered by the impossibility of combining high magnetic fields with photoelectron electron spectroscopy.

Finally the *wide energy range* allows detailed ARPES studies to be performed utilizing soft x-rays, owing to the superb angular resolution now routinely achieved by modern electron spectrometers equipped with 2D detectors combined with the superior flux of ESM. The main advantage of using this energy range is the reduced surface sensitivity. High energy soft X-ray also provides access to the core levels. These provide immediate sample characterization tools (to assess stoichiometry and/or contamination) as well as resonant photoemission channels for selectively probing various portions of the electronic structure.

During FY17, ESM will begin to install and commission the MBE system in partnership with Yale University. This year they will work towards being able to fabricate 2-dimensional quantum materials. In parallel with this work, the design will be started on the "sample highway" to connect the MBE system with the ARPES endstation for sample transfer under ultra-high vacuum. This transfer is essential to ensure no surface contamination. In FY18, depending on available budget, construction will start on the sample highway and integration of the MBE system with the ARPES endstation. During this construction, science commissioning experiments will start on samples fabricated in the MBE system. In FY19 to 21 the combined MBE and ARPES experiments will be offered in general user operations at ESM.

Soft Inelastic X-ray Spectroscopy (SIX, 2-ID). At SIX, resonant inelastic X-ray scattering (RIXS) experiments will be carried out with a world-leading energy resolving power of 70,000 and the ability to continuously vary the momentum transfer. This will enable studies of low-energy collective excitations of the charge, spin, and orbital degrees of freedom of the electrons in both 2D and 3D materials.

The research on electron correlations has recently started to make inroads into energy science applications, inspiring new ways to improve the efficiency of solar cells and rechargeable batteries. While this is encouraging, a deeper understanding of the underlying physics still needs to be gained before electron correlations can have a significant impact on clean energy technologies. At SIX, novel experiments on correlated electron materials will be carried out with the aim to advance the quest for real-world smart energy solutions.

In FY17, the SIX beamline will complete its construction and transition into operations with commissioning. We expect that this beamline will start taking science commissioning users in FY18. In FY19-21, the core RIXS capabilities at SIX will be fully operational and will enable research on investigations of collective electronic excitations in a variety of hard condensed matter systems including the following classes of technologically relevant materials:

- High-temperature superconductors: RIXS, as a phase and bulk sensitive technique, has tremendous potential for probing the superconducting order parameter. At SIX, this potential will be exploited for the first time thanks to the world-leading energy resolving power. Element and momentum-resolved measurements of excitations across the SC gap will become possible in various Cu and Fe-based high-temperature superconductors, which will help address long-standing questions about the importance of spin and orbital fluctuations in the pairing mechanisms of these systems.
- Topological insulators: SIX will join the recent quest for topological phases in correlated electron systems, especially in lanthanide-based materials where the combination of spin-orbit coupling and hybridization between the f and conduction orbitals provides a seedbed for robust topologically insulating states. RIXS measurements of excitations across the bulk hybridization gap in an element, orbital and momentum-resolved fashion will be an important stepping stone in this quest.
- Heterostructures: Studies at SIX will help improve our understanding of the connection between emergent phenomena in heterostructures and the interfacial electronic structure, by applying the x-ray standing wave technique to RIXS. Of particular interest will be the study of 2D high-temperature superconductivity emerging in heterostructures.

Frontier Infrared Spectroscopy / Magneto-Ellipsometric & Time-resolved IR Spectroscopy (FIS/ MET, 22-ID/22-BM). FIS/MET is a pair of IR beamlines currently under development located in the cell 22 floor space using 23-BM as its source. Infrared spectroscopy serves as a highly flexible probe of both low-energy electronic and vibrational excitations of materials under a wide range of conditions (temperature, pressure, magnetic and optical fields), complementing other spectroscopic and structural probes. It is expected that the FIS/MET beamline will finish its construction and start commissioning in FY18, and that the beamline will quickly ramp up its science programs in FY19 in the following areas.

Materials Under Extreme Conditions: NSLS-II will continue its partnership with the Consortium on Materials under Pressure (COMPRES) for the study of materials as a function of both pressure and temperature. The main focus is the behavior of crystalline and molecular solids under conditions found in planetary interiors, resulting in novel phases and physical properties. These include the capacity of the Earth's mantle to store water and the behavior of metallic hydrogen. The combination of pressure and temperature can result in complex electronic reconfigurations that lead to phenomena such as superconductivity. NSLS-II will work with COMPRES to provide this capability to the scientific user community.

Condensed Matter Physics: Infrared and THz spectroscopy will continue to be important for investigating novel solid state systems, in concert with other tools for tuning material properties. These include temperature, pressure, field and light-excitation (e.g. photo-doping). Systems of interest include complex oxides displaying competing orders, topologically controlled phases and 2D materials such as graphene, h-BN & metal dichalcogenides, and nanomaterials. Ideally, the spectroscopic and "tuning" ranges should match the behavior to be studied. In some cases, expanding these ranges with access to higher fields & pressures, and lower temperatures, will be important. To fully explore a material's phase space will require combining the various tuning methods into a single endstation.

Materials Physics: Infrared and THz spectroscopy senses electronic properties relevant to transport and light energy harvesting. Photo-induced and time-resolved spectroscopies can detect exciton binding energies and lifetimes, while magnetospectroscopy can sense effective masses and carrier mobilities. For time-resolved spectroscopies, existing laser systems will serve for some measurements, but access to a 500 MHz synchronized laser system will expand our capabilities for utilizing the NSLS-II normal operation mode.

Chemical / Environmental / Biomedical and Space Mineralogy: Infrared will continue to be a powerful probe of molecular vibrations and have substantial impact across most of the sciences. This is especially true when spectroscopic imaging is included for the study of heterogeneous materials as found in the natural environment.

4.1.2 Hard X-ray Spectroscopy

The Hard X-ray Spectroscopy program operates and develops three facility beamlines ISS, TES, and QAS, and three partner beamlines SST-1, SST-2, and BMM in partnership with NIST. With these world-class beamlines, the Hard X-ray Spectroscopy program provides a wide range of spectroscopic tools in the soft, tender and the hard X-ray energy range that are often combined with simultaneous diffraction techniques such as powder diffraction. Its scientific focus is aimed toward the science of energy conversion and energy storage, *e.g.* battery research, electrochemical catalysis with emphasis on fuel cells and heterogeneous catalysis, and materials growth, especially the development of thin film growth methods, growth suppression, atomic layer etching, and structural and chemical changes during heat, plasma, and radiation treatments. A second aspect of the program is dedicated to the carbon-cycle and to carbon-sequestration, including grain-scale biogeochemistry, bioavailability, transport and global cycling of essential nutrients (Mg, P, K, Ca, Fe), and heterogeneous catalysis for biofuel production.

The objective of spectroscopy is to probe the chemical and structural nature of matter independent from any long-range order. In concert with other averaging techniques like small angle X-ray scattering or resonant and non-resonant diffraction experiments, a complete picture of the sample ensemble is provided regarding chemical structure, morphology, and ordering effects, and is used to guide additional microscopic investigations if needed.

In comparison to other facilities worldwide, the program beamlines are state-of-the-art by providing not only exceptionally high flux in the various energy ranges, but also fast energy scanning capabilities at high data quality. As a consequence, data acquisition times for a full EXAFS spectrum are feasible in a seconds time scale, allowing researchers to follow the dynamics during processing. In addition, it also permits the use of X-ray spectroscopy as a high-throughput technique for combinatorial materials research for the first time. Building on this fast-scanning capability, the program will focus on *operando* characterization of complex hierarchical structures like those typically used in energy conversion and storage, and on *in-situ* experiments in the materials growth and processing area for kinetic and/or dynamic studies.

A characteristic of these scientific areas is a strong diversity of the user community bridging basic science, applied, and industrial sciences. The challenge in the coming years will be to provide appropriate user support for these communities, including appropriate access modes and data management, developing the necessary laboratory infrastructure to pre-characterize and operate sample materials, and to establish the beamline suite as an important resource in the funding landscape of these areas. We plan to work with the user community and integrate community interest in mutually beneficial partnerships, such as the Synchrotron Catalysis Consortium, into strong research programs at our suite of beamlines.

To provide excellence in user support, essential for this community, and at the same time to steer the scientific program we will combine a strong and well organized support group which focuses on the direct user support and handles most of the day-to-day user needs, with a strong in-house science program in battery research, electro- and heterogeneous catalysis, materials growth, and carbon cycling, allowing scientific interaction at the highest level with key user groups driving their respective research fields. Our specific plans to do this are outlined below.

<u>Inner-Shell Spectroscopy (ISS, 8-ID)</u> is a high-flux hard X-ray spectroscopy beamline based on a damping-wiggler source and is optimized for *operando* and *in-situ* experiments. By the end of FY17, all existing hardware at ISS will be commissioned and the controls software developed. This work will include the integration of the automated sample changer of the sample chamber, the Gas Handling System (GHS) and the commissioning of the two von Hamos spectrometers. As of March 2017, a high throughput setup with a hundred samples capability has been installed in 8-ID-B2 and commissioned. To enable high resolution spectroscopy a fast scanning three-element backscattering analyzer system, synchronized with the monochromator, will be developed; this system will be integrated into the sample chamber and can be replicated as additional resources become available (up to three systems can be integrated).

The science program we plan to pursue at ISS includes the following. In *battery research*, we will develop the first test experiments to evaluate high throughput capabilities and create baseline experiments. We will start to develop a data-mining project which combines structural, electronic, and functional data; In *electrocatalysis*, we plan to develop an electrochemical cell that can be used as a half and full cell for gaseous and liquid fuels; the system will allow one to probe the cathode and anode independently, and can be used on other program beamlines and be compatible with tomographic investigations. In *heterogeneous catalysis*, we will evaluate various gas flow reactors, provide baseline experiments for time resolution and the GHS, and demonstrate modulation spectroscopy with proper data analysis tools. We also plan to create a support laboratory to enable these in-house and user research and development projects on catalysis. In *materials growth*, we are focusing on high-throughput ex-situ experiments with the goal of testing new access modes and developing semi-automatic data processing.

In FY18, we plan to construct and commission an initial set of sample environments, compatible with the automated sample changer for battery research, electro-chemical cells, and chemical gas-flow-reactors. These cells will be also used at QAS and TES. The high throughput setup will be equipped with a 100-element electro-potentiostat allowing high throughput battery and electro-chemistry experiments, and the sample chamber will include an integrated powder diffraction detection system available for baseline experiments. In addition, a first Atomic Layer Deposition (ALD) test reactor will be installed and commissioned in 8-ID-B2.

The science projects we plan to pursue in FY18 include the following. In *battery research*, we will continue to pursue high throughput battery research and create an associated industrial user program. We will expand our capabilities to develop a reliability research program by starting long term experiments, and evaluate experimental techniques to study degradation of the cathode/anode. In *electro-catalysis*, we plan to focus the in-house program on nanoparticle stabilization and create lab infrastructure to plasma treat samples. We will develop multimodal analysis tools to analyze TES and ISS EXAFS data simultaneously, and develop a MEMS-based cell. In *heterogeneous catalysis*, we will develop a high-pressure reactor sample cell, and focus the in-house program on nanoporous catalytic systems with a focus on selectivity, developing broad user base for low pressure experiments at ISS, and exploring the multimodal data analysis approach that includes EXAFS and XRD data. In *materials growth*, we will develop a large area (full wafer) spectroscopy probe and focus the in-house program on commissioning of the first ALD test reactor with Ti-O and Zn-O growth baseline experiments for sensitivity and time resolution calibration. We will also develop multimodal data analysis approaches for spectroscopy data and diffraction data at ISS and BMM.

In FY19-21, we envision that key *operando* experiments, like the high throughput battery system, the heterogeneous catalysis flow reactor, and the MEMS-based electro-chemistry cell will be fully implemented at ISS, and our main focus will be to continue to broaden our user base and produce high-impact science. In addition, the program will work with the other Programs to provide common sample and data analysis platforms.

Quick X-ray Absorption and Scattering (QAS, 7-BM) is a high-throughput hard X-ray beamline based on a 3-pole wiggler source, with combined spectroscopy and diffraction capabilities. The beamline will start commissioning by end of FY17. Our development plan in the next five years for this beamline is outlined below.

In FY17, QAS will be fully constructed and installed, and first beam is expected at the end of FY 17. In addition to the beamline, the highest priority for QAS in this year is the upgrade of the monochromator system including updated controls. This will allow the use of all scanning software developed at ISS at QAS. To allow heterogeneous catalysis operando experiments we will also evaluate various options for GHSs and implement (ongoing in FY18) a minimal version.

In FY18, the main focus of QAS is to commission existing capabilities and bring the beamline into general user (GU) operations. At the end of the year, battery and electrocatalysis experiments will be available for GU experiments and the general catalytic experiments will be ready for scientific commissioning. Budget permitting, the GHS will be optimized for the fast scanning capability of the beamline and extended to the full gas range, including toxic and corrosive gases.

In FY19-21, QAS will be in mature GU operations, and will fully support the wide range of science programs within the hard X-ray spectroscopy beamline suite, including battery research, catalysis, and materials growth and characterization.

Tender Energy Spectroscopy (TES, 8-BM) is a unique X-ray beamline optimized in the tender energy range of 1-8 keV using a bending magnet source. The TES beamline is undergoing science commissioning and will start general user operations by end of FY17. Our development plan in the next five years for this beamline is outlined below.

In FY17, the TES beamline is in commissioning phase. The main focus is to establish its core capability in tender-energy micro-spectroscopy, focused on environmental and geobioscience studies. TES will be able to provide baseline capabilities for spatially resolved XRF and XAS and will implement the necessary data analysis tools. In addition, we plan to explore the use of TES for battery research to enable spectroscopy measurements on next generation batteries at e.g. Na, S, and P edges.

In FY18, we will start general user operations at TES with its tender-energy spectroscopic microprobe endstation. The in-house program will initially focus on nutrient biogeochemistry and cycling for sustainability, and will be correlated with the electro-catalysis program at ISS.

To allow *in-situ* and some *operando* experiments at TES we plan to design a liquid flow cell with infrastructure support. This system will be compatible with the ISS and the QAS beamlines. The controls system of this beamline will be upgraded to be compatible with the data architecture used at ISS (budget permitting). An additional GHS, possibly based on a mobile system using lecture bottles with limited gas selection will be implemented allowing *operando* heterogeneous catalysis experiments.

In FY19-21, TES will be in mature user operations, providing its unique capabilities as a tender-energy microprobe for all science programs across TES, ISS, and QAS, as well as XFM, with a broad user base. Budget permitting, an additional vacuum compatible miniature endstation will be combined with the existing environmental chamber. This chamber will allow the use of all ISS sample environments at TES. In heterogeneous catalysis, we plan to establish a user base for pressure-dependent experiments at TES including the development of a high pressure capability. We will also pursue studies on the poisoning of catalysts including corrosive gases. In the materials growth area, we plan to develop a growth reactor for the tender energy range, develop a CVD reactor for SiC (budget permitting), and further enhance integration with field studies in BNL and with communities at large.

Partner beamlines:
The three partner beamlines SST-1, SST-2, and BMM significantly extend the experimental capabilities of the program beamlines in the hard, tender and soft energy range. Funded and supported by NIST and IBM, the beamlines will be fully operated by the partner team (including the GU fraction) providing 40% PU time, up to 10% beamline staff time, and 50% GU time; the program will provide additional support for maintenance and data management as needed.

Spectroscopy Soft and Tender (SST-1 and SST-2, 7-ID) is a canted insertion device beamline which provides a soft energy branch (SST-1) with an energy range from 100eV to 2.2keV and a tender energy branch (SST-2) with an energy range from 1keV to 7.5keV. With seven different endstations, the beamline allows a wide range of XAS experiments with micro- and nano- spatial resolution, full-field imaging, and X-ray Photoelectron Spectroscopy. Truly unique feature of the beamline is the capability to use both sources simultaneously in two of the endstations, providing an energy range of 100eV-7.5keV. The scientific program of the beamline is focused on materials science in the area of soft matter, hard matter, and compound materials utilized in energy storage, energy conversion, and electronics.

In FY17, SST-1 and SST-2 will be under construction and mostly installed; first beam is expected in the middle of FY18. A detailed commissioning plan will be prepared as a part of the Instrument Readiness Review, laying out when the individual capabilities will be available. It is expected that first science commissioning experiments will be performed at the beginning of FY 19 and the full suite of tools be available to general users by end of FY19 or beginning of FY20.

Materials Measurement (BMM, 6-BM) is a high flux 3-pole wiggler beamline optimized for hard X-ray spectroscopy and diffraction. Providing two end-station setup, the beamline offers an EXAFS setup with large flexibility for sample environments and a six circle diffractometer allowing various diffraction techniques, including pole figure, crystal truncation rod, anomalous diffraction, and powder diffraction measurements. The scientific program is focused on hard matter materials sciences, heterogeneous catalysis, battery research, and electro catalysis.

In FY17, BMM will be fully constructed and installed, and first beam is expected at the beginning of FY 18. In FY 18, the beamline will be fully commissioned and the XAFS and diffraction capabilities will be fully developed. To ensure a fast ramp up of the beamline a strong collaboration between the BMM staff and the program staff is envisioned; this includes exchange of sample environments for operando and in-situ experiments, software developments, and the utilization of a transportable gas handling system currently developed by ISS. In FY 19-21, the beamline will be transitioned to general user operations and fully developed.

4.1.3 Complex Scattering

The Complex Scattering Program focuses on soft matter and nanomaterials research that can be captured under two main scientific themes:

Theme 1 – Studies of relationship between function, structure and dynamics in hierarchically ordered and engineered nanomaterials to understand

- how order and fluctuations, both position and orientation, and phonon band structure relate to macroscopic material properties and then to use this knowledge to develop improved materials, and
- functional and structural behaviors under variable environmental conditions (temperature, pressure, stress, flow) and in responsive systems.

Theme 2 – Processing & printing of soft/bio/hybrid materials (films & fibers) for energy, advanced manufacturing & filtration applications with an objective to

- improve our understanding of equilibrium and non-equilibrium dynamics in polymers, colloids, membrane, and composite materials with the aim of controlling functional properties, mass transport and other macroscopic properties, and

- use advance manufacturing processing approaches to develop nanoarchitectures and hierarchical order with the aim of producing functional devices with enhanced properties.

Research covered by the first theme supports the BNL Laboratory Agenda to *Expand Nanoscience Research* while research covered by the second theme is a new direction that strives for a more fundamental understanding of the physical principles underlying advanced manufacturing processing of soft materials and nanoscale architectures into devices. The theme addresses the DOE Grand Challenge to *Understand and Control Systems Far from Equilibrium* and, as described in section 7.8, is a collaborative effort between *NSLS-II, CFN, NIST, and the AFRL*.

The beamlines in the Complex Scattering Program, combined with the NIST SST beamlines, provide a complete suite of scattering and spectroscopy techniques that cover energies from 100eV to 24 keV. Soft X-rays provide contrast between different polymers while hard X-rays allow exploration of deeply buried interfaces; soft and hard X-ray photon correlation spectroscopy, inelastic X-ray scattering, and time-resolved SAXS/WAXS/GISAXS all probe fluctuations and kinetics; micro-focused beams resolve spatial inhomogeneities; wide q-range capabilities enable the study of ordering on multiple length scales; robotic sample handlers and machine learning approaches intelligently map processing and materials parameter space; and spectroscopic imaging maps chemical states. The suite of beamlines supports collaborative research efforts of the NSLS-II and CFN staff and impacts an even broader range of soft and hard complex materials science for the user community. A representative research example is shown in **Figure 7**.

The following subsections describe the four existing NSLS-II Complex Scattering Program beamlines in more detail, the schedule for commissioning different capabilities, planned beamline enhancements, and their impact on the broad user community. There is also a subsection on the proposed jump-start of a new liquids and processing capability that will form the basis for the future PLS beamline described in section 4.2.

Inelastic X-ray Scattering Beamline (IXS, 10-ID). The inelastic X-ray scattering (IXS) beamline is dedicated to ultrahigh resolution studies of phonon dynamics in an energy and momentum space important for understanding the properties of industrially relevant materials systems that exhibit complexities and inhomogenieties at mesoscopic length scales. The IXS beamline incorporates a novel spectrometer based on an angular dispersion crystal optics scheme, operates at a medium energy of 9.1 keV, has a demonstrated energy resolution of 1.5 meV with substantial gain in spectral contrast, and a momentum resolution of 0.2 nm^{-1}. Further technical improvements will focus on improving the energy resolution to sub-meV and the counting efficiency by 5-10 times through upgrade of the insertion device and multiplexing the analyzer system. In addition, to take full advantage of the small focused beam (5-10 μm), sample environments for extreme pressure and temperature, including a dynamic DAC to create conditions far from equilibrium or for metastable states, will be developed to expand the accessible range of thermodynamic conditions; and data acquisition and analysis software will be streamlined to improve user productivity at the beamline. *Improving the counting efficiency requires substantial investment but is crucial for the IXS to be truly competitive with sustained scientific productivity.*

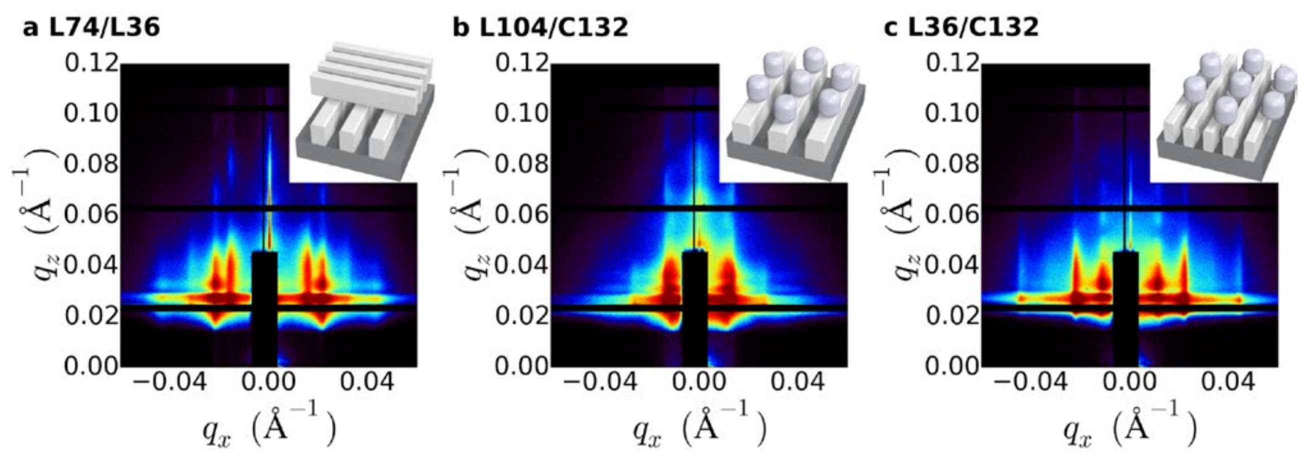


Figure 7: *A representative study undertaken in the Complex Scattering Program: GISAXS patterns from multi-layered alumina nanostructures fabricated using block-copolymer self-assembly. (a) Two lamellar layers, with the second-layer oriented perpendicular to the first and thus ordered with an unperturbed repeat-spacing. (b) Roughly commensurate lamellar and cylindrical layers. A single set of scattering peaks is observed, since the repeat-spacing of the cylindrical layer distorts slightly to match the underlying lamellar layer. (c) Example of two-layer ordering where the lamellar and cylindrical layers have very different repeat-spacings. In this case, the cylindrical layer distorts its spacing to become commensurate (1:2) with the underlying lamellar layer. The GISAXS measurements, carried out at CHX, provided structural confirmation that soft self-assembling block-copolymer phases can be manipulated to form a diverse library of previously unreported morphologies [10].*

The improved energy resolution with significantly enhanced spectral contrast will be a key and unique strength of the IXS spectrometer at NSLS-II compared to other existing IXS facilities around the world. It will enable studies of low-energy vibrational dynamics from nanoscopic to mesoscopic length scales at low Q, which is expected to lead to new insights on phononics in functional nanostructured soft materials with potential applications in thermal management; on fast dynamics of bio-molecular systems and their roles in biological functions; and on the relaxation processes underlying the rich variety of phase transitions in the intermediate regime in liquids and glasses. Beyond soft and/or disordered materials, IXS is expected to contribute strongly to the study of thermoelectric and ferroelectric thin films and the composite materials where the coupling of phonons with electron and spin degrees of freedom plays an important role in their material properties.

In FY17, we plan to pursue the following developments (in priority order): (a) Develop/procure a single-reflection paraboloidal multilayer mirror to replace the Montel mirror of the analyzer optics to improve the reflectivity by nearly a factor of 2; (b) Identify and establish collaboration with external vendors to improve the quality of the high-resolution crystal optics with the goal to improve the energy resolution of the IXS spectrometer to below 1 meV; (c) Improve the thermal stability of the high-resolution crystal optics to limit energy drift to less than 0.1 meV over 12 hours to facilitate long data collection time; (d) Complete the development of sample environments for humidity and temperature control for bio samples, and the integration of a membrane DAC with the existing cryostat; and (e) Implement and develop streamlined software for experimental control, data acquisition and online analysis within the NSLS-II standard BlueSky framework.

In FY18, we plan to (in priority order): (a) Achieve routine operation at sub-meV resolution; (b) Pursue the possibility of obtaining a prototype superconducting undulator as part of the APS-U R&D effort; and (c) Complete the development of the dynamic DAC and the integration of the online Ruby system for pressure characterization.

In FY19-21, we plan to (a) pursue multiplexing of the analyzer system to 3 or 5 analyzers, and (b) work with user community to discuss further improvements to IXS beamline.

Coherent Hard X-ray Scattering (CHX, 11-ID) Beamline. The Coherent Hard X-ray (CHX) beamline offers its user community a best-in-class instrument for coherent scattering and X-ray Photon Correlation Spectroscopy (XPCS) in the 6-16 keV range with beam sizes between 2-10 µm. The beamline has started user operations with a coherent-SAXS capability and will develop coherent-WAXS and coherent-SAXS/WAXS operations using coherent, silicon-resolution, monochromatic beams. CHX will also add the capability of a wide-bandpass monochromator, which will increase its coherent flux by a factor of up to 30 over existing facilities, thereby enabling the measurement of dynamics on time scales 900 times faster than previously possible.

The development of the coherent-WAXS capability will enable the study of dynamics approaching atomic length scales, an area which may be uniquely addressed by X-rays and cannot be covered by other techniques. The technique capabilities of CHX will be enhanced by the addition of advanced sample handling instrumentation, such as

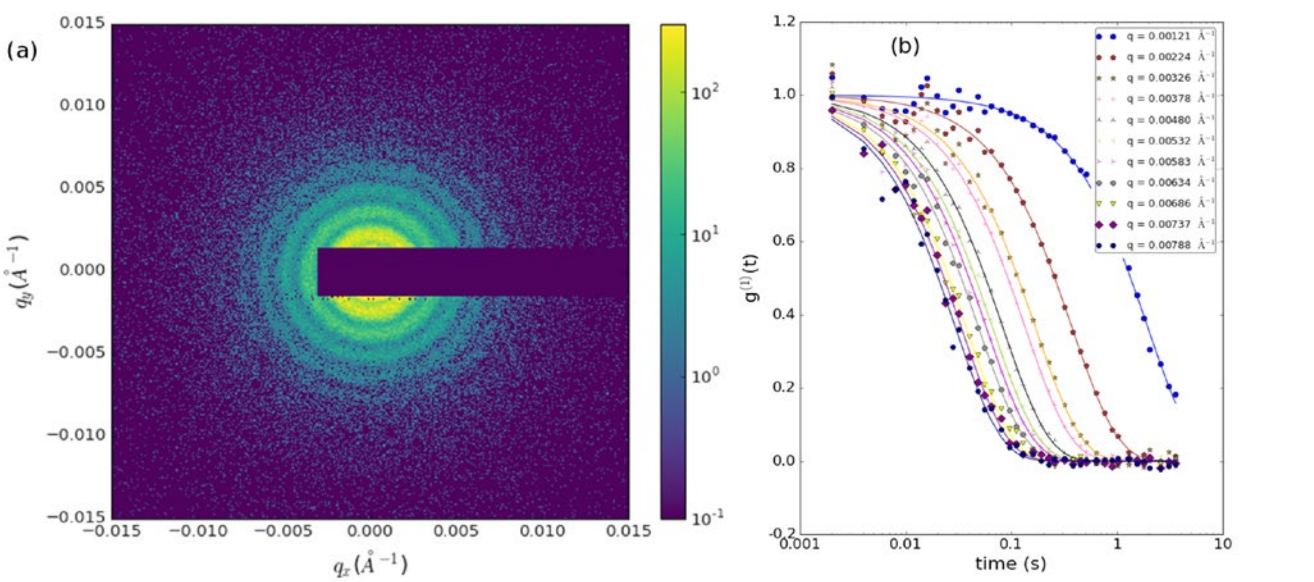


Figure 8: XPCS calibration studies on CHX: *The Brownian diffusion of 500nm diameter silica colloidal particles suspended in a polymer solution of polypropyleneglycol (PPG) in water. (a) A single speckle pattern recorded in 2 ms from the colloidal suspension. (b) Intermediate scattering function (dynamic structure factor) calculated from a sequence of 20,000 speckle patterns recorded at a frequency of 500 Hz using an Eiger 4M area detector [11].*

microfluidic flow cells, to study the interplay between macroscopic properties and nanoscale dynamics. Set-ups for in-situ measurements will also be developed to achieve better control of complex manufacturing processes such as 3D printing or complex materials response under tensile stress or nanoindentation. Finally, by using state-of-the-art detector technologies such as VIPIC (area detectors with 20 ns resolution), Avalanche Photon Diodes, are possible upgrades on the Eiger detectors, the beamline will continuously push the XPCS capabilities towards microsecond time scales.

In FY17, our main focus is on early user science operations. We plan to: (a) Complete endstation construction work, with a particular focus on the control systems for the SAXS and WAXS instruments; (b) Fabricate and test kinoform focusing optics for two spot sizes (2 μm and 10 μm) and several energies spanning the operating range, and (c) Extend user operations to coherent scattering in WAXS or SAXS/WAXS geometries.

In FY18, we plan to mature beamline user operations, and will (a) achieve routine user operations with all planned beamline capabilities including the complete range of working energies (6-16 keV), beam focused to ~2 μm for WAXS, ~10 μm for SAXS, and with a range of different sample environments, and (b) develop wavefront-preserving multilayer optics for coherent scattering. We will also develop scattering capabilities with wide-bandpass monochromatic beams for coherent-SAXS, resulting in a 5-10 times increase in coherent flux (and hence up to 100 times faster time scales).

In FY19-21, we will pursue operations with enhanced capabilities. First, we will expand the capabilities of XPCS towards faster time scales and shorter length scales. Options include, but are not limited to: i) use of advanced detector technologies such as VIPIC; ii) pushing the time resolution by synchronization of the detection process with the SR time structure; iii) synchronization of the correlator(s) with the SR structure. Second, we will pursue enhancement options with a full suite of sample environments for in-situ studies, including but not limited to: devices for tensile stress or nanoindentation, microfluidic cells, in-situ studies of self-assembly of patchy colloidal systems, 3D printing, active nanomaterials, etc.

Complex Materials Scattering (CMS, 11-BM) Beamline. The CMS program aims to facilitate the discovery, design, and optimization of functional materials by developing capabilities for (i) in situ structural characterization under processing conditions and (ii) intelligent exploration of large parameter spaces. To build up these capabilities, the SAXS detector and flightpath will be upgraded to improve data collection efficiency; a series of *in situ* sample cells will be developed or procured to expand the accessible materials parameter space; a prototype sample exchanger will be implemented to increase sample throughput; and data collection, analysis, and visualization software will be improved or developed to enhance the integration and automation of the beamline work flow and to improve the user productivity at the beamline. As a Partner User, the CFN will play a major role in these efforts.

Functional materials are inherently complex, and optimizing their structure-function relationships depends crucially on the ability to efficiently and intelligently explore the vast parameter space associated with these materials. The planned technical developments will allow CMS users to quickly map and focus on a set of compositional, thermodynamic, and processing parameters that result in desired structural properties. These capabilities will be essential to studies of self-assembled hierarchical materials (*e.g.*, nanoparticles, block copolymers, biomolecular materials); polymer nanocomposites under processing conditions (*e.g.*, additive manufacturing); and liquid-solid interfaces (*e.g.*, battery electrodes).

In FY17, our top priority is to install the new SAXS detector (a vacuum-compatible Dectris Pilatus3 2M), which was ordered in September 2016 and scheduled for delivery in May 2017. The existing SAXS detector stage and flight path will be modified to accommodate the new detector. Development and procurement of *in situ* sample cells will start, with initial emphasis on heat and tensile stages and a solvent annealing cell. The prototype sample exchanger will be installed. The approved Partner User program with CFN will commence, and a strategy to automate beamline workflow through hardware and software enhancements will be finalized.

In FY18, an initial set of in-situ sample cells for general users will be installed, tested, and integrated into beamline control. High-throughput operation based on the prototype sample exchanger will be commissioned. In collaboration with CFN, the design, fabrication, and procurement of hardware enhancements for automation will be completed, and the installation work will commence.

In FY19-21, the CMS hardware and software capabilities for intelligent parameter-space exploration will continue to be developed. The portfolio of *in situ* sample cells and processing capabilities will be expanded. Budget permitting, the SAXS flight tube will be upgraded to one that houses the SAXS detector under vacuum and on an internal rail, to enable efficient and versatile control of the sample-detector distance. The WAXS detector will be upgraded from the existing CCD to a faster, photon-counting alternative.

Soft Matter Interfaces (SMI, 12-ID) Beamline. In FY17, SMI completes construction under the NEXT Project. SMI has a 2.1–24 KeV energy range, windowless vacuum sample environment, 500 Hz detectors, low divergence, and micro-focus optics for static and time-resolved SAXS/WAXS measurements, in transmission and grazing-incidence geometries. SMI is advanced in its range of capabilities compared to peer beamlines, and will enable soft matter and bio materials researchers to explore novel types of hierarchically ordering, metastable phases, and heterogeneities.

SMI is one of a very few beamlines worldwide that provide SAXS/WAXS in the tender X-ray range. Resonant experiments from P, S, K, and Ca will provide new contrast mechanisms for the study of membranes, liquid crystals, ionic liquid systems, and biomaterials respectively. SMI's microbeam accompanied by relatively low divergence also offers world-class performance. SMI will develop data acquisition and analysis protocols that will enable SMI to deliver the greatest impact to the research community. This includes making quantitative assessments of beam damage and creating methods to reduce beam induced changes and extrapolate to zero-dose features where feasible.

In FY17, our technical and science commissioning priorities include: (a) Technical commissioning of the photon delivery, sample positioning, and data acquisition/management systems; (b) Science commissioning of the time resolved GI-SAXS capability. No new equipment is requested for this year. Transferred equipment will be used for testing, to strategically make the case for FY18 equipment purchases; and (c) Technical and science commissioning of the wide/medium angle (WAXS/MAXS) detectors. The MAXS detector is provided by the CFN Partner and the science priorities will be developed in coordination with the CFN.

In FY18, we plan to start General User (GU) operations and continue technical commissioning of additional capabilities, including (a) GU beam time available in cycle 2017-3 for time resolved GISAXS, adding WAXS/MAXS to the GU program as early in FY18 as possible; (b) Characterize the micro-focused beam over the full energy range and offer as soon as possible to GUs; and (c) develop tender X-ray capability.

In FY19-21, our development plans include the following: (a) Develop liquids sample methodologies in 12-ID-C in FY19. Tender x-ray science at liquid surfaces has been requested. This requires re-engineering the sample vacuum environment, and (b) Develop multi-mode opportunities in tandem with other NSLS-II beamlines and with CFN capabilities. Multi modal science in important systems such as energy materials, biofuels, and others have not historically utilized SAXS to the fullest extent possible and the SMI program will be developed to move science forward in key areas.

4.1.4 Diffraction & In-Situ Scattering

The '*Diffraction and In-Situ Scattering*' program focuses on the structural characterization and modeling of materials ranging from single crystals to powders to thin films. Often real or functional materials contain defects, surfaces, interfaces, and have particular morphologies and heterogeneities on different length-scales. The program offers a comprehensive suite of elastic scattering and diffraction techniques, tailored to studies of such complex or heterogeneous samples preferably under in situ and operando conditions, for advancing our understanding of the underlying material dependence of functional properties. The program also explores the combination of diffraction/scattering with imaging techniques (*e.g.*, diffraction-tomography analysis of the bulk, coherent beam imaging of surfaces). As shown in **Figure 9**, the objective is to examine the structure-function relationships that occur at different spatial and temporal scales, from Å to meters and from seconds to months. The research scope comprises:

- Studies of the atomic order and electronic order of functional interfaces & surfaces and 3D structures
- In situ, real time diffraction & scattering with environments inaccessible by other probes (for example, electron or neutron beams), e.g. in various gas environments and partial pressures, including hazardous gases, during thin film growth, surface processing, and materials synthesis and reaction processes
- Nanostructures, stacks, nanopatterned structures
- Interrogation of materials ranging from crystalline or polycrystalline to highly disordered or amorphous materials, and materials with short range order only
- Structure solving, structure refinement and structure-property relationships.

The program mission is articulated around such fundamental questions as: how are the atoms arranged (including magnetic/orbital ordering) in single crystals, polycrystalline materials, thin films and nanostructures? How do the atoms assemble and how can they be manipulated as a function of time, temperature, E/H field, polarization, pressure and other process variables? The program develops the theoretical and experimental tools to provide structural/chemical pathways to either improved or new materials and to optimize process parameters. Length scales range from the atomic scale to nano- and meso-structures (atomic clusters, domains, grain boundaries, surfaces and interfaces) to the bulk. The program strives at experimentally and computationally bridging the current gulf between these scales. Materials and structures (thin films, single crystals, powders) under study are very diverse, including strongly correlated electron materials (electronic ordering), batteries, fuel cells, catalysts, multiferroics, nanocomposites, photovoltaics, etc. The program research supports the BNL Laboratory Agenda and addresses several DOE scientific grand challenges.

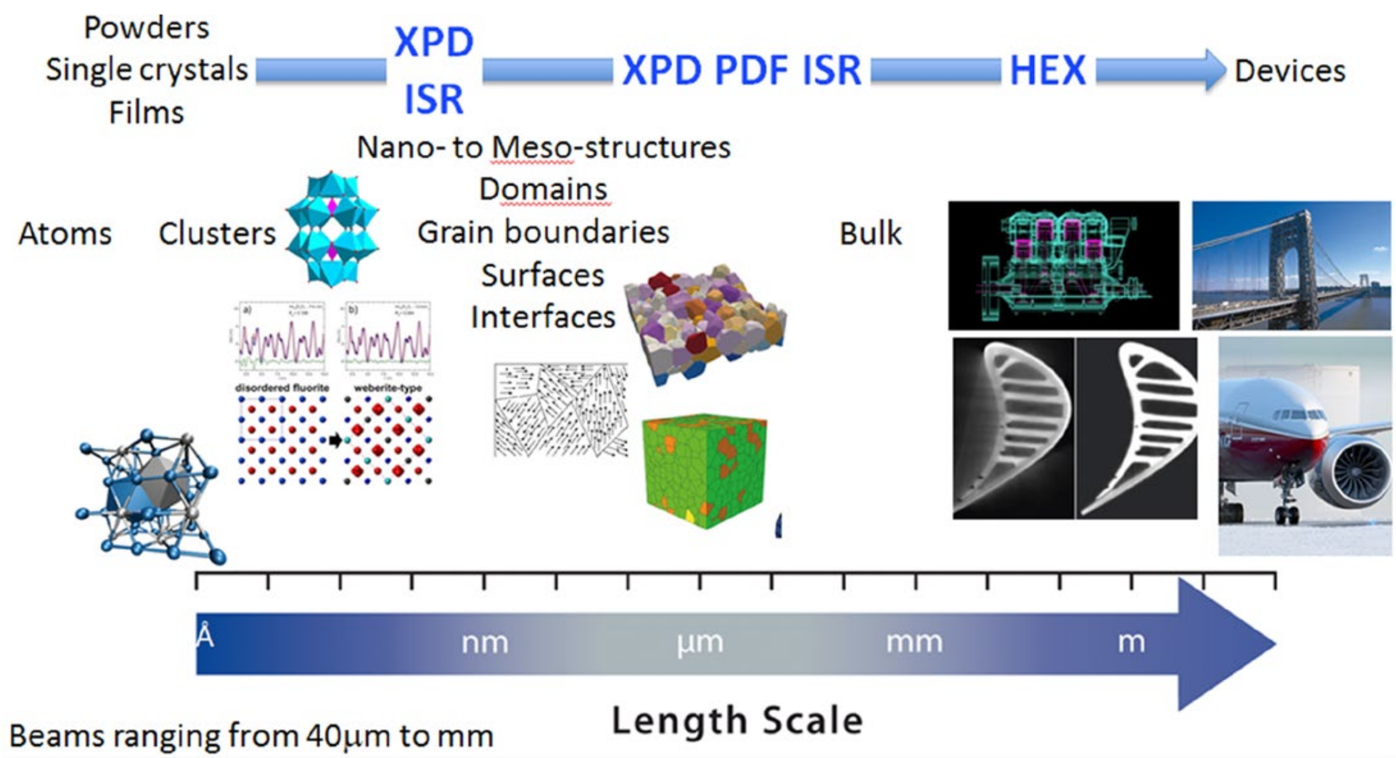


Figure 9: *Representative research examples undertaken in the Diffraction and In-Situ Scattering Program*

The program manages a suite of world-class x-ray instruments that utilize photon beams whose energy ranges from 2.4 keV to 150 keV, and offers to the science communities a comprehensive array of powerful techniques: surface scattering, resonant scattering with full polarization control and analysis, temperature range of 6.5-350 K, and magnetic vertical field of 0-10+ Tesla, reflectivity and diffuse scattering with area detectors, powder diffraction with temperature 10-2000 K and pressure 0-20+ GPa and reactive environments (gases, liquids below 150 bar), and pair distribution function analysis.

The following subsections describe in more detail the three existing NSLS-II beamlines (ISR, PDF, XPD) that form the technical portfolio of the *'Diffraction and In-Situ Scattering'* Program, the schedule for commissioning different capabilities, planned beamline enhancements, and their impact on the broad user community.

In-Situ and Resonant X-ray Studies (ISR) Beamline. The In-Situ and Resonant X-ray Studies (ISR) beamline targets materials physics challenges in the areas of growth and processing, surface and interface structure, and magnetic and electronic structure (**Figure 10**). ISR supports an array of x-ray scattering techniques (e.g., resonant x-ray scattering, crystal truncation rod measurements, x-ray reflectivity, grazing incidence small-angle x-ray scattering, and grazing incidence diffraction) in order to improve our understanding of novel materials. Specialized optics provide polarization control and focusing down to ~40 µm (V) x 200 µm (H) in Hutch C, and ~2 µm (V) x 20 µm (H) in Hutch D. ISR operates between 2.4 and 23 keV, and a flexible range of environment chambers can be accommodated for *in-situ* studies of materials.

ISR employs a flexible and broad range of capabilities to study (top-down) as well as to design and grow (bottom-up approach) novel materials that can potentially enhance devices in energy and information technology applications (*e.g.,* solid state lighting, fuel cells, solar energy conversion, thermoelectrics, information processing and storage media). One area of interest at ISR is x-ray monitoring of growth and surface/film processing: nucleation, growth modes, roughening and coarsening mechanisms, interface formation, surface reconstruction, spin control, etc. Various growth methods are envisaged such as ALE, MBE, PLD, sputter deposition, etc., on materials that include nitrides, complex oxides, semiconductors, photocathode materials, and photovoltaic materials.

Another area is the characterization of surface and interface structures to probe chemical reactions at surfaces, evolution of surface morphology and defects during growth of epitaxial thin films and multilayers, self-organization of surfaces, engineering of interfaces for improved or new properties, and behavior of liquid crystalline order. Finally, magnetic and electronic structures (magnetic order and anisotropic charge distributions in strongly correlated electron systems) can be examined by resonant and polarization-dependent techniques. Studies of the electronic order at ISR will be enhanced through a multi-modal strategy that engages other x-ray techniques at other beamlines: powder diffraction,

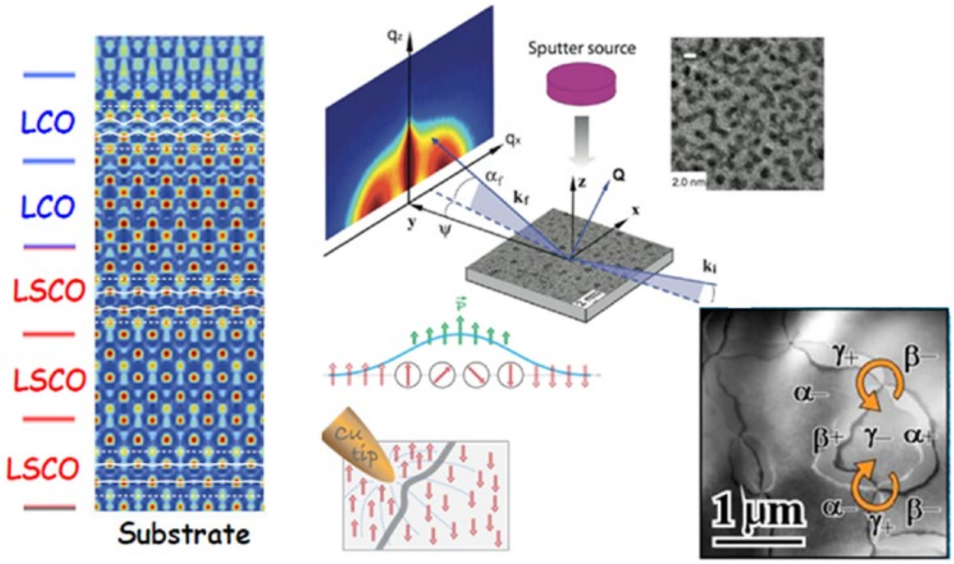


Figure 10: *Examples of science to be carried out at ISR. (Left) Sub-Angstrom resolution electron density map from CTR measurements of a LaSrCuO4 epitaxial film (Zhou et al., PNAS 2010). (Top) Real-time GISAXS patterns during first stages of WSi2 film growth showing nano-particle formation and corresponding TEM image (Zhou et al., PRB 2010). (Right and bottom) In-situ imaging of evolving ferroelectric domains— important for exploring the physics of domain wall motion controlled by electric field in multiferroics (Choi et al., Nature Materials 2010).*

soft resonant x-ray scattering, photoemission, resonant inelastic x-ray scattering, coherent scattering, and imaging. ISR aims to offer the possibility to grow a thin film while investigating the growth processes with real-time techniques, then determining the atomic structure at the interface with crystal truncation rod (CTR) analysis, and finally relating the atomic structure to the electronic structure as measured *in-situ* with resonant x-ray scattering.

Potential new science areas include: (a) sulfur K edge resonant x-ray scattering (application to superconducting FeS, magnetic spinels, transition metal dichalcogenides, (b) high pressure, high magnetic field, low temperature scattering, (c) roll-on capability for growth and processing of thin films, (d) growth of graphene, MoS2 and other transition metal dichalcogenides, (e) microwave assisted etching processes, (f) polarization-dependent surface interface phenomena, (g) evolution of nanoparticles in the PLD laser plume prior to surface deposition, and post deposition, and (h) coherent beam methods such as visualizing nanoparticles on a surface.

FY17 developments (in priority order) include: (1) complete endstation fit-out, (2) complete commissioning of 6-circle diffractometer for hard x-ray scattering with full polarization control and analysis, and with displex cryostat. (6-300K), (3) complete commissioning of in-situ diffractometer endstation, (4) test primary focusing optics at several energies spanning the operating range of the beamline, (5) begin the task of implementing and developing streamlined software for diffractometer and beamline control, and data acquisition, (6) begin identifying and implementing appropriate software for visualization and online analysis of volume reciprocal space data that area detectors will enable, (7) investigate experimental methods that will allow one to operate detectors over the wide dynamic range required for surface/interface diffraction data: from bulk Bragg peaks (strong signal) to broad nano-sized growing surface domains (weak signal), (8) bring on-line the basic functionality of the Gas Handling System (GHS) for non-hazardous gases, (9) bring on-line the laser for PLD growth, and (10) commission the KB focusing optics.

FY 18 Developments (in priority order) include: (1) achieve routine general user operations with all planned beamline capabilities including tender x-ray scattering down to 2.4 keV, (2) expand environmental parameters: temperature range, magnetic field direction, and high pressure, (3) begin design of in-situ chamber, (4) introduce hazardous and pyrophoric gases to the gas handling system for in situ growth study e.g., GaN deposition, (5) integrate the mass flow controllers and switching valves of the gas handling system with the beamline controls, (6) implement timing synchronization between the pulsed laser and the x-ray area detector, (7) measure the coherent flux and properties of the beamline, and determine paths for improvement, and (8) implement kinoform focusing for the 6-circle diffractometer in Hutch C.

In FY19-21, we plan to conduct operations with the following enhanced capabilities: (1) commission the 10T magnet, (2) enhance operations by expanding the capabilities of ISR towards shorter time scales and coherence (e.g., XPCS, ptychography and microscopy/imaging of surfaces). Options include, but are not limited to, integration of a compact electromagnet for the 6-circle diffractometer, (3) enhance operations with an extended suite of sample environments for in-situ studies, (4) finalize design and obtain funding for an upgraded, vibrationally stable, UHV endstation that can be used for micro-diffraction and ptychography studies on surfaces in hutch D, (5) develop kinoform lenses for submicron beam in Hutch D, and (6) pursue development of a large magnet to replace and/or complement the capabilities provided by the existing 13 T magnet.

Pair Distribution Function (PDF) Beamline. Properties of most next generation materials are governed by imperfections in their atomic structures, such as, defects, nano- and multi-scale structures, heterogeneities, nanoscale disorder, stacking faults, surface relaxation, etc. It is important to understand the structure-property relationships in these materials to optimize their desirable properties. Diffraction patterns of such materials (**Figure 11**) show broadened Bragg peaks and weak (or strong) diffuse scattering making them difficult candidates for traditional crystallographic approaches. Under this situation, the pair distribution function (PDF) method that utilizes both Bragg and diffuse scattering emerges as a powerful tool to study these materials. PDF beamline at NSLS-II is dedicated for the atomic pair distribution function technique. PDF will operate at 4 fixed energies (39, 64, 75 or 117 keV), and is optimized for total scattering measurements over a large Q range with extremely low background. PDF also provides Small-Angle X-ray Scattering (SAXS) and medium resolution Wide-Angle X-ray Scattering (WAXS) data enabling studies of the atomic structure on multiple length scales. PDF offers rapid data acquisition rates (30 frames/s) and high flux required for in situ and operando studies with beam size ranging from 0.1 × 0.1 to 1 × 1 mm2. A wide variety of sample environments is available at the beamline, including a 80–500 K liquid nitrogen cryostream, a 5-500 K Helium cryostat coupled with a 0-5 T superconducting magnet, and gas flow-cells. The beamline is equipped with an automatic capillary sample alignment system, and a steel bridge that facilitates positioning of two large area detectors to enable fast switching between SAXS, WAXS and PDF configurations. The beamline is currently under construction and expected to start user operations in Summer 2018.

The science program includes, but is not limited to: structural studies of fuel-cells in action, battery electrodes and electrolytes under real operating conditions, supercapacitors, nanoparticles with interesting optical properties, and many drugs in the discovery pipeline that have limited solubility in the crystalline state, theory driven synthesis of novel materials, catalysts under real operating conditions, and strongly correlated materials under magnetic fields in the temperature range 5-500 K. Probing the structure-property relationships in novel materials using combined techniques (e.g. PDF and IR) will provide unique experimental input for the complex modeling approach (in collaboration with BNL's computer Science Initiative and Columbia University).

In FY17 the PDF beamline construction will be completed, and preparation for the beamline IRR will be in progress. In FY18, the beamline will start commissioning and start routine user operations with all planned capabilities including SAXS and WAXS, and commissioning of the gas handling system. The development of software for automation of various measurements and data analysis will be underway.

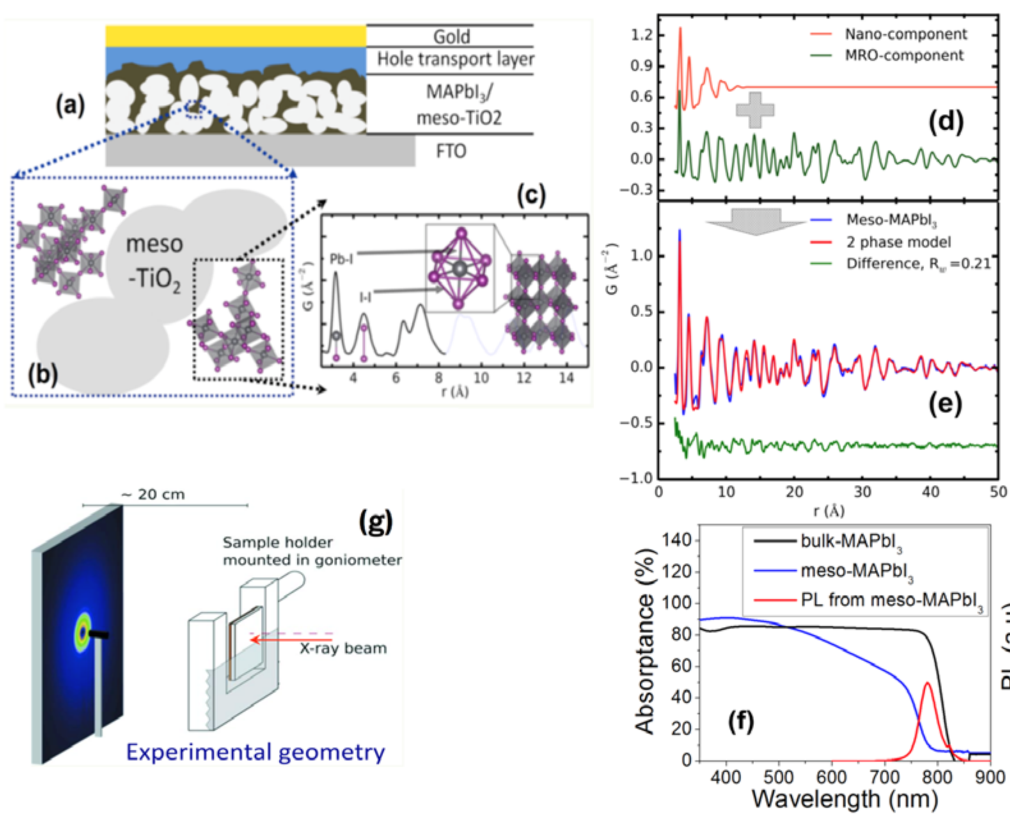


Figure 11: Schematic diagrams of (a) A perovskite-based solar cell, (b) Possible configurations of meso-MAPbI3 within the active layer of the cell. (c) PDF of MAPbI3 providing quantitative information on all atom-atom correlation lengths. (d) PDF of the meso-MAPbI3 reveals disordered nanostructured and medium range ordered (MRO) phases. (e) Resulting 2-phase model fit. (f) Due to the nature of this atomic arrangement, optical absorption (blue) and photo-luminescence (red) spectra illustrates strongly modified optical properties relative to the pure bulk material (black). (g) Experimental geometry for thin film PDF measurements.

Reference: Choi et. al. Nano Lett., 14 (1), pp 127–133 (2014).

In FY19-21, we will continue operation of the PDF beamline with the following priorities: (1) enhance operations and broaden the user base by developing an IR setup allowing simultaneous PDF and IR measurements, (2) explore the possibility of including other probes (*e.g.*, Raman), (3) develop complex modeling software (in collaboration with the CSI and Columbia University) and deploy and test it at the beamline, and (4) fabricate and test kinoform focusing optics.

X-ray Powder Diffraction (XPD) Beamline. The X-ray Powder Diffraction (XPD) beamline serves a very broad and diverse user community ranging from physics, chemistry, and materials science to earth science, environmental science and engineering science. XPD operates with photon beams whose energy is fully tunable between 40 keV and 70 keV, with a nominal beam size of 0.6 × 0.2 mm2. Hard X-rays provide the opportunity to probe high-Z or bulk samples, buried interfaces, and inside sample cells and devices. The core mission of XPD is to observe materials under conditions that are far from equilibrium, ambient or static, *i.e.*, as a function of a process parameter like T, P, pH, reactive gases, electric or magnetic field.

XPD is configured for near-field (higher Q coverage) and far-field (higher Q resolution, *i.e.*, better peak separation) 2D diffraction. For this purpose, endstation C hosts two large-area detectors that consist of flat scintillator panels (16”×16” active area, CsI coated, 200µm pixels). They can be quickly interchanged at any time in the course of a reaction or a process. This dual detector arrangement is ideal for total scattering measurements that provide both long-range and short-range order information on any material in exactly the same environment and set-up. The crystalline fraction of the sample is determined by Rietveld refinements using the XRD data and the model is subsequently imported as a .CIF (Crystallographic Information File) for use in the modeling of the short-range order based on the PDF data.

Thanks to the high energy of the photon beam, a significant portion of the diffraction space can be captured in one shot by the large-area detectors (*i.e.* without scanning). Therefore XPD is well suited for sub-minute data collection times, ideal for time-dependent measurements of transformations or transient processes. A robotic sample changer is available for high-throughput measurements. XPD also offers a large variety of sample environments (commercial, user-custom or in-house systems) that include: furnaces, cryostats, flow cells, etc. Together, these make XPD a world-class facility in the field of *in situ* and *operando* structural science.

XPD will offer the option of a high-resolution configuration (for structure solving and line profile analysis) by trading its 1D and 2D detectors for a unique system composed of 8 channels fitted with analyzer Laue crystals. It uses two distinct detector units developed in house, that are angle-scanned simultaneously and collect the sample-diffracted signal with and without the analyzer crystals. One unit is an array of photomultiplier tubes associated with GYSO scintillator crystals, The second unit is an array of 8 × 8 CdZnTe chips.

A second endstation (hutch D - not in use yet) of XPD will accommodate more elaborate/complex setups: large pressure cells, non-routine reaction chambers, combined spectrometry, gas handling, user-custom devices, etc. Hutch D can also be used for those measurements that require long lead-time preparation, *e.g.*, a gas rig or a spectrometer. Alternatively the beam can be sent intermittently into hutch D to enable short and repetitive measurements at regular intervals over a long period of time *i.e.*, corrosion studies, slow growth processes, charging and discharging of batteries, degradation of cathodes and anodes in fuel cell research, environmental effects on solar cell materials.

Major focus themes of XPD are: 1) *in situ* synthesis (e.g., high temperature solid state growth, colloidal nanoparticles from solution, flash sintering of ceramics/oxide materials, nucleation & growth of MOFs, and microwave-assisted synthesis) and 2) *in situ* structure evolution (e.g., catalysis, oxidation reduction reactions using gases, hydrogenation reactions, gas adsorption and separation, and cycling of energy-storage devices). Theory and experiment can be integrated in a closed loop in exploratory syntheses, where theory can identify theoretical desired materials that are thermodynamically stable, and *in situ* XRD synthesis could then be used to pinpoint the feasible synthetic routes. This new approach has great potential to accelerate materials discovery.

FY17 developments include: (1) mature instrumentation and automation of existing equipment, (2) develop hardware, controls and software for high resolution operations, (3) develop quasi real-time data processing, pipelining and visualization that build upon the XpdAcq/Bluesky software (in collaboration with Columbia University). This will provide in-line processing and automated analysis of data as they are flowing off the 2D detectors, in addition to search and database mining engines on processed data, (4) develop and test an in-house 1D Ge strip detector, that consists of 384 0.5 × 0.125 mm2 germanium elements mounted with a closed-cycle cryostat, and (5) develop additional sample environments in collaboration with users: high temperature cell for a combined differential scanning calorimeter and diffraction, microwave reactor for in-situ synthesis, and a high-pressure gas loading system.

In FY18 we plan to enhance General User Operations with the following activities: (1) commission a photon-counting pixelated 2D detector with 130 µm pitch, (2) develop robot operations for high-throughput, combined with database mining, machine learning and Principal Component Analysis of the pre-processed data for guiding the user in real-time decision-making, (3) fit-out hutch D for stress-strain-time characterizations (in the 10 MPa, 10^{-5} range) of a multi-anvil system that consists of a 1,000 ton press using 25 mm3 anvils with a uni-axial stress capability (applications are: rheology, elasticity, anelasticity and kinetics measurements), (4) commission the high-resolution configuration, (5) install and commission the gas handling system, (6) migrate the PDF program to the new PDF beamline, (7) develop micro-focusing optics in the D-hutch, using either kinoform-lenses and/or a set of in-vacuum Kirkpatrick-Baez mirrors, and (8) develop the fast diffraction tomography set-up in Hutch-D (in collaboration with Nuclear Science and Technology Department at BNL).

In FY19-21 we plan to pursue the following tasks to expand the science program at XPD: (1) enhance the SAXS capability in hutch C, (2) purchase commercial, new generation large-area, photon-counting detectors (pixelated CdTe sensors), to substitute the a-Si/scintillator technology that is being currently used (3) design hardware and software to allow operations beyond the current trial-and-error approaches, and develop machine-learning and other theory-assisted predictive tools, (4) adapt, install and test container-less measurements, (5) develop the long lead time experiments in the D hutch *e.g.*, measurements on batteries and fuel cells over long periods of cycling, measure the corrosion reaction over periods of days, and (6) expand the frontiers of extreme environments by including Diamond Anvil Cells (DAC) for p-V-T equation-of-state of Earth materials. The addition of laser-heating or resistive heating allows one to study phase transitions, reactions between minerals at high T,P, or melts.

4.1.5 Imaging & Microscopy

The Microscopy & Imaging Program at NSLS-II focuses on the imaging of heterogeneous materials over a broad length scale range from millimeters to nanometers in two- and three-dimensions, and includes both static and real-time measurements. The program employs multiple contrast mechanisms (*e.g.* absorption, fluorescence, phase, diffraction) in order to resolve morphology, structure, chemistry, and elemental variation in these systems.

The program currently has two operating beamlines, the Hard X-ray Nanoprobe (HXN) and the Sub-micron Resolution X-ray Spectroscopy (SRX) beamline. Two additional beamlines are currently under construction: the X-ray Fluorescence Microprobe beamline (XFM) and the Full-Field Transmission X-ray Microscopy (FXI). Two additional beamlines are in the planning stages: the Soft X-Ray Spectromicroscopy beamline (SMF) and the Coherent Diffraction Imaging beamline (CDI).

The scientific applications for the program reach widely into many scientific disciplines, due to the breadth of techniques that can be provided by this suite of beamlines. That said, relevant science areas of growth include energy storage & conversion, catalysis, nanomaterials and nanosynthesis, bioenergy and biofuels, and climate science.

The high brightness and stability of NSLS-II make certain techniques/capabilities unique to the facility and thus we focus in these areas. Specifically, the program is focusing on (1) high-resolution structural and chemical (spectroscopic) imaging, (2) fast three-dimensional imaging, (4) multi-modal, multi-technique, multi-beamline imaging, and (3) imaging in situ systems that from operando capabilities; e.g. catalytic materials, energy materials, other dynamic systems.

In order to achieve the program's technical objectives, a number of short-term and longer-term goals must be met. In FY17-18, the top priorities program-wide include:

(1) Deliver what we've promised on the operating beamlines
HXN and SRX are actively doing user science but commissioning and optimization need to be done. For SRX, the high resolution endstation, submicron EXAFS, the Maia detector, and fluorescence tomography need to be commissioned and made available to users. Much of this development is hindered by a lack of IT/controls resources, which is a top priority to remedy. For HXN, the beam stability will be addressed for differential phase contrast (DPC) and ptychography to be successful and for higher resolution MLL optics to be implemented.

(2) Deliver two new beamlines (XFM, FXI)
Two gaps in the imaging portfolio will be filled by the XFM and FXI beamlines. XFM will be a workhorse microprobe/micro-EXAFS beamline that will address science that does not need the highest possible spatial resolution and/or has large, real-world samples that cannot be manipulated/processed for high resolution imaging. XFM will also dramatically enhance the efficiency of SRX and HXN by provide the ability to "image the forest through the trees." Most often, large-area mapping is necessary to define regions of interest for high-resolution mapping. FXI will be a high-throughput, full-field, absorption and phase contrast nanoprobe for fast tomography with <30 nm spatial resolution. The speed of the instrument will produce a 3D image in seconds, enabling a wide range of dynamic measurements on the nanoscale. Many applications with operating devices such as batteries and fuel cells will be possible.

(3) Improving beamline throughput and efficiency to accommodate more users
The user throughput on imaging beamlines is typically slow; users often want to image large regions at high resolution with many replicate samples. This requires a lot of beam

time. In order to optimize beam time use, we will pursue improvements including automated sample handling, sample mounts that hold multiple samples, and software that can define batches of maps at once. Better offline sample pre-characterization is also invaluable, so users will be encouraged to use SEM or VLM to pre-define their areas of interest. IT support will be pursued to integrate these SEM/VLM images into the beamline software for defining regions of interest for X-ray mapping.

(4) Optimize output and enhance capabilities to deliver more high impact science

A common bottleneck in scientific productivity (i.e. publication) is the processing and analysis of the data. This barrier can be lowered by providing users with better software for data collection, real-time visualization, and user-friendly analysis. This must extend beyond data from a single beamline and incorporate similar tools and approaches to combine multidimensional and multimodal images. In addition, the capabilities of the beamlines cannot stand still and must continue to advance with improved technology. NSLS-II has a very successful optics group and we will utilize their expertise to improve the X-ray focusing optics, including spatial resolution, efficiency, and working distance. Higher resolution optics all call for improved beam stability, which will be a focus of the beam stability task force.

In FY19-21, we plan to: (1) Streamline the use of multi-modal, multi-beamline, high-throughput, and operando imaging techniques across all beamlines in the portfolio and across the programs (see Section 6.4), and (2) Pursue the growth of our suite of beamlines to fill the gaps in the technique portfolio (e.g. CDI, SMF/ARI); These two additional beamlines have been proposed to fill gaps in the Microscopy and Imaging portfolio. The SMF/ARI beamline will provide unprecedented spatial resolution (<5 nm) for soft X-ray microscopy including scanning transmission modes, nano ARPES, and nano RIXS. See Sections 4.2.3 and 4.2.4 for more information.

The development plans for the individual beamlines in the Microscopy and Imaging program are described below.

Hard X-ray Nanoprobe (HXN, 3-ID) beamline. HXN is an undulator beamline in general user operations at sector 3-ID providing X-ray imaging capabilities with a world-leading spatial resolution. It offers a suite of X-ray analytical tools for structural, elemental and chemical imaging, with a resolution of 10 nm and an ultimate goal of 1 nm. The combination of unique detection capabilities and the unprecedented resolution enable noninvasive materials characterization at the nanometer scale, critical for studies in many areas of science and technology.

In FY17, our main focus is on user science operations. We will (a) optimize user operations on 2D X-ray fluorescence (XRF) imaging using the MLL microscope and the zone plate microscope, (b) enhance visualization and analysis of multi-modality imaging, which include elemental distribution (through fluorescence) and nanoscale morphology (through differential phase contrast (DPC) and ptychography), and (c) enhance robustness of 3D data collection through XRF tomography using the zone plate microscope.

In FY18, we plan to mature beamline user operations by offering additional imaging capabilities. We will (a) optimize 3D XRF imaging capability using the MLL microscope, (b) provide a ptychography capability for general user experiments with a goal of achieving sub-5 nm resolution, (c) optimize in-situ experiments using electrochemical controls (for battery and corrosion research) and current/voltage measurements (for solar cells or other functional materials) where chemical (oxidation state) imaging will be carried out under in-situ controls, and (d) expand Bragg ptychography imaging capability for quantifying strain distribution within single crystal grains.

In FY19-21, we will pursue operations with enhanced capabilities. We will (a) streamline all of the on-line analysis tools, so that even non-expert users can perform experiments without difficulties, and (b) perform experiments with variable sample temperature controls (from ~90K to ~900K). We will reduce the level of technical commissioning from year to year in favor of accommodating more users. At the same time, working together with the NSLS-II optics group, we will continue to improve the MLL optics with a goal to reach sub-10 nm focus in this time frame.

Sub-micron Resolution X-ray spectroscopy (SRX, 5-ID) beamline. SRX is an undulator beamline in general user operations at sector 5-ID that specializes in X-ray fluorescence microprobe and XANES spectroscopy with a spot size of ~0.7 microns and an energy range from 4.65 – 25 keV. Elemental imaging can be performed in 2D and 3D. A second endstation at SRX is currently under development that is expected to provide similar capabilities with sub-100 nm spatial resolution. Scientific communities such as environmental, life, nuclear, planetary and material sciences take advantage of this beamline to understand complex natural and engineered systems that are heterogeneous on the micron to nanometer scale.

In FY17, our main focus is on user science operations. We will (a) complete the implementation of sample fly-scanning to optimize routine XRF mapping, (b) resolve the heating issue with the monochromator motor so that XANES measurements are improved and EXAFS will be possible routinely, and (c) continue to commission the Maia detector.

In FY18, we plan to mature beamline user operations. We will (a) commission the high-resolution KB optics to enable chemical imaging at sub-100 nm spatial resolution, (b) continue to work on complex sample environments such as in-situ/operando cells for research on functional materials or a cryostage for radiation-sensitive soft materials, (c) make the Maia detector available for routine user operations to enable fast XRF mapping of large sample areas, (d) commission XRF-tomography to enable elemental mapping in 3D with sub-micron resolution.

In FY19-21, we will pursue operations with enhanced capabilities. Specifically (a) XRF elemental mapping and XANES / EXAFS spectroscopy shall be available for routine user operations with sub-micron and sub-100nm spatial resolution, (b) we hope to pursue micro-diffraction as a measurement simultaneous to XRF, yielding structural information, (c) we want to push for XRF tomography with sub-100 nm spatial resolution, and (d) we will investigate X-ray ptychography as a tool to increase spatial resolution with SRX even further. We will reduce the level of technical commissioning from year to year in favor of accommodating more users.

Full-field X-ray Imaging (FXI, 18-ID) beamline. FXI is a damping wiggler beamline currently under construction at sector 18-ID that will house a Transmission X-ray Microscope (TXM) with 30 nm spatial resolution and 20-40 micron field of view. At 500 mA NSLS-II operation, the expected exposure time per image is < 100 ms. FXI will also be capable of nanoXANES, which will allow for elemental imaging and speciation. The scientific scope of the beamline will focus on 3D in-situ and operando dynamics of sample morphology and oxidation states imaged at 30 nm spatial resolution. Scientific areas include energy storage devices, materials science and environmental science.

In FY17, we plan to finish construction of the beamline, with the Instrument Readiness Review (IRR) planned for September 2017.

For FY18, our goals are (in priority order): (a) getting the TXM instrument operational – in particular, the data acquisition, management and analysis (DAMA) aspects, (b) achieve 30 nm spatial resolution with projection image exposure times below 1s, (c) begin science commissioning with expert users, (d) establish external collaborations for in-situ sample environment cells and x-ray optics, and (e) participate in multi-modal science with other NSLS-II and CFN capabilities. The main challenge will be (a), as we delve into the new territory of world-leading full-field tomography with fly scans at 30 nm spatial resolution.

For FY19 through FY21, we plan to start General User Operations and continue technical commissioning of additional capabilities including: (a) development/prototyping of one or two dedicated sample environment cells (based on collaborations in FY18), (b) developing and testing new x-ray optics from collaborators – the goals are to (i) increase the working distances to better accommodate sample environment cells, (ii) stack zone plates to increase efficiency and (iii) offer a wider range of spatial resolutions (not just 30 nm) for users, (c) continue to implement/develop new analysis algorithms into the data workflow, and (d) design/develop a robotic sample changer for the TXM.

X-ray Fluorescence Microprobe (XFM, 4-BM) beamline. XFM is a 3-pole wiggler beamline under construction at beamline 4-BM that will provide unique spectroscopic microscopy capabilities because it will span the tender (2-5 keV) and hard (5-23keV) energy range (P to Tc K-edges), and also offers a polychromatic “pink” mode ideal for rapid 2D and 3D fluorescence imaging and tomography. It will employ compound focusing to achieve a tunable spot size from 1 to 10 microns while maintaining a long working distance for physically large samples and custom in situ environmental cells. XFM will specialize in spatially-resolved characterization of elemental abundances and chemical speciation in heterogeneous samples spanning applications in the biological, environmental, geological, and materials sciences.

In FY17, we plan to finish construction of the beamline, with the Instrument Readiness Review (IRR) planned for September 2017.

In FY18, our main focus will be beamline characterization and technical commissioning activities. Our science commissioning priorities will be fast, on-the-fly 2-D X-ray fluorescence imaging (i.e., XRF mapping) and microbeam X-ray absorption near-edge structure (μ-XANES) spectroscopy.

In FY19-21, we plan to start General User operations and technical commissioning of additional capabilities (in priority order): fluorescence computed microtomography (fCMT) in monochromatic and pink-beam modes, on-the-fly microbeam X-ray absorption near-edge structure (μ-XANES) and extended X-ray absorption fine-structure (μ-EXAFS) spectroscopies, and microbeam X-ray diffraction (μ-XRD).

4.1.6 Structural Biology

The NSLS-II beamlines for biological investigations are sited close together on the experiment floor covering the region from 16ID (LIX) through to 19ID (NYX) the suite of beamlines have been created through the cooperation of DOE-BES, the NIH and Partner user groups who have together contributed to the creation of a “bioVillage” to support the needs of this research community. The NSLS-II source will enable the delivery of x-ray beams of unrivalled brilliance, thereby enabling the examination of vanishingly small crystals of proteins and other macromolecules. The performance of the beamlines that is being demonstrated represents a leap in the performance hitherto available to the structural biology community.

Our overall development strategy in structural biology is to harness the x-ray beams through sophisticated automation and instrument control to allow the elucidation of the structures of the molecular machinery underpinning life in its function and dysfunction. Taken in isolation the structures do not reveal the full complexity of the underlying processes thus we expect that in addition to molecular biology experiments undertaken in the home laboratory, it will be beneficial if access is possible to a complementary suite of biophysical measurements and imaging, thus we will work to enable simple, coordinated, access to the full suite of biological beamlines. In addition the development of our capability for bio-imaging will be closely coupled to the work describe here and aimed at enabling the beamlines to become productive.

In FY17-18, the first priority for all structural biology beamlines is to continue technical and science commissioning to achieve initial benchmarking experiments and to transition into general user operations with the goal to stabilize their operations - both hardware and software - sufficiently that routine general user operations are possible. All five of the beamlines will be establishing operational processes during FY17 and into FY18, one of the beamlines (XFP, 17BM) will also extend the range of techniques available by adding an additional capability to cover x-ray absorption spectroscopy - this development will occur in a phased fashion and should not materially affect the science program under development on the host beamline.

The three crystallography facilities, 19ID (NYX), 17ID-1 (AMX) and 17ID-2 (FMX) will face similar and specific problems. At FMX, achieving the design goal of enabling Frontier macromolecular crystallography will require the instrument to achieve a performance that is yet to be matched at existing beamlines. Establishing this performance and developing a science program using the full capability will need time and effort, we plan to establish the tools for using the tiny beam we will be able to make - software and hardware will need to be tuned and made user friendly. Once available the exploitation of a capability orders of magnitude brighter than other available in the US will be the main focus for the beamline team.

The level of automation on 17ID-1 (AMX) will be brought into full utility during the next year. Establishing a clear, automatic data collection and analysis pipeline with an x-ray beam size of 5 μm^2 will not be a trivial matter. In the short to medium term our efforts will be contained to the practical aspects of beam and sample delivery along with the associated effort in data management to enable the structure determination process to proceed smoothly and efficiently.

The third of the MX beamlines 19ID (NYX), the beamline developed by the New York structural biology center, is the youngest in the development process having, late in 2016, successfully met the safety review criteria before commissioning with x-ray beam started. The beamline will aim to deliver high intensity x-ray beams with higher energy resolution than is the norm for MX beamlines, this superb energy resolution will allow finer examination of the anomalous dispersion so vital to *ab initio* structure determination by x-ray phasing methods. Commissioning and development of the beamline will continue during FY17 with a smooth transition into general user operation in FY18.

Two of the beamlines in the structural biology suite will be handling non-crystalline samples. First, LiX, which was constructed as part of the NIH investment that also provided the MX beamlines 17ID-1 and 17ID-2. LiX has a broad science program envisaged and the first parts of their remit are now available to the research community. The LiX team offers static protein solution scattering, online chromatographic purification with solution scattering (online HPLC) and have started to roll out the next technique - microbeam scanning scattering. Protein solution small angle scattering has had a profound impact on our ability to understand protein structure in solution and as such it offers a powerful counterpoint to the structures obtained through MX. Through the delivery of automated high quality data collection and analysis we expect to be able to bring this powerful technique to the wide community of structural biologists. Microbeam scanning reveals the spatial distribution of the macromolecules within biological materials – to date root systems and plant leaves have been examined. Analysis of the properties is challenging and will provide a link to the data analysis efforts at other beamlines and with the Computational Science Initiative developing at BNL.

The final beamline to note is the x-ray footprinting beamline developed by a second partner. The Case Western Reserve University has a long standing interest in understanding the dynamics of the structure and function of proteins. X-ray footprinting provides a unique viewpoint on the spatial arrangement and dynamics of macromolecules in solution. This Partner team brought their footprinting beamline online in the latter part of 2016 and initial experiments have been performed and the stabilization and build up of the user program will continue through 2017 and 2018. In addition, the team will also continue to develop their capabilities in another of their areas of expertize viz biological x-ray spectroscopy. To do this, they will enhance the capability of their 17BM beamline through the addition of a scanning monochromator and a bio-EXAFS experimental facility. Construction will occur during FY17 with commissioning and first experiments during FY18.

In the longer term FY19-21, the NSLS-II source offers us significant advantages when considering the design of beamlines and then the experiments to make significant contributions to the field of structural biology. As described above we have invested well in providing state-of-the-art synchrotron beamlines and have a compelling suite of beamlines with room for growth. How we will develop the priorities and scale of our program will be in some part governed by what we learn as we understand how to harness the new regimes these beamlines will give us access to. However, our approach may be summed up in the following principles.

First, we must continue to innovate to create the best sorts of experiments that will make optimal use of the light-source. Given the projected lifetime of biological crystal samples in our x-ray crystallography beams (on the order of ~ms) we will integrate the best ideas from x-ray free electron laser sources to develop the sample delivery systems for highly fragile samples, in achieving this goal we will collaborate with the leaders in the field. To enable measurement of dynamic process we will develop microfluidic mixing and injection schemes to allow for the study of transient interactions and enzymatic reactions, novel sample handling schemes and mixing cell construction will benefit from collaboration in the community and with BNL's Center for Functional Nanomaterials. Development of tools for in vivo measurements will allow us to understand proteomics in the cell using footprint tools to be established, whilst imaging techniques exploiting the coherence of the source will allow LiX to image biological objects with sub-micron spatial resolution.

Second, drawing together the necessary tools to study complex problems will require us to establish correlated research programs. It is our intention to enable access such that diverse data can be brought together to inform scientific deliberation - transient complexes described through scattering experiments will be married with high resolution structures enabled by our crystallography beamlines. Together these will be coupled with the structures of higher order complexes enabled through the electron-microscopy efforts described in other sections. Biological or cellular context can be enabled by the imaging tools and techniques under development and through the construction of new instruments. We have made a start in this direction through investments afford by the operational support grant for the LSBR resource and also through the laboratory, but much work is to be done and we will need serious efforts to ensure success.

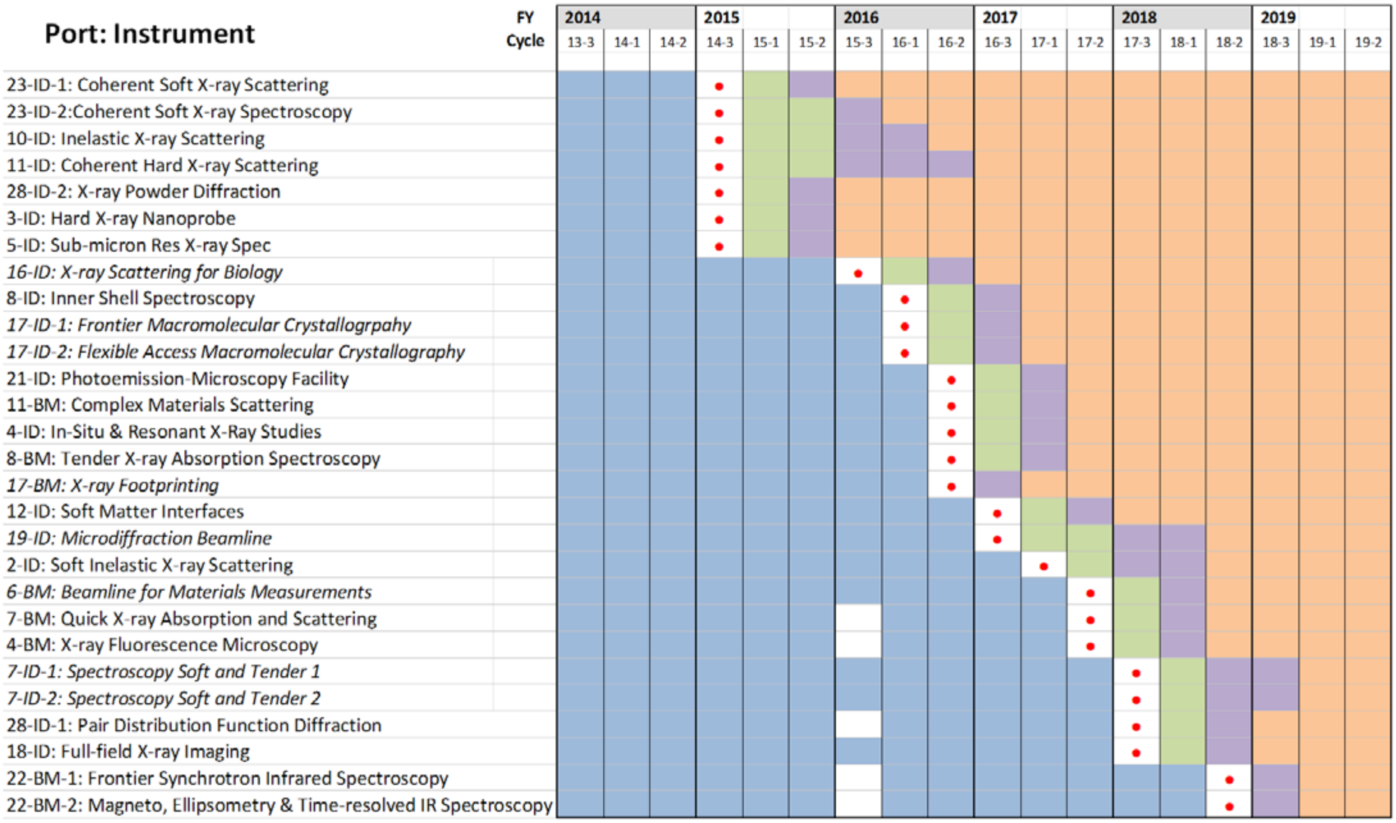
Third, the type of experiment we perform to understand structural biology will change due to the source. The need for new computational approaches affects each beamline within the structural biology program. Rather than attempt to be complete in the enumeration of the problems, one example suffices to demonstrate the scale of the problem: the lifetime of the typical protein crystals in these beams is estimated to be about 10 ms and thus the collection of data sets from a single protein crystal will be essentially impractical without X-ray attenuation factors of 99% or greater. Traditional MX experiments require one or at most two (a low and a high resolution) sweep data collection. More complex strategies are possible, based upon the radiation robustness of the crystal, however NSLS-II will bring scientists into completely new regimes where data sets will be generated from thousands of crystals. We expect to provide software capable of rapidly and reliably sorting partial MX data sets such that an ensemble is achieved that creates a complete data set with accuracy appropriate to the question posed by the experiment. Many similarities exist to the types of problems that face experimenters using x-ray free electron lasers, thus we are reaching out to learn best practices whilst also developing methods adapted to our experiments and our needs.

Finally, we are aware that the science of structural biology is going through a period of rapid change. The impact of the cryo-electron microscopy revolution has been and continues to be astounding, free-electron laser sources continue to develop and major upgrades are planned at highly successful facilities. How this situation will eventually work out is still difficult to interpret. However, we believe that there will be a need for further beamlines supporting this science area and for communities not yet well represented at NSLS-II. We plan to investigate several use cases and elaborate potential beamline designs consistent with those use cases. Speed of construction, cost effectiveness and integration within the NSLS-II program and the wider DOE complex view of capabilities will all form part of the development process.

4.2 DEVELOPMENT OF NEW BEAMLINES

Section 4.1 focused on development activities that we plan to pursue on currently operating beamlines or beamlines currently under construction. These beamlines, twenty eight in total, represent the current suite of beamline programs that either have already transitioned into operations from construction, or are soon to transition into operations in the coming two years. The overall timeline of these twenty eight beamlines are summarized in **Figure 12**.

With these twenty-eight world-class beamlines, NSLS-II is poised to make significant contributions and deliver high-impact science in a wide range of research disciplines. While this current beamline portfolio constitutes an essential part of NSLS-II operations in the next five years, a number of capabilities gaps exist in the current portfolio that will limit the NSLS-II's scientific impact and potential. It is thus critical for NSLS-II to continue the development of new beamlines to provide new state-of-the-art capabilities to meet the additional research needs of the scientific com-



	13-3	14-1	14-2	14-3	15-1	15-2	15-3	16-1	16-2	16-3	17-1	17-2	17-3	18-1	18-2	18-3	19-1	19-2
Development	28	28	28	21	21	21	15	17	12	10	9	6	2	2				
First light - In Service				7			1	3	5	2	1	3	4		2			
Technical Commissioning					7	3		1	3	4	2	2	3	4				
Science Commissioning						4	3	2	2	4	4	1	2	5	4	4		
General User Operation							4	5	6	8	12	16	17	17	22	24	28	28

Figure 12: *Development schedule for the current suite of twenty-eight beamlines in operation or under construction.*

munity. This section outlines our development strategy and the first suite of such additional beamlines that we have identified to pursue.

4.2.1 Development Strategy

To fully realize the scientific potential of NSLS-II, future development of additional beamlines is clearly needed. The current NSLS-II beamline portfolio (**Figure 13**) occupies ~60% of insertion device (ID) straight sections and ~30% of the BM/3PW/IR ports. Among the remaining open ports, there are 11 insertion device straights plus three canted undulator sources, and 22 available BM/3PW/IR ports.

Given that the majority of the highly-demanded ID ports are already under development and the overall facility is more than half full, it is important to develop a high-level strategy for allocation of the remaining open beam ports. We have been actively engaging the NSLS-II SAC and the community at large to discuss this topic in the past few years, including a strategic planning workshop held at BNL in fall 2015. During these interactions, we have considered several factors in order to make informed decisions on future strategic directions, including a capabilities gap assessment of the current NSLS-II beamline portfolio based

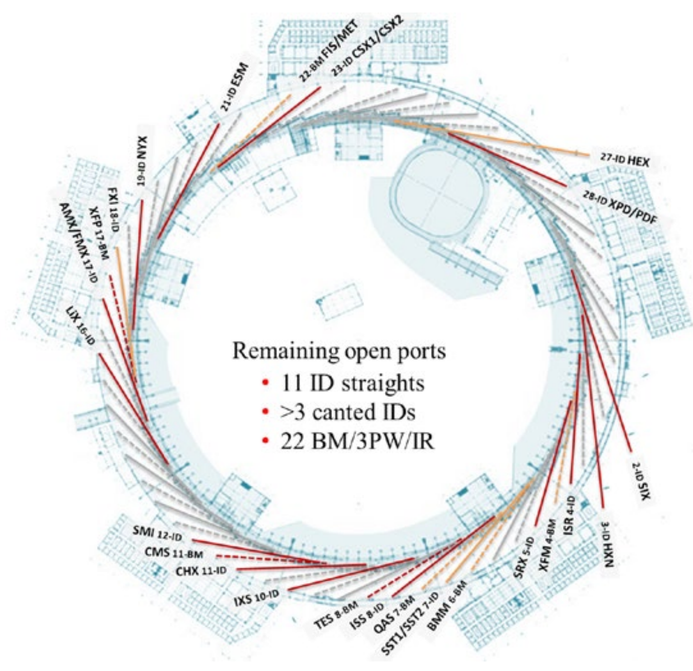


Figure 13: *Current beamline suite at NSLS-II, showing also remaining ID straight sections and bend-magnet/3-pole wiggler/infrared ports to be developed.*

on the research needs of the scientific community, capacity estimates for both high-throughput beamlines as well as high-end beamlines in the current beamline portfolio, NSLS-II strengths in the national and global context, and the relevance and alignment to the NSLS-II strategic directions.

Following our standard beamline development proposal (BDP) solicitation and peer-review process, we have identified and selected six new beamlines as the next suite of beamline programs to develop. Further, there is an additional beamline that was selected from the previous rounds BDP calls but its funding commitment from New York state has been ongoing for the past couple of years. These seven beamlines, as well as our current plans to develop them, are described in more detail below.

4.2.2 Bragg Coherent Diffraction Imaging (CDI)

Bragg Coherent Diffraction Imaging (CDI) will be a state-of-the-art beamline that takes full advantage of the world-leading coherent photon flux in a 6-15 keV energy range available at NSLS-II, and will enable cutting-edge research on structural evolution in a wide-range of materials systems under in-situ conditions. By taking the advantage of largely empty reciprocal space at large momentum transfers, BCDI has the unique capability to single out materials of interest in highly complex systems, leading to imaging of defects, dislocations, and strain fields in single grains of heterogeneous materials with relatively high signal-to-noise ratios (**Figure 14**). Additional capabilities include Bragg ptychography to allow mapping single grains in polycrystalline and extended specimens, and time-resolved measurements for both reversible and naturally occurring processes.

The CDI beamline is well aligned with all three NSLS-II strategic science directions – in complexity induced emergent behavior, in in-situ and operando science, and in multiscale structures and function of materials systems. It matches well with the strengths of NSLS-II, particularly in nanoscale imaging, and complements and strengthens other existing beamlines such as HXN, CHX, and ISR. A strong national and local research community already exists for this new beamline and, with the increased interests worldwide on diffraction limited light sources, it can be expected that the CDI community will continue to grow over time.

NSLS-II plans to develop the CDI beamline on a green-field ID port that has the possibility to extend beyond the ring building. This development plan, as outlined below, will be accomplished by allocating a portion of its operating funds each year in the next five years.

In FY17, NSLS-II will identify a lead scientist for the CDI beamline, form a BAT by holding its first meeting, finalize the beamline conceptual design, including the determination whether the beamline would need to go long beyond the ring building, complete the preliminary cost and schedule, and start the preliminary engineering design of the beamline.

In FY18, NSLS-II will complete the beamline preliminary design of the CDI beamline, baseline its cost and schedule, and start the long-lead time procurement of beamline subsystems, and conduct a construction readiness preliminary design review.

In FY19-21, NSLS-II will start the construction of the beamline infrastructure and the installation of beamline utilities, continue the procurement and installation of all beamline components, and start to receive and test com-

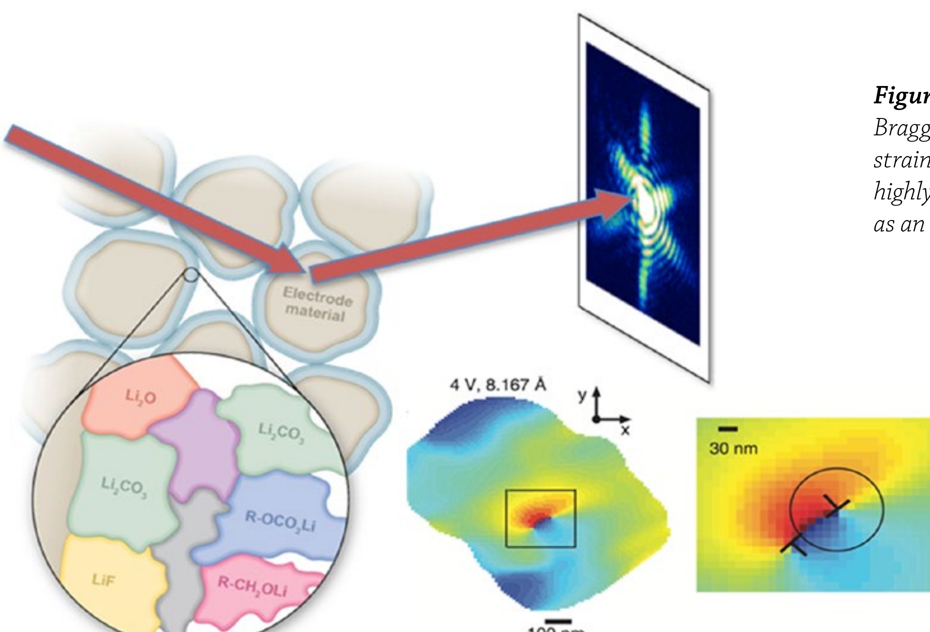


Figure 14: *Schematic illustration showing the Bragg CDI technique would allow imaging of the strain fields in a single grain of crystallite in a highly complex and heterogeneous specimen such as an electrode in a lithium ion battery.*

ponents and subsystems, with the goal to complete the construction and transition into operations of the CDI beamline by end of FY21.

4.2.3 ARPES and RIXS Nano-Imaging (ARI)

The ARI beamline will be a cutting-edge soft X-ray spectroscopy facility with two experimental capabilities - Angle-Resolved Photo Electron Spectroscopy (ARPES) and Resonant Inelastic X-ray Scattering (RIXS), combined using a nano-focused soft X-ray beam on the same spot on the sample with a world-leading spatial resolution of ~100 nm. Its chief science mission is to address the basic R&D needs in the development new quantum materials as driven by new information technologies & new directions in microelectronic & computer industry.

The ARI beamline is well aligned with the NSLS-II science themes on emergent behavior due to complexity and on in-situ and operando sciences. It leverages the NSLS-II strengths in soft X-ray spectral range, wide experimental floor space that enables long working distances for soft X-ray spectrometers, and the infrastructure that provide stable beams and good ground vibration characteristics. It will offer great synergy with existing soft X-ray programs at CSX-1, CSX-2, ESM, and SIX at NSLS-II, as well as with strong research interests at BNL and from the national condensed matter materials communities.

Another novel feature of the ARI beamline is a zone-plate based spectrometer for RIXS imaging. This unique capability will offer a large solid-angle collection of the RIXS signal, with a possible simultaneous observation of ARPES spectrum from the same illuminated nanoscale region on the sample. With this combined nano-ARPES and nano-RIXS at ARI, it will be possible for the first time to provide a complete picture of near-Fermi-edge excitations and interactions with collective modes at the nanoscale in complex hard condensed matter systems in their realistic in-situ environments, leading to a critical understanding of the nanoscale origins of emergent macroscopic materials properties.

NSLS-II plans to develop the ARI beamline on a canted green-field ID port. The ARI beamline will be located on the low-energy canted branch in 40-150 eV, with the affordance of a low-energy scanning transmission X-ray microscope (STXM) upstream of the ARI endstation on the same branch. In addition, affordance will be made for a high-energy branch on the same port that will accommodate an independent high-energy STXM instrument. The current development plan for the ARI beamline is outlined below, funded through NSLS-II operating funds for the R&D and conceptual design activities. Construction funds have yet to be identified.

In FY17, NSLS-II will pursue the R&D to demonstrate the novel concept of the zone-based RIXS spectrometer, finalize the beamline conceptual design, and complete the preliminary cost and schedule. NSLS-II will engage DOE-BES and others to explore the possibility of alternative funding to support the construction of this beamline in future years.

In FY18, NSLS-II aims to secure alternative funds to continue the development of the ARI beamline. Activities will include the completion of the beamline preliminary design, baselining its cost and schedule, conduct a construction readiness preliminary design review, and starting the long-lead time procurement of beamline subsystems if alternative funds are in place.

In FY19-21, assuming the alternative funds are in place, NSLS-II will start the construction of the beamline infrastructure and the installation of beamline utilities, continue the procurement and installation of all beamline components, start to receive and test components and subsystems, with the goal to complete the construction and transition into operations of the ARI beamline by late FY22.

4.2.4 Soft X-ray Spectro-Microscopy Facility (SMF)

The Spectro-Microscopy Facility beamline will be a world-leading soft X-ray beamline consisting of two cutting-edge scanning transmission X-ray microscopes STXMs – one low-energy STXM with full polarization control that will cover the energy range from Li K-edge at 45 eV to Si K-edge at 1.5 keV, and one high-energy STXM from C K-edge 250 eV to Au/Pt M-edges at 3.5 keV. Both instruments will have best-in-class focused soft X-ray beam sizes down to 10-15 nm, wide temperature range sample environments to LN2 temperatures, modular sample holders compatible with other imaging beamlines as well as TEM, and integrated ptychography capabilities to reach ~5 nm spatial resolution.

Together this new soft X-ray microscopy facility will take full advantage of NSLS-II strengths in the soft X-ray regime and enable element-specific chemical analytical microscopy at 10-20 nm spatial resolution with an extremely rapid 100 μs/pixel scan speed for a wide-range of studies on complex materials and devices under in-situ and operando conditions. The unique capability of the low-energy STXM will allow access to the Li K-edge, enabling direct imaging of Li chemistries and distributions in Li-ion batteries for the first time. Both STXM microscopes will fill the energy gap in the soft X-ray range among the existing cutting-edge X-ray imaging and microscopy tools at NSLS-II, and complement the research activities at HXN, SRX, TES, XFM, and FXI, allowing multiscale imaging of hierarchical structural and chemical organizations in complex systems that affect their functional behavior. In addition to cutting-edge capabilities, it is expected that this SMF beamline will also fill a capacity gap in the STXM user base and be able to quickly accommodate a very broad user community ranging from energy and materials research, soft matter and polymer sciences, to geo-environmental and biosciences.

NSLS-II plans to develop the SMF beamline on a canted green-field ID port, sharing with the ARI beamline. The low-energy STXM will be located on the low-energy canted branch, sharing with the ARI endstation downstream. The high-energy STXM will be located on the high-energy branch on the same port that will be fully independently operated from the low-energy branch. The current development plan for the SMF beamline is outlined below, funded through NSLS-II operating funds for the conceptual design activities, and through alternative funds for its construction.

In FY17, NSLS-II will continue low-level activities based on a phased approach to develop the three endstations on the combined canted ARI/SMF beamlines – low-energy STXM 45-1200 eV, ARI endstation on the low-energy branch, and finally high-energy STXM 250-3500 eV on the high-energy branch. NSLS-II will engage DOE-BES and others to explore the possibility of funding to support the construction of this beamline in the coming years.

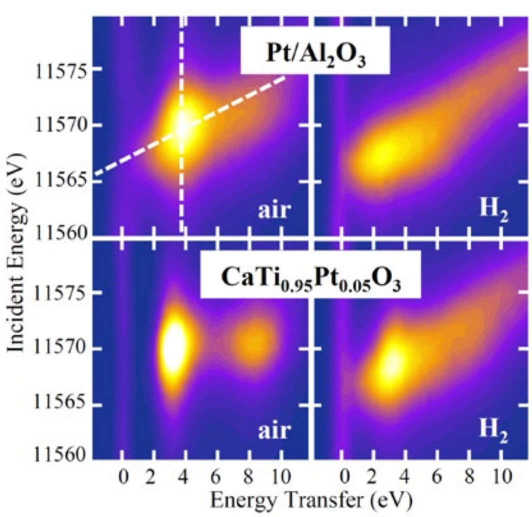
In FY18, NSLS-II will seek to secure funds to continue the development of the SMF beamline. Activities will include the completion of the beamline preliminary design, baselining its cost and schedule in the phased approach, conduct a construction readiness preliminary design review, and starting the long-lead time procurement of beamline subsystems once the alternative funds are in place. Depending on the availability of the alternative funding from DOE-BES, NSLS-II may also pursue funding the high-energy STXM from other funding agencies such as DOE-BER or NSF.

In FY19-21, assuming the alternative funds are in place, NSLS-II will start the construction of the beamline infrastructure and the installation of beamline utilities, continue the procurement and installation of all beamline components, design, fabricate, and assemble the low-energy STXM, start to receive and test components and subsystems, with the goal to complete the construction and transition into operations of the low-energy STXM on the SMF beamline by late FY21.

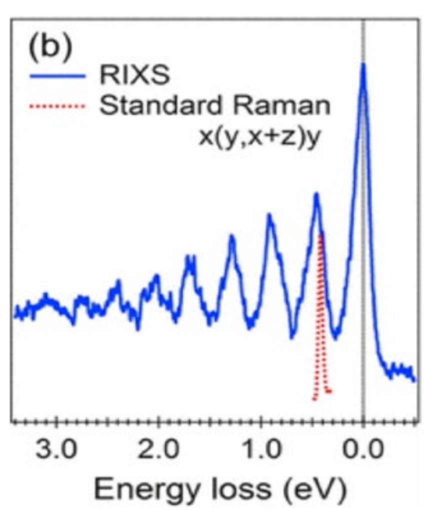
4.2.5 Quick RIXS Beamline (QIX)

The quick resonant inelastic X-ray scattering (QIX) beamline will be a soft X-ray RIXS/XES beamline with best-in-class photon flux and throughput for investigation of static and dynamic behaviors of advanced energy materials in realistic conditions. This new instrument will have a resolving power ~10,000 at 1000 eV in an energy range of 200 – 2000 eV, with a focused beam spot of 1 μm x 10 μm. Taking advantage of the NSLS-II spectral brightness in this energy range, this soft X-ray capability will enable very fast RIXS data acquisition on the level ~1 sec for a 2D RIXS map over a few eV energy window, providing time-dependent (sec. to min.) snapshots of chemical, orbital, charge, & site-resolved electronic structures relevant to catalysis and chemical sciences and meeting the research needs of a strong and active spectroscopy user community (**Figure 15**).

NSLS-II plans to develop and implement the QIX instrument as an additional endstation on the CXS-2 beamline which can already provide high photon flux in the desired energy range for QIX. In FY17 NSLS-II will engage DOE-BES and others to explore the possibility of funding to support the construction of the QIX instrument in future years.



RIXS maps measured for two distinct Pt catalysts in air and H_2



OH-stretch vibration in H_2O at O K-edge

Figure 15: *(Left) RIXS maps measured for two distinct Pt catalysts in air and* H_2 *[12]. (Right) Vibration spectrum, measured using RIXS, of the OH-stretched bonds in water at the O K-edge [13].*

In FY18, assuming the availability of funding, NSLS-II will complete the QIX preliminary design, produce its baseline cost and schedule, conduct a construction readiness preliminary design review, and start the long-lead time procurement of beamline subsystems once the alternative funds are in place.

In FY19-21, assuming the funds are in place, NSLS-II will start the construction of the QIX instrument in FY19, continue the procurement and installation of all components, including the design, fabrication, and assembling any in-house developed items, with the goal to complete the construction and transition into operations of the QIX by late FY22.

4.2.6 Processing and Liquid Scattering (PLS)

The Processing and Liquid Scattering beamline will be a versatile x-ray scattering facility sharing a canted straight section at 12-ID. Its science mission is to support a world-class scientific program for operando studies of soft matter interfaces, especially polymer thin films during processing and liquid surfaces, both these in contact with air and with a secondary liquid. Through the use of a canted undulator this facility will operate independently (and in parallel) with the Soft Matter Interfaces (SMI) beamline at 12-ID.

The PLS capabilities will provide new scientific opportunities at NSLS-II that are not currently addressed by existing beamlines, in part since the design allows the sample to remain level while the beam is tilted downward over a wide angular range. The high flux and tight focus of the NSLS-II source will enable unprecedented time-resolved studies of soft matter specimens undergoing industrially-relevant formation, processing, additive manufacturing, as well as structural transformation, weathering, degradation, and aging. These studies will encompass polymers, liquids, liquid crystals, granular materials, gels, and biomolecular materials, all of which lack the three-dimensional crystallinity characteristic of conventional hard materials. Soft materials are increasingly called upon to address national needs in energy, health, the environment, and national defense and security.

The PLS beamline will play an important role in addressing our strategic directions in emergent behavior from complexity and in *in-situ* and *operando* science. In particular it will help strengthen NSLS-II connections to the advanced manufacturing and flexible electronics initiatives, and complement the existing scientific scopes at SMI and CMS. Its cutting-edge liquid scattering capability will help recover lost capacity for liquid interface community in US and connect to strong in-house expertise. The facility is also well suited to take advantage of new funding opportunities associated with BES/DOE's interest in the Energy-Water Nexus where the oil/water interface is a major topic of discussion.

The NSLS-II strategy to develop the PLS beamline will be to leverage the significant interests in the advanced manufacturing community and industry to explore the external funding opportunities in the national network of manufacturing institutes (NNMI), potentially in partnership and close collaborations with the National Institute of Standard and Technology (NIST), the defense threat reduction agency (DTRA), and the Department of Defense (DoD) services laboratories.

In FY17-18 the Complex Scattering Program team will enhance engagements with NIST, with NNMI, and with DoD agencies and pursue funding initiatives relevant to the PLS program. The lead beamline scientist for PLS, will refine the PLS conceptual design, particularly the concept of the processing endstation, during the process. Activities will also include pursuing joint research projects using existing NSLS-II beamlines to demonstrate benefit to the community and to help identify the gaps in our current suite of capabilities. Our goal is form a realistic approach to allow funding of this beamline by FY19.

Recognizing the level of uncertainties in the timeline for funding, NSLS-II has developed a plan to construct an interim liquid spectrometer on 12-ID by adapting existing instrumentation from the former 9-ID liquid spectrometer at the APS, recently transferred and shipped to BNL, in a time-shared operating mode with the SMI SAXS/WAXS endstation, This will allow the addition of the state-of-the-art liquid scattering program at NSLS-II while we continue to pursue funding for the enhanced PLS beamline scope which includes a liquids instrument that keeps the sample height fixed as the incident angle is varied and parallel/independent operation of a processing and liquids instrument.

In FY19-21, assuming the new funding is in place, NSLS-II will finalize the conceptual and the engineering designs of the PLS beamline, develop a baseline cost and schedule, and start its construction of the PLS beamline, with the goal to complete its construction and transition into operations by late FY22.

4.2.7 Infrared Near-Field Nanospectroscopy (INF)

The infraread near-field nanospectroscopy (INF) will be a new infrared beamline for nanospectroscopy and vibrational spectroscopy of materials central to current problems in condensed matter physics and chemical catalysis (**Figure 16**). Apertureless near-field nanospectroscopy, based on synchrotron infrared light scattered from an atomic force microscope (AFM) tip, offers broadband spectroscopy of materials with better than 10 nm spatial resolution across the important range of wavelengths from 2μm to 100μm

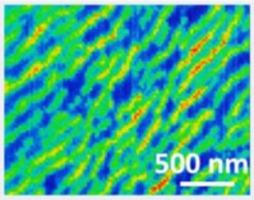
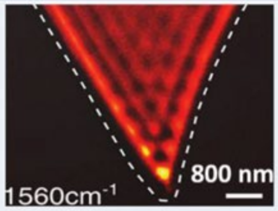
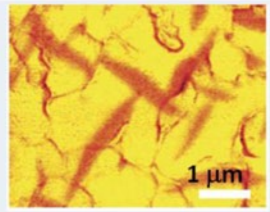
Strongly correlated electron materials	Low dimensional materials	Organic materials and chemical compounds
Phase inhomogeneities Drude response, collective electronic excitations	High momentum coupling of plasmon, phonon polaritons	Structural resonances
		
Metallic stripes in VO_2 film on $[110]_R$ TiO_2	Phonon polariton in hBN	local crystallinity of organic thin films (pentacene)

Figure 16: *Representative inhomogeneous systems of interest under broadband IR near-field investigation. From left to right: Phase inhomogeneity in strongly correlated electron materials (VO2), high momentum polariton coupling in low dimensional materials (hBN), and phase mixture and structural identification in organic thin films (pentacene).*

that probes many intrinsic electronic and vibrational excitations. Applications of this novel method will include a wide range of studies in such areas as phase transitions and intrinsic inhomogeneities in Mott insulators, high Tc superconductors, magnetic and multiferroic domains in complex oxides and heterostructures, elementary excitations in low dimensional and plasmonic materials, spectroscopic and chemical catalysis of nanoparticle catalysts, and phonon vibrations in oxide nanoparticles or organic thin films.

The scope of the INF beamline consists of three endstation programs – near-field IR spectroscopy for condensed matter and materials physics, near-field IR spectroscopy of nanomaterials for catalysis, and IR reflection-absorption spectroscopy (IRRAS) of catalytic systems under ambient pressure. The latter is in combination with the CSX-2 branch program in partnership with CFN, and will also provide conventional mid-IR microspectroscopy of materials with ~50% time share. This suite of state-of-the-art instruments is well aligned the NSLS-II strategic directions in emergent behavior from complexity and in multiscale structures and functions. It will place NSLS-II at the forefront of synchrotron IR nanospectroscopy, extending conventional IR microspectroscpy far beyond the diffraction-limit and complementing other NSLS-II nanoscale probes – existing or currently under development.

NSLS-II plans to develop the INF beamline on the 23-BM floor space, utilizing the 24-BM bending magnet as the IR source. This location is in close proximity to other IR beamlines already under construction (FIS and MET) on the 22-BM space, and also next to the AP-PES as well as the new QIX instruments at CSX-2 on 23-ID. This synergy will greatly enhance the programmatic interactions in the condensed matter physics and chemical analysis communities.

Under consideration for the INF funding strategy is the potential to apply for and obtain major research instrumentation (MRI) funding from NSF to support its construction. Specifically, in FY17 NSLS-II will work with partner institutions such as Stony Brook University to submit a grant application to the NSF Major Research Instruments (MRI) program. It is expected that such funding, if successful, will constitute the bulk of the required budget for engineering design, IR extraction system, and endstations and cabins for the INF beamline.

If funding is realized in FY18, the construction of INF will proceed as rapidly as possible, with the potential to complete the final designs of the beamline and start long-lead procurements of the IR extraction system by early FY19. It is expected that the construction will be completed and the beamline will transition into operations by late FY21.

4.2.8 High-energy Engineering X-ray Scattering & Imaging (HEX)

The HEX beamline will be a new beamline facility to provide a suite of most advanced hard X-ray tools required for engineering-scale materials studies using hard X-ray diffraction, scattering, and imaging. The beamline will be located on a short-beta straight section using a superconducting wiggler as the high-energy high-flux X-ray source. It will consist of three independent endstations in a satellite building to provide hard X-ray diffraction and imaging probes in the 20-200 keV range for studies of engineering material systems under real operating conditions. Key science areas will be in the areas of structural analysis of the chemical reaction fronts and their evolution in real battery systems during charge and discharge cycles, materials microstructural changes under external extreme conditions such as high mechanical stress, high pressure, high temperatures, and corrosive environment, and phase contrast hard X-ray imaging with a large field of view in real space for studies of micro-crack formation and propagations under realistic operating loads, etc. (**Figure 17**). These studies will have significant impact on the economic competitiveness of industries in New York state as well as in the nation.

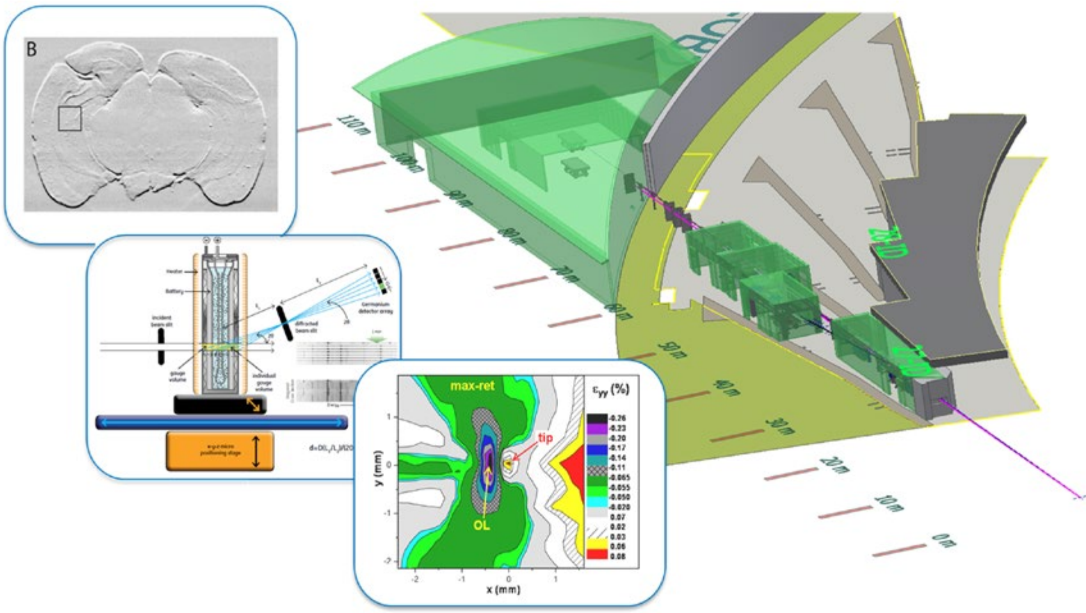
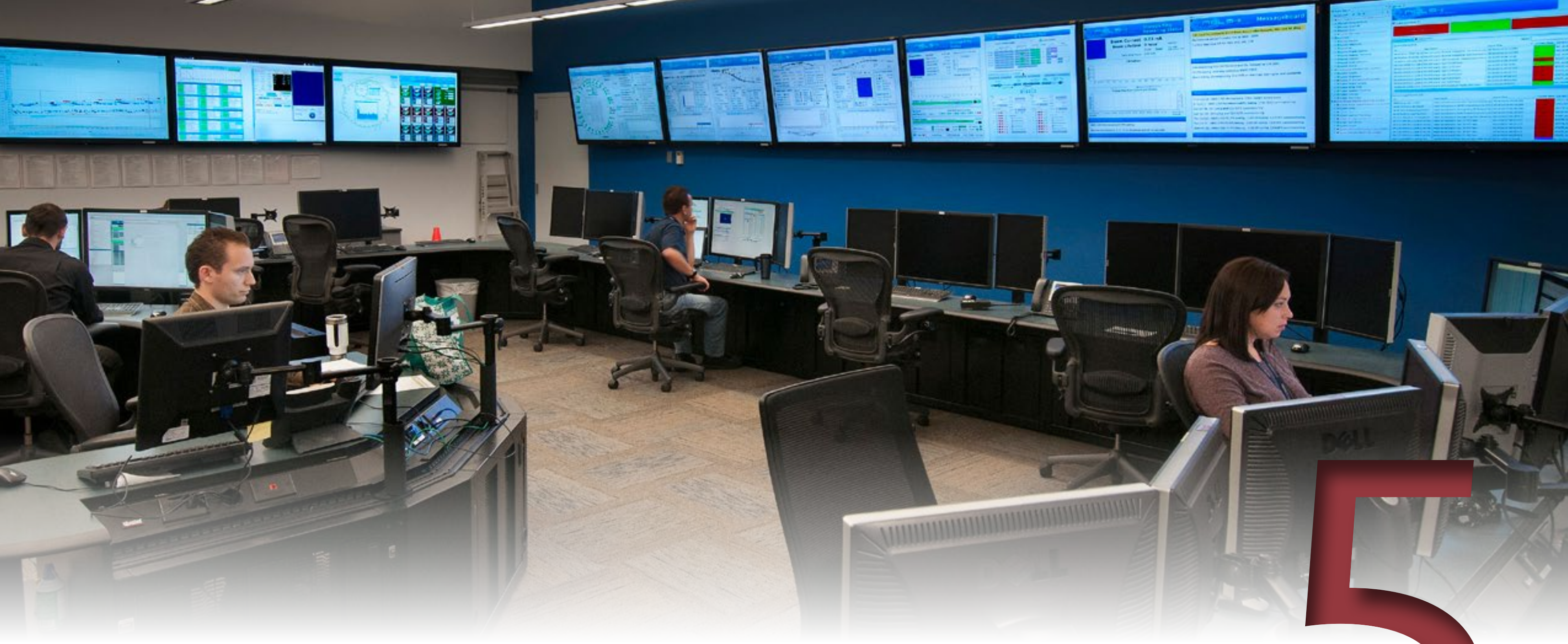


Figure 17: *Illustration of the High-energy Engineering X-ray Scattering & Imaging (HEX) beamline, and its three cutting-edge programs for engineering systems studies (strain-stress map-ping under mechanical load, operando studies on real systems e.g. batteries, and large field of view phase contrast imaging using hard X-rays.*

NSLS-II will develop the HEX beamline using funding that is already committed by New York State. In FY17, it is expected that State funding will be received by mid fiscal year, which will allow commitment of NSLS-II staff to complete the conceptual design of the HEX beamline. NSLS-II will form a BAT for the HEX beamline consisting of key researchers and industry program managers relevant to the applications of this beamline.

In FY18, NSLS-II will complete the engineering design of the beamline including the satellite building, and conduct a construction readiness review with a goal to start long lead procurements by end of FY18 and the start of the satellite building construction by early FY19.

In FY19-21, NSLS-II will start the construction of the HEX beamline hutches and utilities, continue the procurement and installation of all components, including the design, fabrication, and assembling any in-house developed items, with the goal to complete the construction and transition into operations of the HEX beamline by late FY22.



5

CONTROLS AND DATA SCIENCE

Accelerator and beamline controls and high-level data acquisition, management and analysis play a mission-critical role in the productivity and impact of all NSLS-II science programs, and serve as the front-end interface between the facility and our visiting users. Our main objective in controls and data science is to provide our users a suite of reliable, flexible, and open-source software codes that meet the science needs and are at the leading-edge and well maintained and documented. In this Chapter, we outline our action plans in these areas to meet our objective.

5.1 CONTROLS

Every major facility like the NSLS-II uses computing software and hardware prolifically to achieve the facility aims. We universally use computers for almost every aspect of our daily operations, from monitoring of the smallest physical quantity of the accelerator, exploring trends, capturing and analyzing the scientific data, generating models and both communicating and storing the data for long term archival. It would be impossible to operate the facility without extensive computing networks, servers, computer desktops and many differing software resources.

To meet the needs of the facility, we rely on a combination of computing and electronic hardware – purchased off the shelf where we can, developed in house where we must and software, again sourced either commercially or via collaborations where we can and developed in house where we must. The use of both custom hardware and software, and the deployment, maintenance, debugging and backup of these hardware and software systems primarily for monitoring and control of all NSLS-II equipment is known generically as "Controls". We note that outside of the Controls program, there is excellent expertise in the mechanical engineering team, the accelerator team, the operations team on many beamlines and elsewhere producing outstanding software and hardware. They will work closely with the Controls program to build on the infrastructure created by Controls.

The Controls program scope of work consists of the production and maintenance series of specialist technologies that are used for the monitoring, control, data acquisition, and data analysis of systems used in both the production and utilization of synchrotron radiation. As such, the Controls program encompasses the monitoring and supervisory control of most of the NSLS-II accelerator systems and is an integral part of each of the beamlines. The data acquisition and analysis is more beamline specific, though we strive to exploit commonalities.

Systems monitored and controlled by the Accelerator Controls program include RF systems, vacuum, magnet power supplies, equipment protection systems, diagnostic equipment such as beam position monitors; and insertion device control which crosses into beamlines. Systems monitored and controlled by beamlines controls are typically front-end equipment, optical components, endstation equipment, equipment protection systems, detectors, vacuum, and data storage and analysis.

Constant monitoring and reporting of abnormal conditions lead to improvements and high uptime of accelerator.

Certain systems are used by all control systems, among which networks, software distribution, user interface support and EPICS data archiver support are good examples.

The monitoring and control of these various systems is performed using the application of electronic systems. These systems include networking, computer servers, workstations, large data storage facilities, high performance computing, embedded micro-computers and the provision of software to drive it all.

The NSLS-II has, in concert with most other U.S. and worldwide Synchrotron facilities chosen EPICS for some of its software requirements and the use of EPICS as the "glue" or middleware has greatly enhanced the ability of the Controls Group teams to deliver the solutions at ever decreasing low cost compared to scratch developing systems.

For the beamlines controls, the NSLS-II Data Management Acquisition and Analysis group develops a suite of higher-level software and user interfaces, building on common platforms of EPICS and Python and through collaborations with other institutions, to ensure that the controls at NSLS-II beamlines are optimized for different types of experiments. In addition, the beamline controls group provides support for specialized high-level applications that may be run as part of a science experiment.

5.1.1 Accelerator Controls

The accelerator controls systems are required to run twenty-four by seven, often even during machine downtimes and machine maintenance periods. If a major component fails during operations, then the facility is down and every beamline is affected. If certain components fail – even during maintenance it can delay maintenance work or the eventual normal operations.

Currently there are over 1.3 million different process variables (PVs) either monitored or derived by the accelerator systems. The original estimates were for around 350,000 at the NSLS-II first light.

This growth is expected to continue at a substantive rate, perhaps at around 20% per year, over the next five years and will lead to improvements in accelerator performance, in such areas as beam stability, emittance, timing accuracy, beta function and lifetime. It will also improve the ability to both diagnose and repair faults, thus increasing the already high uptimes. The cost per PV, particularly derived PV's is also dropping as the cost for CPU time drops.

The Accelerator control systems were assembled and deployed early in the construction phase of the project, nominally ending at the CD-4 review in 2015. As a result, certain components are now approaching end of life. The strategy for replacement is to target the components nearing, but before the end of life, using the familiar engineering "Bathtub" model and a variety of analysis tools for failure modes, effects and cause analysis, based on a widely used industry methodology not dissimilar to many of the project risk assessment methodologies. It helps to make logical replacement decisions for high uptimes and high quality installations.

For controls hardware, it is primarily intended to replace hardware to maintain high uptimes and to provide for off the shelf replacements as equipment falls out of manufacturer support, both for hardware, firmware and software. However it is also inevitable that the performance of the newer hardware will also allow for faster responses times and increased processing support for the servers, and increased network bandwith and lower network response times for networking equipment.

Based on our failure modes analysis, our plan is to replace the oldest portion of the accelerator controls including many IOC's, servers over five years old in FY17, replace at least 50% of all servers, network switches in FY18, and replace all operator workstations and all remaining commodity server hardware in FY19-21. Also in FY19-21, we plan to rewire to newer network standards as applicable, and replace or supplement the network core switch.

For controls software: On EPICS, our strategy is to follow closely the latest release of EPICS. If too far behind, the ability to get community support is diminished, and if too far ahead, the incidence of bugs increases. The sweet spot varies, but for EPICS, the stability of a release at around 12-24 months is close to optimal. It is also important to stay near the current version of EPICS in order to gain benefits from the community support – bugs are still being found. This adds to reliability and the ability to diagnose problems quickly, in addition to help recruiting and retaining the needed staff with relevant experience.

Specific plans for EPICS include the following: In FY17, we plan to maintain at or near the current release of EPICS. In FY19-21, we plan to diverge systems – retaining low level IOCs at EPICs V3 and progressively introduce certain servers to EPICS V4 as the features unfold. We expect EPICS Version 4 to have a pvAccess Protocol for structured data. Some expected features include: an Introspection interface, "pvData", dynamic typing, standard scientific types, smart database, Codec based, APIs in C++, Java, Python and Matlab, and other high performance, high reliability features.

For Operating Systems, we plan to issue upgrades to keep to a near current version of Linux and RTEMS, primarily for cyber security reasons, although community support for more recent operating systems is also an important factor.

In addition, we plan to explore the possible introduction of a components database. There are increasingly large amounts of data, based on our PV estimates. There will be staff turnover and not all engineering staff in the future will be the same ones as those who created the systems. It is important to keep track of the ever increasing versions of software, hardware and components. A components database is one very effective way of performing these functions.

5.1.2 Beamline Controls

Beamline controls allow experimental procedures to proceed by enabling motion and parametric controls of beamline optics and components as well as specimens, detectors, and sample environments manipulations in endstation instruments. Beamline controls systems use similar basic controls software to the accelerator, but with significant complexity, variations, and specialization to suit different hardware and different experimental techniques.

Typical beamline controls are accomplished with low-end server-class computers for basic input output controls, with networking done using higher-end networking equipment. Timing and a few specialist components use VME and RTEMS as the OS. At NSLS-II, Delta Tau Geobrick LV is the standard controller for stepper motors. There is also a lot of specialist hardware, ranging from detectors, robot arms to pico motors, sample environments and more, that are required to conduct optimized experiments.

As with the accelerator, the widespread use of commodity IT components means that the average lifetime of five years for servers and networking equipment. Fortunately these components span a variety of years and were not purchased at the same time. In addition to networking equipment, there is considerable need for expanded data storage – local to the beamline, centralized to NSLS-II, central to BNL (the Computational Sciences Initiative, CSI), and finally delivered to the end user either at their home institution or on a cloud service.

Beamline controls hardware. For beamlines, one additional driving factor is the increasing needs in computing and data (network) speeds that is driving the desired technological updates. Our plan for the next five years include the following: In FY17-18, in addition to replacement of ~15% servers and network switches, upgrades to faster networks switches are required at certain beamlines in order to move data from detectors and onto local, near local and remote storage arrays. In FY19-21, we will plan to update all beamline workstations, replace all remaining commodity server hardware, rewiring to newer network standards as applicable. Towards FY21, we envision replacement or supplement of the network core switch due to the current hardware being obsolesced by the vendor.

Beamline controls software. We plan to follow a similar updates schedule on EPICS as to the accelerator controls, as the newer versions of EPICS have many features – particularly with the drivers like SYNAPPS that support an increasing variety of beamlines devices. The same process will be followed for beamline workstation operating systems updates.

One new area of beamline controls we plan to implement in the FY17-18 timeframe is the remote access for beamline users. There are three major use cases for this, as follows. (a) The user is currently performing an experiment and wishes to monitor and control the experiment as it happens. Typically a user may set up an experiment and then, perhaps overnight monitor the progress from the lodging and modify accordingly. (b) The user is performing a “standard” experiment and controls the progress of the experiment remotely from their home institution, with samples mailed-in to NSLS-II. (c) The user is not performing an experiment and wishes to access or process previously gathered data remotely.

Techniques for safely and securely performing these remote access cases (and other variants) will be developed in a manner that is both consistent within a beamline and across beamlines, with special attentions paid for security of data, security of control, and authorizations consistent with BNL-wide policy. Such development will require coordinated efforts among multiple groups on beamlines, beamline controls, IT, data acquisition, management & analysis, BNL computational science initiative, user office, experimental safety, and cyber security. It is expected that there will be ongoing working groups as this is a very complex area, and naturally subject to a cyber security safety component.

Detector and DAQ Support. One area of responsibility of the beamline controls group is to provide controls support to new X-ray detectors that will be developed or procured in the coming years by the NSLS-II detector group and beamline groups. Integration of these new detectors into the individual beamlines will be provided on a case by case basis. Similarly, new experiments may be conducted at NSLS-II beamlines that require new ways of collecting experimental data. Thus the beamline controls group will also need to work beamline staff to provide data acquisition support to implement new experimental protocols. In these cases, complexities in controls may arise due to the bandwidth required for each of the new detectors, the amount of data generated, EPICS integration, fly-scan algorithms, motion controls, insertion device coordination, and timing devices with fast or slow glue logic.

In FY17, we will survey the beamlines and the detector groups to gain knowledge and understanding of new detectors and new data acquisition (DAQ) modes under development or that may be acquired in the near future, along with their functional requirements and data rate and characteristics. In FY18 and beyond, we plan to deploy and develop timing and glue logic as part of a general DAQ architecture, and start to develop large scale data storage that will meet the beamlines data requirements.

5.1.3 IT systems

The IT system of the NSLS-II accelerator controls network consists of gateways and a dedicated, multi-tiered private local area network for control of the NSLS-II accelerator complex: LINAC, booster synchrotron, and storage ring. Construction of this system was completed in 2012. The accelerator controls system adheres to a modern distributed control model consisting of (a) global timing achieved utilizing a GPS network time protocol appliance refined through a rubidium oscillator and distributed via event generators and receivers, (b) low level controls of e.g., magnet power supplies, vacuum, RF systems achieved utilizing a mixture of modules for analog and digital I/O running EPICS on an embedded real-time operating system (RTEMS), and commodity servers acting as EPICS I/O Controllers (IOCs) on Linux, and (c) high-level controls e.g., Controls System Studio (CSS), channel archiving, alarm handling and applications e.g., Matlab Middle Layer Toolkit, pyEPICS, Elegant, and Bluesky running on Linux servers and workstations.

NSLS-II capitalizes on modern network and computing hardware. For the network, managed Brocade switches and routers are used exclusively. Since 2015, all purchased IOC and infrastructure servers are variants of the same manufacturers family. Servers purchased prior to 2015, many still in service, are IBM systems. Workstations utilized by operators and engineering staff are variants of the Hewlett Packard (HP) systems . All systems exclusively run Debian Linux. Other Ethernet-based devices include, but are not limited to, beam position monitors (BPMs), cell controllers, instrument controllers (e.g., motor, power supply, vacuum), cameras, oscilloscopes, radiation monitors, and serial-Ethernet converters. These devices run simple, embedded operating systems, some Linux-based, some proprietary.

It is important to anticipate the beamline experimental programs needs in the next five years as these needs will have impact on NSLS-II IT systems. We currently envision two new trends from beamline programs. The first is the need for remote access by users from institutions outside of BNL, which will drive the requirements on IT security and flexibility. The second is the need for fast transfers of a greater amount of data at a greater data-rate (see **Figure 18**) to a central storage and processing facility. This will drive the need for faster network links.

Our plans to meet the beamlines needs are as follows. In FY17, we plan to update the core switch and develop a plan for separation of the beamline network for greater security, flexibility and reliability. In FY18, we plan to deploy the secure beamline network, update all Linux machines, and develop and implement a prototype plan for remote access by external users. In FY19-21, we will plan for increased data rates at certain beamlines and implement 40 and 100 Gb/sec links to all network nodes.

5.2 DATA ACQUISITION, MANAGEMENT AND ANALYSIS

It is clear that the full impact of scientific understanding from experimental results can only be realized by having a successful computational strategy and therefore data management and computing is an essential component of the NSLS-II strategy. A description of the data challenges that NSLS-II is facing, the approach that is being taken to address these challenges, and the plans to develop theoretical simulation and modelling in support of the user science at NSLS-II is presented below.

An encompassing attribute of all modern scientific facilities, especially light sources and other data producing user facilities is how the successful implementation of data acquisition, management and analysis strategies has the ability to transform the user experience and become an integral part of improving the experimental process as a whole. We have already seen a tremendous growth in the number of publications that combine the analysis and interpretation of their synchrotron experiments with data from other sources, both experimental and computational. This has an impact on all aspects of computing, namely;

- acquisition and coordination of disparate and varied data sources,
- management and tracking the provenance of the data
- utilization of varied data analysis and modeling techniques.

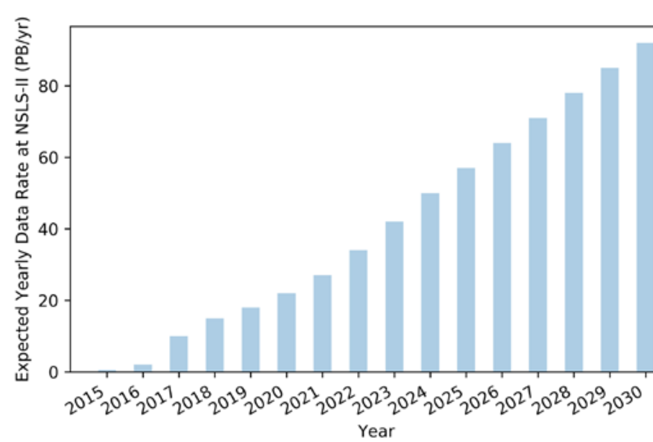


Figure 18: *Estimates of NSLS-II beamline data growth rates in 2016 - 2030. This estimate was based on the current information on data capabilities at existing beamlines and those presently under development, along with their schedule to start operations in the 2015-2021 timeframe. It also takes into account estimated increases in both detector technology and in beamline operational reliability.*

5.2.1 Big Data' Challenges

As the newest synchrotron facility with high-brightness and high-flux beamlines serving a broad and diverse scientific community, NSLS-II faces significant challenges in data management and scientific computing. These challenges primarily arise from three factors.

Data Complexity: Many of the NSLS-II beamlines support cutting-edge scientific capabilities that make use of the most advanced systems for specimen positioning and manipulation as well as photon detection. In order to ensure all experimental techniques are conducted in the most optimal way and not constrained by a 'standard' data acquisition system, NSLS-II has adopted, by design, the strategy that the data acquisition system at each beamline is developed to match the intrinsic data collection needs dictated by the specific experimental technique in sample and photon beam manipulation as well as in photon detection methods. As such, the data structures and formats may be complex and can vary substantially from beamline to beamline, making follow-up visualization and analysis of the data challenging.

Data Management: The high brightness and high flux available at many of the NSLS-II beamlines coupled with advanced high-speed megapixel detectors will drive much higher data rates and volumes compared to situations at most existing synchrotron beamlines. Indeed, all synchrotron disciplines are increasingly using multi-element detectors to efficiently measure and record the results of the experiment, and certain techniques often utilize detectors that can produce multi-megapixel images with frame-rates in the kilohertz range. The volume of data associated with an experiment may therefore now exceed several tens of terabytes so simply moving data from one location to another is prohibitive. As such, it may not be possible for external users to take a copy of all the data on portable media or to transfer over the internet. Thus it will require high-performance data storage systems and a front-end processing facility to allow users to access the data both during- and post-experiments.

Data Mining and Analysis: Broad uses of new megapixel detectors in new techniques drive a new paradigm for data processing and analysis at NSLS-II and at synchrotron sources worldwide, where individual users are often unable to write the sophisticated algorithms required to process, analyze, visualize, interpret or otherwise extract the important information from raw detector data. In addition, visualization and analysis of 3D or multi-dimensional data are intrinsically more difficult, particularly if one wants to extract scientifically relevant information from a multi-dimensional dataset, often requiring specialized data reduction and manipulation algorithms and routines not readily available to individual users. In addition, in the future it will be important to simultaneously analyze data sets from different sources. Examples include electron probes at the Center for Functional Nanomaterials and computational models simulated using CSI HPC clusters. Such "data complexing" or "complex modeling" will have broad application in areas where NSLS-II will have impact and the data architecture is being constructed with this in mind from the initial conception.

In addition, as synchrotron experiments become more and more sophisticated, there is an increasingly greater need for theoretical **modelling and simulations**. For example in experiments depending on high degree of x-ray beam coherence, the experimental results have a greater dependence on coherent properties of the beamline optics and beam defining apertures. Therefore a better understanding of how a complete experiment works, including the effects of optics, is important to being able to interpret the experimental data correctly. NSLS-II plans to address this issue by working with the community and exploring the development of a complete "start-to-end" simulation chain from radiation sources through beamline optics and sample to detectors for certain experiments. This would ensure more optimized experimental design with correct matching of different links in the experimental setups, including source, optics, sample, detector and data processing, leading to a more efficient use of resources and beam time at beamlines and timely and correct interpretations of experimental results. Second, new and enhanced experimental capabilities at NSLS-II will lead to new experimental results that may require new theoretical development and interpretations. Therefore, there will be greater needs for theoretical modelling and analysis to lead to high-impact and scientifically relevant conclusions. NSLS-II will work closely with the scientific community to tackle this challenge, through collaborative efforts on joint research projects with key members of the community and through forming targeted initiatives to outreach to specific expert groups in the community.

Together these theory, simulation and modelling efforts will greatly enhance the NSLS-II capabilities in experimental planning and design, in interpretations of experimental data, and in arriving at research results with a greater impact on the research activities in variety of scientific disciplines.

5.2.2 NSLS-II Data Science Strategy

NSLS-II has developed a preliminary data science strategic plan and is currently executing according to that plan. Key elements of the plan are outlined below.

Flexible Modular Data Acquisition Architecture: NSLS-II beamline data acquisition system is built to provide an essential infrastructure that can grow and evolve over the life of the facility. NSLS-II has developed a suite of open source software packages that not only support new detectors and new techniques as they continue to evolve, but also allows the analysis of the quality of the data as it is being collected and the performance of the beamline (**Figure 19**). The user facing package is called Bluesky and is for experiment control and the collection of scientific data and metadata. Bluesky interacts with the beamline hardware through the standard programming language, Python using the EPICS interfacing software.

During FY17 we will define the requirements for a Bluesky v1.0 release. The baseline features will be defined to fulfil the day-to-day requirements of the currently operating beamlines. Some of the high level functionality includes (not an exhaustive list): complex step scans including N-dimensional, complex spiral trajectories, etc., fly scans, reciprocal space scans, adaptive scans (e.g. feed measurements back into plan), sophisticated streaming analysis (e.g. live tomographic reconstruction), manual and automatic suspend/resume (e.g. in response to beam dump), simulation mode, and the requirement that all known hardware on operational beamlines is supported.

In FY18, we plan to deliver the Bluesky next release (after 1.0). The main area of development for the new release will be focused towards providing a more streamlined user experience with more graphical user interfaces (GUI) for composing and executing scans/plans, together with beamline specific GUIs that will be tailored for specific techniques. Future releases will be planned according to the timescales of future beamline requirements.

In order to promote the use of Bluesky, we are committed to continue running tutorials and training courses both onsite and at other facilities to stimulate active collaborations. It has been presented at ORNL, APS, SLAC, and the Australian Synchrotron, and installed for testing on beamlines at SNS and at APS.

Data Stores and Data Broker Application Interface: At the core of the NSLS-II data acquisition and data management system is an essential set of flexibly structured data stores. These store all data and metadata related to an experiment. A data broker application interface retrieves and manages data and metadata from a distributed set of data stores. This set of data stores are tailored for specific types of experiments, and store not only the raw data from a detector, but also additional metadata from the beamline, accelerator, logbooks, proposal, sample management and scheduling systems. The data broker is a key piece of data handling interface software. It enables the development of data analysis procedures for visualization and analysis of the real-time data to allow decision making, and for post-processing of all data after the actual experiment.

During FY17 we will define and release a version 1.0 of *Databroker*. Its high level features include search on arbi-

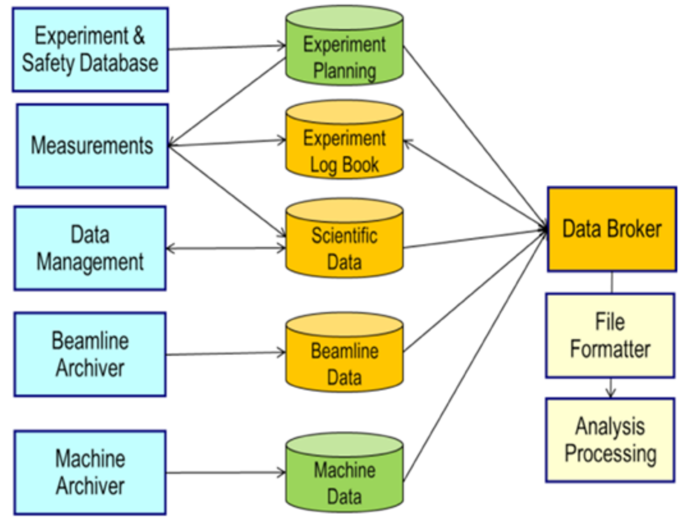


Figure 19: *Schematic representation of the experimental data acquisition architecture at NSLS-II beamlines.*

trary metadata (user groups can use whatever systems make sense to them), automated end-of-run data export to industry-standard formats (TIFF, CSV, HDF5, etc.), sample management inventory database, remote access to streaming data via ZMQ, a basic GUI for browsing saved data, basic feature for commenting on or tagging datasets, and a service architecture to allow remote access to DataBroker functionality.

In FY18, we plan to issue the next release (after 1.0). The main features for this release will include role-based security, improved graphical tools for data discovery, improved provenance handling, integration of cloud services (e.g. Dropbox, Google Drive and Amazon Web Services), integration of Globus, support for more data export formats, and integration with the NSLS-II PASS (proposal system).

On the topic of meta-data content, we have agreed on a small set of meta-data items that will be stored for each dataset for the NSLS-II, APS, ALS, SNS and HFIR. This will allow better data discovery, which is important for a single user group on a single beamline, but it becomes critical when we start to make use of multi-modal or multi-facility data sets and experiments.

Multi-tier Data Management System. To be able to accommodate high data-rate and high data volume data at beamlines, NSLS-II is implementing a multi-tier data management system to ensure efficient and adequate storage for complex experimental data from beamlines. Initially, this multi-tier system will consist of one or two tiers (depending on the beamline requirements), namely local to the beamline and central NSLS-II storage. This will be then extended by adding connections to CSI for long-term storage and near-computer level storage. The investigation, planning and initial prototyping of this expansion will take place during FY17-18 with an implementation by FY19.

The storage local at each beamline is only intended for use as a cache layer for fast data collection. The data will be cloned onto a central repository as soon as it has been collected (but at a lower priority so as to not effect data collection). The data location will look to reside in the same place irrespective of whether it is stored locally on the beamline or centrally. This strategy will mean that we can provide high speed access from a central analysis facility without effecting the beamline performance. In order to meet this goal for all operating beamlines then there will need to be an investment consistent with the number of beamlines. Assuming sufficient funds, this could be fully operational before the end of FY17. Based upon current estimates (**Figure 18**) we will need to have 25 PB available initially in order to support operations up to FY20, this assumes that we will only store data for a period of one year.

Data from each beamline will be replicated and archived at a centrally managed data center for longer-term storage. Here the same visualization and analysis tools for evaluating and processing will be made available as at the beamline. This centrally managed data center will be established in close coordination with BNL's Computational Science Initiative. In order to identify potential issues and bottlenecks we will perform a test of the full end-to-end data pipeline by transferring experimental data from the beamline to central archive storage in FY17. In the first half of FY18 we will select a final architecture and then roll out to all beamlines through the rest of FY18 and FY19. During the remainder of FY17 and into FY18 we will investigate and subsequently define what data format we will use for long term data archival.

As part of our plan in data science, it is crucial that we update our data management policy so that our users have a clear understanding and expectation on what NSLS-II and BNL will provide in terms of data storage, retention and access. We will have a draft plan available for comment in FY17. This plan will have larger implications on resources and procedures (e.g. user authentication) both at NSLS-II and within BNL as a whole.

Functional Library of Analysis Software Tools: Based on the data architecture and the data broker interface, a library of software routines and tools is being developed within the multi-tier data management system. These tools are being tailored to meet the needs of specific types of techniques, experiments, and scientific disciplines. Recognizing the large effort required to meet all the needs from the diverse community, NSLS-II is developing the analysis tools in a phased approach consistent with the NSLS-II beamline development timeline. The software and tools developed are released under the 'scikit-beam' umbrella project, which has users and contributors from multiple facilities.

It is important to state that our approach will be to reuse and collaborate on the development of exisiting software that meets our requirements. During FY17-18 we will evaluate existing software that is available (both internally and externally) and develop a project plan for each to meet the requirements of the beamlines. One example of a development effort that is currently in the planning stages, is to standardize on a single SAXS processing software, this is updating an existing package to make use of modern processing techniques and architectures, which will be completed in FY18. There have been initial discussions with the APS and ALS on how we can work together more effectively and maximise the impact of the software produced by each facilities by eliminating areas of overlap.

Post-Experiment Data Processing Facility: Anticipating the greater need for post-experiment data mining and processing, NSLS-II will work with other stakeholders on computing within BNL to develop and operate a central data processing computing facility as part of the multi-tier data management system. The main goal of this facility is to provide front-end computing and centralized data storage/archiving system for NSLS-II users. This will allow them to access their data on-site during the experiment and also later when they return to their home institutions. The archived data will be made available to users for a length of time that is will be determined by policy and resource constraints. This post-processing facility on archived data is an essential component of the NSLS-II scientific capabilities portfolio. It is required to enable effective and efficient workflows from experimental data to publications and solutions for high scientific productivity and societal impact.

The facility will consist of multiple components, each tuned to a different data processing pattern or activity. The users will be able to make use of which type of computational platform is appropriate for their needs. As an example, for a case where a user has a problem that requires a large amount of physical memory and lots of tightly coupled compute cores, then they will make use of the general user systems within the NSLS-II. But, for a use case that can be parallelized more efficiently and can make use of large parallel HPC like machines, then they will make use of compute clusters situated within CSI. We are currently working with CSI (and have a successful ASCR SBIR) to benchmark some standard codes, such as accelerator physics and ptychography (based upon the SHARP code from the CAMERA project), in order to determine which computational platforms would be best suited for the various NSLS-II use cases.

The archived data will be made available to users for a length of time that is will be determined by policy and resource constraints, but as of this time we are planning on keeping data for at least one year. During FY17 and FY18 we are working with CSI to evaluate a system that can be used for long term data and software curation. The software, Invenio was developed by CERN and is starting to be used and investigated by other institutions, such as Caltech. This system will act as a 'digital library' for data, which included not just the raw experimental data, but the processed data together with the software used. Together with CSI experts we are investigating how we can capture and subsequently store the workflow and provenance of the data lifecycle in an effort to aim scientific reproducibility.

It should be noted that this post-processing facility on archived data is an essential component of the NSLS-II scientific capabilities portfolio. It is required to enable effective and efficient workflows from experimental data to publications and solutions for high scientific productivity and societal impact.

Community Participation: No one facility or organization will have the expertise and resources required to develop all the software necessary to cover all the use cases in the wide variety of science that will be done at the NSLS-II. Therefore, we are actively working with other facilities and the user community on sharing software, knowledge and experiences. BNL held the first of what has become a series of "hackathons" for staff members representing the DOE Office of Science User Facilities. These have been a success and we intend to continue this series and encourage the participation of NSLS-II, CFN and CSI staff.

In order to provide an independent technical assessment of the overall architecture and direction we will hold a review of the Data Acquisition, Management and Analysis software stack in FY17. The charge for this review will also seek what level of resource is required in order to implement our strategy.

NSLS-II will be hosting the New Opportunities for Better User Group Software (NOBUGS) conference in 2018/2019. The aim of these conferences is to foster collaboration and exchange between scientists and IT professionals working on software for X-ray, neutron and muon sources around the world. Better software for data acquisition and data analysis will increase productivity of facility users and thus maximize the scientific output.

5.2.3 Computational Science Initiative

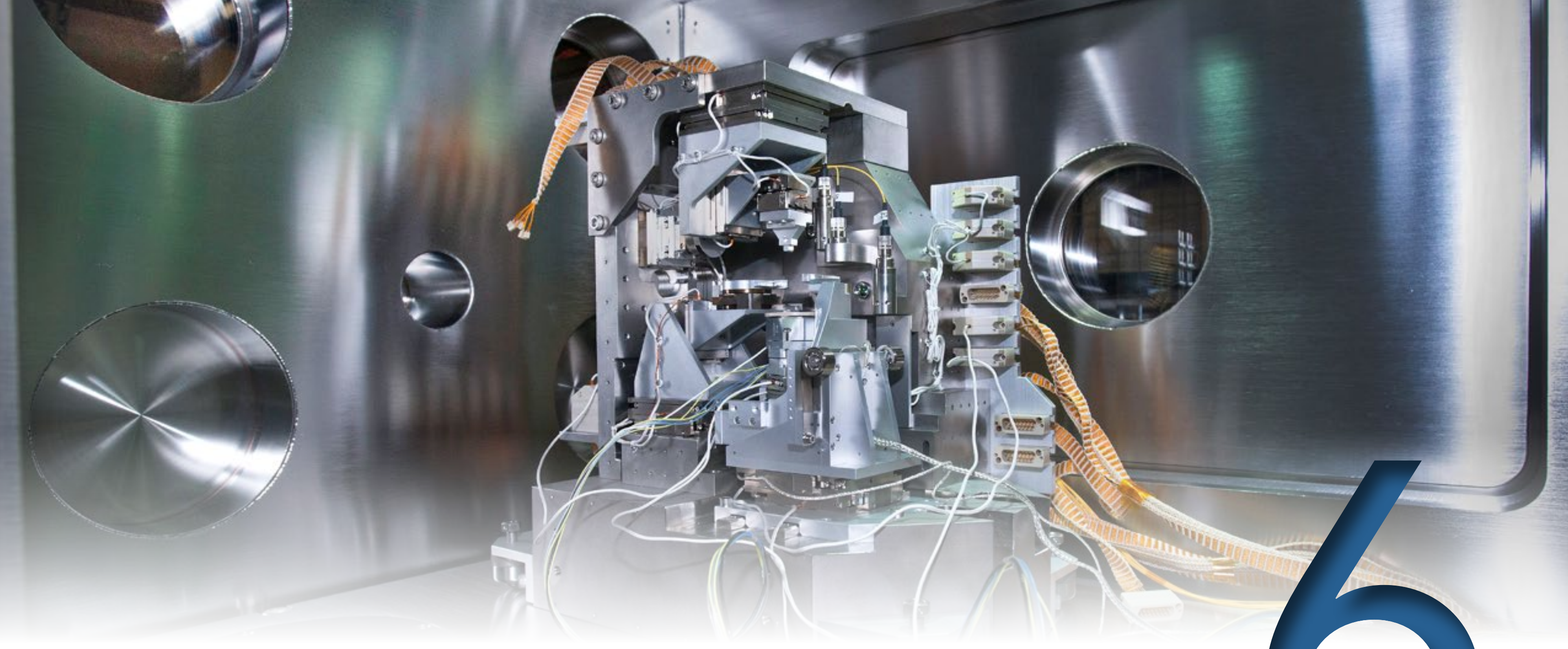
We will leverage developments being made by Brookhaven National Laboratory through the Computation Sciences Initiative (CSI) to mitigate the costs involved in providing computational resources, for large scale storage and compute clusters. By partnering with experts within CSI we can develop a 'flavor' of HPC resources that are geared more towards the needs of scientists that will use the NSLS-II.

One particular example is that we need a more instant on demand access to resources so that we can make use of computational modeling techniques to provide input for both experimental planning and steering. This type of access and usage is significantly different than traditional HPC offerings. Further, leveraging CSI staff for standard computational work will allow NSLS-II staff to concentrate on the problems that are specific to the smooth operation of an experimental facility.

There should also be an active level of general day to day interaction and collaboration between members of the CSI and the Data Acquisition, Management, and Analysis (DAMA) group. In order to encourage this we have allocated office space for the DAMA group within CSI. Another option for closer integration could potentially include joint appointments, both for permanent staff members and for postdoctoral researchers.

As can be seen in the above sections, we already have a good level of interaction between CSI and Photon Sciences. To summarize, this is a list of the high level areas that we are currently interacting with CSI on: software development and release policies, development of Ptychography software, Workflows and Provenance Capture, long-term data storage, computing architectures, GPGPU techniques and developments, cloud computing, application of machine learning, authentication and authorization, and data libraries and catalogues. In addition, we are currently working with CSI to benchmark some standard codes, such as accelerator physics and ptychography (based upon the SHARP code from the CAMERA project), in order to determine which computational platforms would be best suited for the various NSLS-II use cases.

In summary in order for the NSLS-II to become a world-leading facility we will plan to expand our scientific computing efforts substantially, both in terms of staff numbers, development effort on software codes, and investment in fast and reliable IT hardware.



ENABLING R&D AND SUPPORT

6

Facility supported R&D is an integral part of NSLS-II operations. Its role is to advance the current state-of-the-art in targeted areas of synchrotron light source technologies, such as X-ray optics and detectors, that are critical to fulfil the long-term mission of the NSLS-II facility as well as the overall synchrotron community. Through the development of new technologies that enable new science, the NSLS-II R&D program contributes to the overall DOE scientific facilities' mission and sustains the DOE leadership in synchrotron science and technology for the foreseeable future.

Leveraging the experience gained and infrastructure already existing at BNL as well as established during the NSLS-II construction phase, we plan to pursue advanced R&D and engineering using the following strategy:

- Define mission-driven R&D directions: To ensure efficient and effective utilization of resources, the NSLS-II R&D program will focus on those targeted areas that are required to achieve certain strategic objectives in the NSLS-II mission;
- Encourage and develop collaborations and partnerships: To leverage expertise, developments, and resources elsewhere in academia, industry, and other national laboratories, NSLS-II will pursue R&D in coordination with the community and our sister facilities;
- Adopt integrative systems engineering approach: NSLS-II will use a goal-oriented systems-engineering approach to pursue R&D. This approach ensures development and integration of all required subsystems (optics, detectors, nanopositioning, environment, and controls) to meet the NSLS-II R&D goals.

This section describes several strategic R&D and support areas, in both accelerator systems and beamline capabilities, that are critical to enable NSLS-II to achieve its best-in-class performance as well as to remain at the cutting-edge for the coming years.

6.1 ACCELERATOR R&D

Accelerator systems form the backbone of the NSLS-II facility, and play a critical role in keeping the facility at the cutting-edge. In this section, we discuss accelerator R&D activities we plan to pursue, along the following two directions: to develop novel insertion devices to enhance the photon output at NSLS-II, and to explore future high-brightness upgrade options to maintain the NSLS-II's competitiveness in the evolving synchrotron landscape.

6.1.1 Development of Novel Insertion Devices

Cryogenically-cooled Permanent Magnet Undulator (CPMU). After being first proposed in 2004 by T. Hara et al., such devices are now routinely constructed at several synchrotron radiation facilities, including ESRF, Spring-8, SOLEIL, Diamond Light Source and others. A CPMU devise represents a direct upgrade of a hybrid in-vacuum undulator (IVU), and offers a substantial increase in magnetic and spectral performance over IVU, thanks to operation at cryo-temperatures, when both the remanent magnetization (Br) and coercivity of permanent magnet materials increase quite significantly: e.g. the increase in Br can be by ~30-

40%, allowing to reach Br ≈ 1.45 T in the case on NdFeB material, and even higher value, ~1.6 T in the case of PrFeB material. This makes it possible to reduce period length of in-vacuum undulators and reach hard X-ray spectral range at lower harmonic numbers at medium-energy storage ring sources (such as NSLS-II), and obtain a considerable gain in spectral flux and brightness. For NSLS-II, we have developed a few prototype PrFeB arrays and confirmed that bakeable CPMU running at 77K was possible to fabricate. In addition we might consider developing special dysprosium/gadolinium based field concentrators.

Segmented Adaptive-Gap Undulator (SAGU). Calculations show that substantial gain in radiation properties, can be reached by using a segmented undulator design approach. This approach permits the different segments to have different magnetic gaps and periods, yet selecting the periods so that all segments produce undulator radiation at the same photon energies of harmonics, while retaining the electron beam "stay clear" and reducing impedance constraints by the undulator magnet structure along the entire straight section. As a result, the entire undulator will have more periods and larger effective K (deflecting parameter) value, and so higher flux and broader spectral tuning range of harmonics, compared to a constant-gap (and constant-period) undulator of the same length. This approach can be applied to any existing technology, including room-temperature IVUs and CPMUs, resulting in further increase of spectral flux and brightness. The relatively large lengths available for Insertion Devices (ID) at NSLS-II (~4 m in low-beta straight sections and ~7 m in high-beta sections) make the SAGU approach particularly efficient. For the NSLS-II parameters, the expected gains in spectral flux and brightness are from ~30-50% at ~5-10 keV to a factor of 2 or more at 20-30 keV photon energies. Besides the spectral performance gains, the segmented approach may simplify mechanical design and reduce cost of long undulators, facilitate their magnetic shimming and enable more accurate tuning / compensation of residual magnetic field errors during operation. The R&D on SAGU will satisfy the needs of hard X-ray beamlines of NSLS-II (and possibly other low-emittance synchrotron sources) in highly-optimized undulators complementing ID R&D activities carried out at different light source facilities and labs. The SAGU R&D will also contribute to development of new methods of magnetic shimming of IVU and CPMU, and further improvement of magnetostatics and synchrotron radiation calculation software (Radia, IDBuilder, SRW codes) supported by NSLS-II.

Superconducting Undulator Based on APS Nb-Ti Technology. APS has developed a superconduct-ing undulator based on NbTi. The present design has been optimized for APS and can be re-optimized for NSLS-II. The R&D includes optimization of the undulator length and period, as well as development of an effective quench protection system. An optimized design of an undulator based on this technology could exceed the performance of an IVU based on permanent magnet technology. This could be an alternative to PrFeB and HTS technologies. To test the new superconducting devices, a Magnetic Measurement System for Superconducting Wigglers and Undulators will be developed. A vertical test facility is now available for magnetic measurements of a short (max 0.4m long) superconducting undulator (SCU). However, to certify a new superconducting undulator or 1.2-m long superconducting wigglers, which are planned to be installed in the NSLS-II ring for future beamlines in coming years, a horizontal measurement system capable of measuring 2-m long superconducting devices must be developed and built. The new system will offer a benefit of highly precise and fast measurements at various locations across the ID gap.

Test Straight Section. We are planning to equip one of the NSLS-II straight section with a test set-up for experiments with novel undulator concepts. Installing a test undulator into the straight section and studying the radiation properties in the short diagnostic front-end during beam studies will help to gain invaluable insight in small gap, short-period and high field IDs, which are the natural next step in undulator and front-end technology for NSLS-II. The project will be broken into two phases. During the first phase that does not require Front-End we will install a long scraper simulating the undulator gap with temperature and RF diagnostics. Studies with the scraper will show the minimum possible gap together with distribution of wakefields and temperature fields inside the vacuum chamber. During the second phase the actual prototype of the undulator magnetic array will be installed together with the Front-End and the test ID will be commissioned using optical diagnostics. We are assessing the possibility of using future HEX straight section as the home for this experimental set-up.

6.1.2 Upgrade Options for a Lower-Emittance Storage Ring

As discussed in Section 2.2, a number of new and upgraded synchrotron facilities are under development, which promise brighter beams than NSLS-II is able to provide today. In order to maintain the competitiveness of NSLS-II we plan to pursue studies to explore potential ways to increase the brightness of NSLS-II, with the constraint of not having to replace a large fraction of the magnets. Our objective is to quadruple NSLS-II brightness by reducing the horizontal emittance of the NSLS-II storage ring by a factor of three to four.

The horizontal beam emittance can be expressed as

$$\varepsilon_x = F(\nu_x, lattice)\frac{E^2}{J_x N_d^3}$$

where E is the electron beam energy, F is a function dependent on the storage ring lattice, J_x is the horizontal damping partition number, and N_d is the number of dipole magnets. Studying this definition, there are three ways to decrease the emittance of a beam with fixed energy:

1. Increase of the horizontal damping partition number J_x;
2. Modifications of the storage ring lattice to optimize F;
3. Increase of number of dipole magnets N_d.

Increase of the horizontal damping partition. The damping partition number J_x is equal to1 for a storage ring like NSLS-II since its lattice consists of pure dipole magnets without field gradient. J_x can significantly exceed unity if there was a gradient but replacing the dipoles would be very expensive. Alternatively, a dipole magnetic field with gradient components can be introduced into the lattice by operating the ring off its nominal energy by mismatching the RF frequency, which forces the electrons on an off-momentum dispersion orbit to match the circumference with a multiple of the RF frequency. We plan to optimize the lattice taking into account the off-axis passage of the beams through the dipoles, quadrupoles, and sextupoles. Additional emittance reduction can possibly be achieved by adding Robinson wigglers with a quadrupole component to their magnetic field. The first step is to determine theoretically and experimentally how large shift of the damping partition can be achieved by RF frequency shift. To achieve optimum conditions, the beam optics needs to be optimized to take into account the mismatch between momentum and quadrupole strength and the influence of sextupole magnets, which contribute with a quadrupole component. This also requires re-optimizing the geometric sextupoles outside the achromat. Once an optimum solution is established, it will be tested during beam studies.

Modifications of the storage ring lattice. The emittance can be reduced by adjustment of the focusing to approach the theoretical minimum emittance of a DBA lattice. In the current NSLS-II lattice, the emittance is approximately 2 nm without damping wigglers. In principle, it can be reduced to just over 1 nm by adjusting the strength of the quadrupole magnets to optimize the dispersion in the dipoles. This modification of the lattice likely results in significantly reduced lifetime, so more frequent injection and probably a new injection scheme may be required. Simulation codes will be used for particle tracking through the modified lattice to study the dynamic aperture and predict the beam lifetime. It will be explored whether we can continue to use the existing injection kickers with off-axis injection or whether on-axis injection will be required. Experimental tests of the lattice are also planned to see the measured emittance, lifetime, and other beam parameters compared to the predictions.

Increase of number of dipole magnets. Yet another way to reduce the emittance is increase of the number N_d of dipole magnets. Doubling this number gives the emittance reduction by a factor of 2^3=8. To minimize the cost of upgrade, the hardware changes should be minimized. We also have to maintain the existing ID source points. The main idea is to replace existing dipole magnets with the combined-function magnets such as longitudinal-gradient and reverse-bend dipoles. This approach allows us to minimize hardware changes to only two girders per ring cell. There is no major change outside of the dipole girder (DS absorbers should be modified). We plan to pursue a dedicated study program focused on machine optics and beam dynamics, in four steps: (1) splitting the dipole magnets and moving them apart (about 50% emittance reduction), (2) adding a quadrupole between the combined-function magnets (dipole with gradient), (3) using longitudinal-gradient magnets, and (4) using longitudinal-gradient magnets and replacing the quadrupole with combined-function reverse-bend magnet.

For the lattice with modified dipoles, three damping wigglers already installed in NSLS-II provide emittance reduction by a factor of 1.5. This is not a small factor as compared with the original factor 2 for the present lattice. The energy spread grows slower and this is beneficial for brightness at higher IVU harmonics.

6.2 X-RAY OPTICS

Many advances in synchrotron beamline technology, and consequently in the range and quality of scientific applications, continue to be driven by advances in X-ray optics. Optics developments over the preceding decade have encompassed improved performance from existing optics such as mirrors, increasing use of multilayer coatings, and the development of new X-ray optical elements such as refractive and multilayer Laue lenses. This trend is expected to continue in the future, as driven by the demands of the high brightness of the third generation sources and by increasing performance required by scientific experiments. In the *2013 DOE X-ray Optics workshop report* [14], X-ray Optics for BES Light Source Facilities, a roadmap for DOE facilities x-ray optics R&D was proposed.

Meeting NSLS-II strategic objectives to establish and retain NSLS-II leadership in high-spatial-resolution imaging and in high-coherent-flux scattering requires development and characterization of a number of advanced X-ray optics. Therefore, an essential and integral part of the NSLS-II strategic plan is to develop novel X-ray optics and the associated tools to characterize simulate and utilize them.

Leveraging upon the experience gained and infrastructure established during the NSLS-II construction phase, we plan to pursue advanced Optics R&D with following objectives:

- Establish the next-generation of nanofocussing optics (MLLs, Refractive lenses and mirrors) to support NSLS-II strategic objective.
- Expand the optical nanometrology and At Wavelength Metrology/alignment R&D to support NSLS-II beamline operation.
- Provide optical metrology support to already existing and emerging beamlines in order to enhance and optimize their performances.
- Support all these above capabilities with advanced methods of optics modeling.

This section describes these four strategic R&D areas and the support laboratories that are critical to enable the NSLS-II beamlines to achieve their best-in-class performance and capabilities. Throughout these R&D initiatives, NSLS-II plans to coordinate with other BES light source facilities to pursue R&D in complementary approaches in nanofocusing optics R&D and simulation during the next 5 years.

6.2.1 Nanofocusing X-ray Optics

NSLS-II plans to continue to advance the essential nanofocusing X-ray optics R&D towards achieving the ultimate goal of ~5 nm spatial resolution. Two main R&D areas will be pursued as described below.

Multilayer Laue lenses (MLL) and Multilayer Mirrors. Owing to its excellent structural, elemental, and chemical sensitivity and sufficient penetrating power, hard X-ray microscopy has grown in applications in recent. However, existing hard x-ray microscopy tools offer spatial resolution down to a few tens of nanometers, which is not adequate for addressing a wide variety of scientific problems that require the understanding of the interplay between materials' properties and their functionality at the nanometer level. This strong demand is the driving force toward achieving hard x-ray focusing well into the single digit nm regime.

Multilayer Laue Lenses (MLLs) and multilayer mirrors (MLMs) have shown the potential to be the best choices to achieve hard X-ray focusing in the nanometer regime, with complementary strengths. MLLs have the best potential to reach the smallest focal spot possible for hard X-rays, while MLMs are best suited for spectroscopic imaging at the nanoscale. NSLS-II plans to lead and coordinate with other BES light source facilities to pursue R&D in complementary approaches towards MLL and MLM development in the next 5 years. Our plan includes the following two components:

- Development of large-aperture tilted and wedged multilayer Laue lenses (MLL): Leveraging several critical advances in the multilayer Laue lens (MLL) optics development made in the past few years, we plan to continue to lead the development of MLL optics by advancing the necessary thin-film deposition technology including materials selection, sectioning and polishing techniques, and characterization as well as developing related metrology techniques to fabricate and implement tilted and wedged MLLs and their associated mechanical systems to achieve 5 nm focus in the 10-20 keV range.
- Collaborative development of large-numerical-aperture multilayer mirrors (MLM) and stacked Fresnel zone plates: We plan to pursue collaborative efforts with other Laboratories (particularly the APS) and interested industry partners to develop novel methods for fabrications of multilayer focusing mirrors, based on a combination of profile ML coating and controlled ion beam figuring with in-situ optical metrology, and of hard x-ray zone plates based on precision stacking of individual zone-plate optics. Our goal here is to obtain these novel optics for focal spots down to ~10 nm for spectroscopic imaging applications.

It has been widely recognized by the community that these approaches – multilayer Laue lens (MLL), multilayer KB mirrors, and stacked zone plates are the most promising ways to ultimately achieve nanometer-scale spatial resolution with high optical efficiency for hard x-rays. While our main emphasis will be to continue to drive and advance the MLL technique, our strategy to supplement this main R&D with a collaborative effort with APS on ML mirrors and stacked zone-plates will ensure NSLS-II to stay at the cutting-edge in hard x-ray nanofocusing capabilities.

In FY17, we will pursue the following tasks:

- Wedged MLL growth with minimal residual error (<5nm) in order to break the 10nm mark. This will be enabled through continuous developments in deposition, sectioning and metrology technologies.
- Extension of the portfolio of geometries and microfabrication techniques used for MLL/optics fabrication: combined with metrology, this will enable easier incorporation of MLLs onto X-ray microscopes, allow for improved monolithic/bonded multilayer Laue lens (nanofocusing optics) and enable potential use of the MLL optics for full-field microscopy.
- Gain experience in, and expand the use of, deterministic polishing for X-ray optics fabrication
- Determine the viability of the use of VSi_2/Si and VSi_2/AlSi for 25um thick MLL fabrication and/or potential hurdles that will need to be overcome (if viable, such materials will improve efficiency of the MLL optics for hard X-rays)

- Integration of an Atomic Absorption Spectroscopy tool (developed through an SBIR project) onto large deposition chamber and evaluation of performances for in-situ deposition monitoring. This will provide in-situ metrology and the ability to estimate the quality potential of a growth before moving to more accurate but time consuming metrology
- Test of profile coating capabilities of the deposition chamber

In FY18:

- Wedged MLL growth pushing for increased efficiency with high spatial resolution
- Investigation of different materials systems for MLLs fabrication for energies in the ~ 7-15 keV range
- Pursuit of experience acquisition and expansion of the use of deterministic polishing for X-ray optics fabrication
- Profile coating of mirrors with high gradient: pushing the deposition strategy develop for MLLs to other thin film based optics.

In FY19-21, our MLL ultimate goal is two-fold: (a) 5 nm focus beam in the 10-20 keV range, and (b) higher efficiency with larger apertures. Throughout this development, we will be closely coordinating with the Imaging and Microscopy beamlines so that our development priorities and emphases are well matched with the interest and the demand of the NSLS-II scientific user community.

Kinoforms and Compound Refractive Optics. Refractive optics are being widely used at NSLS-II beamlines in one form or another, e.g at the CHX, IXS, HXN, FMX, LIX, NYX, and ISR beamlines. However, the only commercially available refractive optic is a Beryllium Compound Refractive Lens, (Be CRL), and this does not serve all needs. Kinoform optics are a special type of refractive lens that are well suited to the requirements that the excellent phase profile of the source of the source be preserved.

Leveraging our previous experience that started at NSLS, and is currently being supported through an R&D grant from DOE-BES, we plan to pursue Kinoform/refractive lens R&D in collaboration with APS. Our objectives are to (1) make improvements in the lens fabrication processes at the Center for Functional Nanomaterials, (2) characterize the lenses with x-rays; and (3) feedback the information from characterization into improved lens design and fabrication. While this grant award is mostly focusing on high energy (E > 50 keV) applications, the approach and the equipment developed will also be useful for the lower photon energy lenses that will be of interest to many of the NSLS-II beamlines. Specific plans are outlined below.

In FY17-18, we plan to continue R&D efforts in refractive and kinoform lenses using silicon and diamond material at NSLS-II. Our specific aims include the following:

- Establishing a portable (APS/NSLS-II) precision end-station to enable lens characterization. In collaboration with the NSLS-II nanopositionning group we will create a portable endstation with resolution in the tens of nanometers. This end-station will be crucial for characterization of lenses with the detail necessary to allow improvements of design and fabrication.
- Development of lenses with larger useful apertures. The bulk of our effort will be dedicated to improving etch depth and uniformity. In FY16 we improved lens etch depth from 100 microns to 125 microns, a 25% improvement, and some test structures were etched down to 300 microns. For FY 17 we intend to transfer the depths obtained on test structures to actual lenses, aiming for a more conservative 250 microns.
- R&D in novel etching approaches. The process flow for kinoform etching has been the simplest and most straightforward deep silicon reactive ion etching (RIE). However, to achieve our goals, we may need more complicated and time consuming processes. One of these paths is to have a two-step RIE process in which one creates sacrificial features on the wafer, which one removes later, after a second lithography and second RIE step. A second path is to use metal assisted chemical etch (MACetch). In FY 17 we intend to simply learn how to do the RIE process on test structures.
- Using the new end-station at NSLS-II and APS for testing the performance of newly fabricated Kinoform lenses. The goal of the project is to deliver two sets of working Kinoform lenses at high X-ray energies at the spatial resolution in the range of 250 – 750 nm with a large acceptance aperture of 250 microns. One such optic will be used at APS 1-ID and the other will be for NSLS-II XPD beamline.

6.2.2 Optical and At-wavelength Metrology and Wavefront Preserving Mirrors

Many of the high-impact scientific opportunities afforded by NSLS-II, such as coherent X-ray imaging, nano-diffraction, and nano-spectroscopy, require maximum intensity in the focus and minimal wavefront distortion. These applications require X-ray mirrors with ≤0.5 nm rms height errors and sub-100 nrad slope errors for surface spatial frequencies ranging from 100 microns to the full optical aperture of the optic. These characteristics are extremely close to the present noise floor for short flat mirrors and are sometimes beyond the state-of-the art for highly curved mirrors.

To fully deliver such mirrors requires concerted and coordinated efforts in the synchrotron community and targeted efforts in close collaboration with the optics manufacturing industry. Leveraging the unique expertise and the cutting-edge optical metrology capabilities acquired through the NSLS-II construction project, our strategy is to identify and pursue a number of targeted initiatives where NSLS-II will continue to play a significant leadership role in the development and metrology of advanced X-ray mirrors for coherent applications. These initiatives include:

Development of next generation metrology tools and techniques: This is essential to enable measurements of figure errors at sub 100-nrad levels. This targeted R&D strategic plan will be done by upgrading instrumentation in the existing NSLS-II optical metrology laboratory and efforts on the development of new instruments for slope errors measurements to reach 50 nrad slope error accuracy (NanoSurface Profiler and Software Configurable Optical Tests SCOTS) and stitching interferometry capabilities for sub nm rms accuracy both on highly curved surfaces. These efforts will be combined towards the construction of new instruments with stitching capabilities using interferometer and Shack Hartmann and software configurable optical test stations to perform 2D mapping of the optical surfaces in order to feed a deterministic polishing process based on ion beam figuring. This activity will start in FY17 and will follow until end of FY18.

X-ray mirrors are extensively used at NSLSII and are supplied by a small number of industrial companies. The few possible suppliers of state of the art mirrors is a significant risk, the products are very expensive and production times can be very lengthy (multiple years). We propose to set up equipment at NSLSII for deterministic polishing (ion-beam milling or preferential deposition), similar to those at facilities such as ESRF, MAXIV, BESSY and DIAMOND. Such a facility would let us achieve in-house diffraction limited focusing of X-rays mirror development. This effort is being funded by an LDRD grant and will start in FY17 and will follow until end of FY18.

Development of in situ at-wavelength metrology tools (metrology using the x-ray beam): For x-ray component characterization, alignment and beamline performance studies, this is a necessary complementary method of visible light metrology. The availability of adequate measurement tools and adjustments directly at the beamlines will be crucial for a thorough *optimization* of operational performance of individual beamline components and entire beamline systems. One of the major missions of in situ at-wavelength metrology is to provide the required instrumentation and measurement techniques to fulfill these requirements. In situ metrology is complementary to ex situ in the sense that it deals with optics previously tested, characterized, and adjusted at an optical metrology laboratory, and now installed at an X-ray beamline.

The advantage of in-situ metrology is that it allows fine mutual optimization of a sequence of beamline optical elements at the location and under conditions in which the optics are designed to operate. It overcomes the insensitivity of ex situ measurements to the imperfections of the input beam, tolerances of mounting of optics at the beamline, surface shape distortion due to x-ray heat absorption, as well as limited optical quality of the surrounding optical components. Moreover, in situ metrology has the potential to provide direct feedback for active (on-line) correction of the beam by using adaptive optics. At-wavelength wavefront characterization techniques will open up perspectives, for instance, in the in situ optimization of adaptive optics or correction of reflective optics and could also be used as an online setup permitting focusing optimization, for example, by assisting in the alignment of critical x-ray optical components or compensating for the astigmatism of an incoming beam or mechanical deformation due to heat load or mounting stress.

This R&D capability coupled with extensive simulation development is supported through a BES grant in collaboration with LCLS, and will start in FY17 and will follow until end of FY18.

Other Optics and Metrology Projects / Laboratory of Optics and Metrology. In the longer term, it is highly desirable to access a test beamline. Plans are being developed for collaboration with the APS and facilities there for this purpose. This would provide X-ray beams with characteristics similar to the user beamlines to enable testing of coherence and diffraction limited optics as well as instrumentation at 'real' power density loads. With the predicted demand for upgrading existing beamlines, we are also proposing facilities for refurbishing existing optics for higher performance.

6.2.3 Advanced Methods of Optics Modeling.

The development of advanced analysis and simulation tools is essential to enable quick feedback on optics fabrication and characterization as well as forward simulations of coherent wave propagation of combined optical effects, with imperfections, that directly influence targeted experiments. This includes the implementation of efficient analysis codes for phase retrieval and reconstruction of wavefronts based on at-wavelength measurements of X-ray optics at existing NSLS-II beamlines. When making progress in the beamline optical specification, modeling of the effects of imperfect optical surfaces on wavefront propagation along the beamlines must be considered. Geometrical ray tracing used for the design of optics fails when diffraction and coherence effects have to be considered. Therefore, wave-optics simulations of the propagation of partially-coherent radiation are essential.

NSLSII is a world leader on these developing methods and has established collaborations with other synchrotron facilities, but further developments are required. Our plans to further develop and mature these methods are outlined below.

In FY17-18, we will develop an important key software tool – the *Virtual Beamline* environment in the *Synchrotron Radiation Workshop (SRW)* code under newly-developed "Sirepo" interface. We will set up this tool for all existing and planned NSLS-II beamlines, to enable a large variety of potential applications. In parallel, we will further extend the library of optical element "propagators" in the SRW code, to increase the accuracy of the simulations, including such optical elements as multilayer Laue lenses (in collaboration with HXN beamline team), perfect and imperfect compound refractive lenses, zone plates with a very large number of zones, kinoform lenses, mirrors with all practically-important shapes incorporating height profile error data from Optical Metrology and imperfect crystals in different geometries with heat load aspect from Engineering FEA simulation.

There is a need to continue improvement of numerical efficiency and reliability of the partially-coherent wavefront propagation simulation methods. This includes further optimization and parallelization of algorithms implemented earlier in SRW code (i.e. summing-up contributions to final intensity from wavefronts emitted by different "macro-electrons"), testing new algorithms (e.g. based on coherent mode decomposition) and improvement of an automating propagation "driver".

Assessing the performances of all operating / commissioned NSLS-II beamlines is necessary to speed up the beamlines commissioning and to identify and solve problems. This can be done by comparing measured X-ray spectra and intensity distributions at different beamline locations with the calculated ones, obtained using the "virtual beamline" environment. As a result of this activity, it will be possible to define a program of "fixes" and improvements for each beamline (e.g. re-aligning undulator, re-aligning or replacing particular optical elements, etc.) to ensure that in a reasonably short time all beamlines will maximally exploit low emittance / high brightness of the NSLS-II, and deliver higher performance than that of similar beamlines at other light source facilities. This work will be performed in collaboration with beamline staff, accelerator physicists, ID and X-ray Optics group members.

In parallel, the development of in-situ diagnostics and metrology methods provides minimal or no perturbations to existing optical schemes of beamlines, based on forward-simulations of partially-coherent radiation propagation and inverse problem solving; extensive use of these methods to determine, minimize or eliminate existing performance issues at beamlines. This work will be combined with At Wavelength Metrology activity discussed in Section 6.1.2.

We plan to perform simulation of user experiments at beamlines of NSLS-II (and possibly other light source facilities), using the "virtual beamline" environment complemented by special software libraries for simulating samples and detector effects. The priority will be given to coherent elastic scattering types of experiments (such as those that are performed at CHX, CSX-1, and will be performed at the SMI and ISR, and the future CDI beamline). However, simulations of (ultra-)high-resolution microscopy and spectroscopy experiment are technically feasible and are important as well. The main goals of such simulations are: determining optimal beamline settings for a particular experiment (e.g. optimizing radiation degree of coherence, spatial and spectral resolution, flux at sample) and determining relevant "apparatus functions" (i.e. "transfer" or "point-spread" functions) to be used during experimental data processing. This activity will allow to better prepare the experiments, use beam-time more efficiently, and to better process / interpret experimental data. These different activities are highly interconnected with the development of simulation tools for the Accelerator Division like x-ray pinhole camera, visible light monitors and of course development of new insertion devices.

In parallel with the above activities, the development of new efficient data processing algorithms for experiments exploiting partial coherence of X-ray beams at NSLS-II. Strategically, it seems very important for NSLS-II to work on data processing in this particular area, to ensure its long-term competitiveness with emerging lower-emittance light sources producing more bright and coherent X-ray beams.

In FY19-21, we plan to focus the R&D activities on continuing improvement of emission calculations algorithms and functions in SRW code, as well as functions that bridge SRW with other codes describing different sources, for potential applications beyond NSLS-II in collaboration with others, e.g. for time-/frequency-dependent simulations for X-ray free electron lasers, THz range coherent synchrotron radiation sources and others, misc. simulations for future light sources.

6.3 PRECISION ENGINEERING AND NANOPOSITIONING

Precision engineering, nanopositioning and nanometrology are the essential key elements of the NSLS-II integrative systems engineering approach for mission-oriented R&D, as complex instrumentation, nanoscale motion, sensing, control, positional and angular stabilities often determine ultimate performance of the cutting-edge x-ray optical elements. In addition to x-ray optics, all related experimental subsystems, such as sample positioning, beam-defining apertures and complete endstations also require high-precision positioning and stability in order to take full advantage of the x-ray optics or advanced coherence techniques such as ptychographic imaging. In order to meet such needs, NSLS-II has established a state-of-the-art nano-positioning laboratory during the NSLS-II construction project to pursue R&D in precision engineering, nanopositioning, monitoring, feedback, and controls. This R&D effort has been very successful, leading to pioneering designs of a number of prototype systems and culminating in the multiple-awards winning MLL scanning microscope installed in the C-hutch of the HXN beamline (**Figure 20**). It delivers a world record 12 nm spatial resolution in a working X-ray microscope, utilizing in-house developed MLL nanofocusing optics.

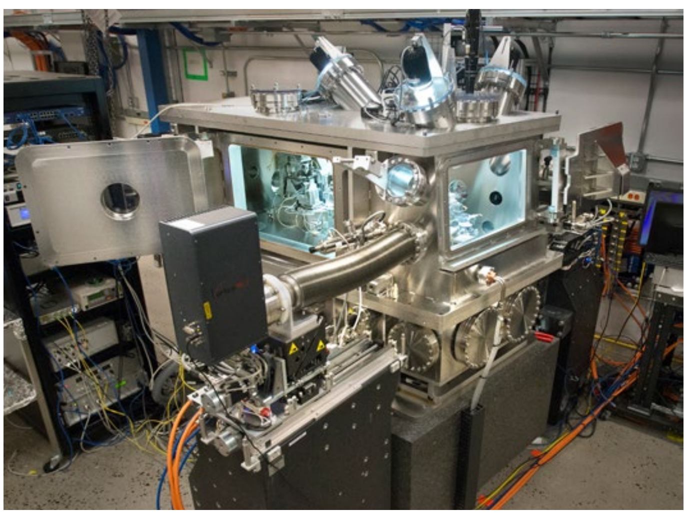


Figure 20: *The awards winning MLL microscope installed in the C-hutch of the HXN beamline*

Building upon the experience and expertise acquired during the NSLS-II project, we plan to further develop advanced capabilities for precision engineering, positioning, actuation, manipulation, sensing and control at the nanoscale, with the overall goal to (a) establish the next-generation precision engineering/nanopositioning platforms in support of the NSLS-II strategic objective to enhance microscopy capabilities, (b) expand the precision engineering, nanopositioning and nanometrology R&D and support to enable a broad range of mission-critical capabilities at the NSLS-II, and (c) provide mechanical metrology services to already existing and emerging beamlines in order to enhance and optimize their performance. Specific areas of future developments are outlined in the section below and arranged in the order of priority and projected timelines.

Bonding of the MLL optics and novel positioning techniques using MEMS technology: The emergence of ultrabrilliant synchrotron sources and recent advances in the development of efficient x-ray focusing optics has stimulated significant efforts aimed to generate and use x-ray nanobeams in many areas of science and technology. The HXN beamline, has been commissioned and is delivering cutting-edge imaging results with unprecedented spatial resolution utilizing MLL nanofocusing optics. The HXN endstation employs state-of-the-art piezo-mechanical components and provides positioning accuracy down to a few nm. Alignment of the two 1D MLL optics is a complex procedure which involves eight degrees of motion and requires nm-scale resolution and nm-scale long-term stability. To push the resolution even further and achieve a focal spot size of 5 nm and below, we are targeting a novel approach. Specifically, we plan to develop a pre-aligned, bonded 2D MLL optics to minimize the number of motions needed for positioning of MLLs with respect to the sample. This approach will scale down the size of the next generation microscope itself and in combination with optics development, will provide a route for imaging experiments with spatial resolution of 5 nm and below.

We will fabricate a Si template to hold two lenses together in a pre-aligned configura-tion. We will utilize mature micro-fabrica-tion and MEMS technology to achieve this goal. **Figure 21** illustrates to-be-developed optics modules. Once developed, such monolithic 2D MLL devices have the potential to become standard nanofocusing optics which could be adopted and easily installed at the imaging beamlines of the NSLS-II with a potential for direct scanning, ptychographic and full-field imaging. In collaboration with the HXN team, such monolithic devices will be implemented in the HXN microscope and will be considered for the FXI full-field imaging endstation. This project is funded through the BNL LDRD program and will start in the middle of FY17.

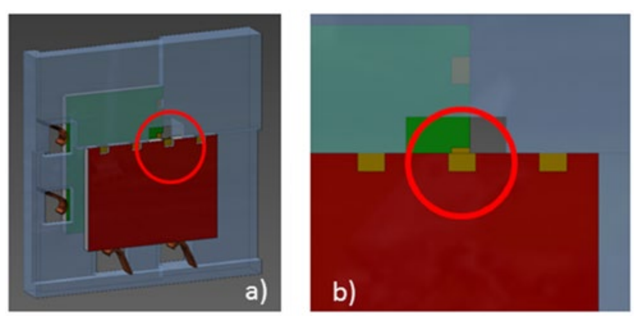


Figure 21: *a) Schematic of a microfabricated template used to align and lock two linear MLLs. Si template accommodates two MLL lenses aligned orthogonally (red and green squares). Si springs secure lenses in place. b) close-up of the active MLL area. The red circle indicates the active MLL area.*

Sample manipulation apparatus for serial protein crystallography at full flux: The flux density of the MX beamlines at the NSLS-II surpasses the flux density of comparable beamlines around the world by orders of magnitude. The dramatic performance improvement offers great opportunities for scientific studies however the expected lifetime of samples falls into the ms range. In collaboration with the FMX team we are developing a novel, ultra-high-speed, high precision goniometer system to support scanning serial protein crystallography measurements and benefit from the flux density of the NSLS-II. The system under development will enable up to 5 Hz rotational speeds with simultaneous scanning frequencies on the order of 100 Hz, making it the fastest sample manipulation apparatus in the protein crystallography community. This is an on-going project funded through an LDRD proposal, and it will continue through FY17-FY18. The final system will be installed at the FMX beamline and will be available for users. In the long term, similar systems are expected to be adopted by other MX or tomography beamlines.

Transmission X-ray Microscope endstation: The FXI beamline is currently under construction, and it targets tomographic imaging of various samples with a spatial resolution of 30 nm. The endstation will be developed in-house and will utilize some of the optical components available from a previous TXM microscope. The conceptual design of the high stability microscope, which utilizes previous design experience acquired during various projects, has been developed. In collaboration with the FXI team the detailed layout and some prototyping and testing will be carried out in FY17 culminating in final design, construction and commissioning of the TXM system. Design, construction, commissioning and optimization will span over FY17–FY18 and are funded through the Beamlines Developed by NSLS-II (BDN) portfolio.

Kinoform lenses microscope: kinoform lenses have been proposed and developed as an alternative way to provide x-ray focusing (see kinoform/refractive optic section in the x-ray optic R&D section for more details). Recently, DOE M&S funds have been allocated for a construction of a prototype instrument suitable for testing and focusing experiments utilizing kinoform lenses. In FY17 the design of the prototype instrument will be completed, components procured and fabricated, and the system will be assembled and tested. In FY18 it will be primarily stationed at the ISR beamline but since it is a stand-alone microscope, it can be moved to different beamlines or APS. The M&S for the project is supported through a dedicated DOE funding; design, construction and assembly are performed through the NSLS-II operations.

Support for emerging and existing beamlines utilizing standard mechanical metrology approaches. The development and performance of state-of-the-art beamlines requires very high precision mechanical systems. Achieving this level of precision requires an equivalent capability of the mechanical metrology instrumentation and resources. It is crucial to perform mechanical metrology of small mechanical setups, mechanical motion, various large pieces of equipment (i.e., diffractometers, monochromators, mirrors, etc.), and vibrometry and its infrastructure prior to and after their installation. The requirements for mechanical metrology range from testing "simple" motion stages to measuring mechanical performance of complex instruments. Limited support in this area has been provided to date benefiting a number of existing and under-construction beamlines. To take full advantage of the mechanical metrology services needed through FY17-FY21 both dedicated staff and instrumentation funding are required above those expected under approximately flat funding scenarios. Beamlines such as HXN, SRX, SMI, SIX, FXI and other emerging beamlines would benefit from this service.

In addition we plan to expand our services to support the development of multi-modal sample environments (in-situ, in-operando) to increase scientific impact of all beamlines at NSLS-II (see multi-modal experiments section for more details).

Development of automatic sample exchange systems: In order to increase scientific throughput of the highly complex microscopy systems developed at NSLS-II, it is of prime importance to enable automatic sample exchange protocol. This becomes especially critical when environmental conditions (temperature/pressure/magnetic field) are considered. To minimize down time due to equilibration processes prior to the measurements, we plan to develop such systems. This will include sample storage containers, universal sample mounts, grippers, translation mechanisms, sensing and control algorithms. The prototype system will be developed for the ZP module of the MLL microscope at HXN. HXN endstation. Similar system (with modifications) can be used for the SRX and SMI endstations. This effort would span over the next five years, and it would require additional funding through NSLS-II or other agencies.

Development of dedicated instrumentation to support fast 3D ptychography measurements: In recent years ptychography has become a standard microscopy tool, especially useful for imaging of low-Z materials. NSLS-II possesses unique ptychography expertise and in order to capitalize on this world-leading knowledge, we consider development of a high throughput, dedicated tomographic ptychography system. It will possess high stability and will allow fast scanning yielding nm-scale resolution imaging in 3D. This project requires adequate funding and support. A DOE early-career award package has been submitted. Based on the outcome of the proposal, the project will evolve over the next five years.

Next-generation microscopy instrumentation developments: The development of nanoprobe and nano-imaging instruments is of critical importance in all high-brightness synchrotron applications and thus has become a highly competitive field as driven by all new and to-be-upgraded synchrotron facilities worldwide. We expect that the pace of the development will evolve rapidly, in such directions as the design and fabrication of more compact and integrated optics/manipulation systems, including taking account of the synergy between nanofocusing optics fabrication and nanoscale motion. Therefore in FY19-21, we anticipate that there will be an urgent need to develop upgraded, next-generation microscopes for NSLS-II imaging beamlines such as HXN and FXI. Such development will focus on monolithic optics/manipulation systems, including combining optics modules (focusing optics and associated manipulation needed for alignment) with integrated order sorting apertures and beam stops, as well as the ability to be easily integrated into existing instruments. This next-generation development will be important for achieving higher spatial resolution and higher stability imaging capabilities, and for maintaining NSLS-II leadership in this highly competitive field.

6.4 X-RAY DETECTORS

As recognized in a recent DOE-BES report *Neutron and X-ray Detectors*, as the synchrotron source characteristics continue to improve over the years, areas of scientific investigations at these sources are increasingly limited by the detectors in certain experiments [15]. This is particularly true for a new synchrotron facility like NSLS-II. Therefore, one of the important strategic R&D directions at NSLS-II is advanced X-ray detector development.

Given the broad range of detector improvement needs in the scientific community, our plan is to coordinate and collaborate with other DOE facilities to ensure that resources are well directed towards targeted strategic areas, benefiting the broader community well beyond the NSLS-II. We are also leveraging the resources available at the Instrumentation Division of BNL such as clean laboratory for prototype sensor and/or ASICs fabrications. Through this approach and taking into account the NSLS-II strategic strengths, we have identified the following detector development projects to pursue.

X-ray Fluorescence Pixel Detector MAIA: MAIA is an award-winning x-ray fluorescence microprobe system which has transformed the way such measurements are made. It is a massively parallel detector system (~400 independent detectors) with unique custom computing elements which provide real-time analysis of the elemental makeup of a sample. We plan to fabricate several MAIA detectors in FY17, in collaboration with CSIRO in Australia, and to install MAIA detectors at SRX and XFM beamlines at NSLS-II in FY17-18.

The MAIA system is also under continuous development which is essential to retain our leadership in this area. Our current emphasis is on improving the energy resolution of the detectors by (a) making a new readout integrated circuit with better noise figure and (b) developing an x-ray sensor array presenting a lower capacitance to the amplifier, again improving noise performance. This SDD-based MAIA is an LDRD-funded project through the BNL Instrumentation Division, with a re-use of a previously developed readout. This change provides the dual advantage of allowing a higher aggregate throughput and a lower capacitance sensor, and would move us away from the current wire-bonded package towards a more modern bonding technology. We anticipate that this development will be an important step towards a MAIA-II, an imaging detector with a spectroscopic energy resolution; it would be ideally suited for spectroscopic imaging experiments at NSLS-II beamlines SRX and XFM.

VIPIC for X-ray Correlation Spectroscopy: A detector optimized for X-ray photon correlation spectroscopy (XPCS) experiments is essential for accessing micro-second time regimes and is ideally suited for a high-coherence X-ray scattering beamline such as the CHX at NSLS-II. The VIPIC (Vertically Integrated Photon Imaging Chip, **Figure 22**) is a unique design for this purpose, based on the most advanced CMOS technology, and proving the viability of this technology for x-ray and HEP detectors. We are currently developing a plan to make a full-scale (i.e. 1 megapixel) version of this detector. This project is funded by DOE-BES scientific user facilities. At the same time we are working on prototyping the next generation of such a detector. It would improve the time resolution by a factor of at least 100 compared with the first detectors, i.e. from 10 ms to 100 ns. That requires testing some circuit ideas. This project is a three-way collaboration between BNL, FNAL and ANL, and we anticipate that the project will be completed by end of FY18.

HEXID (High Energy-resolution X-ray Imaging Detector): This is a prototype detector which provides full spectral information for every pixel, i.e. a true "color" x-ray camera that is essential for spectroscopic X-ray imaging. The device takes ideas from the Maia detector and compacts it into an area on the integrated circuit which is the same size as the sensor pixel. The sensor can then be bump-bonded to the circuit to form what is now known as a hybrid detector. The first prototype integrated circuit of such a device has been received in second quarter of FY17 and is undergoing tests. We are also developing the technology to bond the chips to the sensor. In the future it could become the replacement for Maia in an x-ray microprobe (e.g. at the SRX beamline or in an energy-dispersive XRD instrument at the HEX in the

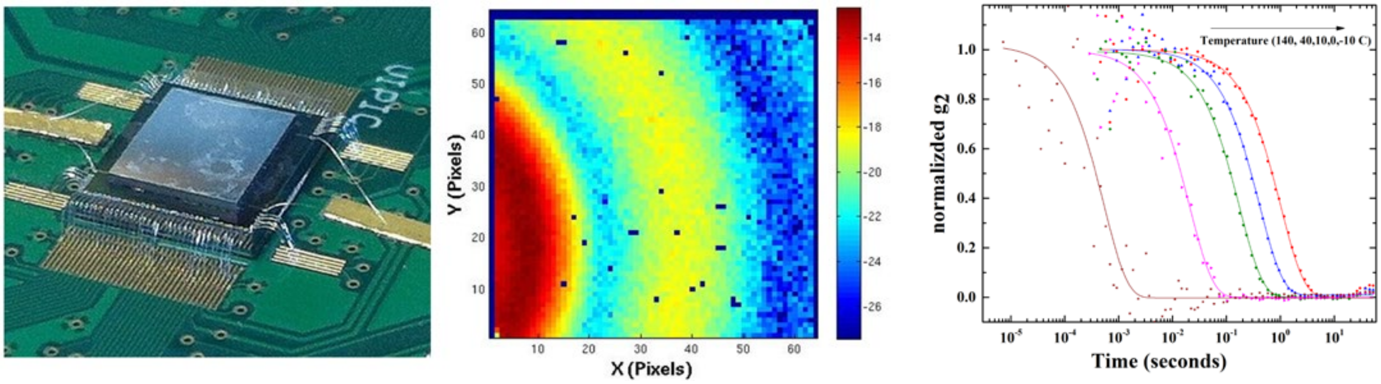


Figure 22: *(Left) Picture of the VIPIC prototype detector - a two-level microchip design that provides twice the area per pixel and allows more on-detector, real-time, processing. (Middle) Reconstructed image corresponding to a few seconds of data collection in a test run using the VIPIC prototype. (Right) Autocorrelation function derived from the data, indicating such detector will enable dynamic studies at ~10 μs level.*

future) and we are pursuing that path. A full-size version will also be useful for full-field x-ray fluorescence imaging and Laue diffraction. Both these techniques are highly restrictive currently because of the inadequacy of existing detectors.

Monolithic Segmented Germanium Detectors. We have built a detector based on a 64-element sensor fabricated by our German collaborators, Semikon Detectors GmbH, and on integrated circuits developed here at BNL. The sensor has 64 strip-shaped pixels, each one 0.5mm x 5mm, and was read out by two of our 32-channel readout chips. This device has shown that our ASICs can function properly in a cryogenic environment, and that the segmented germanium sensors produced by Semikon are of high quality. In order to have this information quickly, we used simple electronics which could only provide spectra from one channel at a time. We are now in the process of building a fully spectroscopic version based on the Maia readout system. This project is funded by DOE-BES and is moving ahead rapidly, and we expect to have several such detectors installed for the NSLS-II supported ED-XRD program at the APS 6-BM beamline, as well as for the APS high-energy X-ray diffraction program at 1-ID, within FY17.

The next step in this project is to implement a microstrip detector for high-energy monochromatic powder diffraction, specifically for use on the XPD beamline at NSLS-II. A 384-strip Ge detector is being fabricated using the MARS chip at its ASIC, modified for higher photon energy range. We plan to complete this system and conduct an X-ray test in the 2017-2 run-cycle at XPD.

Other projects: Detector R&D will also support NSLS-II beamline science in smaller projects that make use of the technology we have developed. This is an important part of NSLS-II operations. We have built a custom microstrip detector for use on the HXN beamline, and are working on a high-spatial resolution 1-D hard x-ray detector for application in a Von Hamos geometry energy analyzer for use on the ISS beamline. For the XPD beamline we have developed a detector based on the high-Z detector material CZT. It will be used to detect the x-rays arriving from a multi-crystal analyzer array. It has 8 channels, matching the number of crystals in the analyzer. It is expected that there will be more such development projects as NSLS-II becomes operational and experimenters realize the advantages of customized detectors for their experiments.

In FY19-21, with the continuing move towards imaging detectors, we plan to make some investments in such developments. We plan to continue the development of HEXID, since it blends our spectroscopic expertise with imaging. The needs to move to a smaller pixel size will drive the design away from bump-bonding and towards 3D-style direct wafer bonding. We have most of the equipment required to do this, but it is labor intensive to develop the process details.

Process, Infrastructure, and Staffing Development: We need to develop several new processes to enable reliable sensor production. These process developments are on-going, and will likely be completed in the next three to five years.

Most of our new designs rely on the availability of two layers of conductors isolated by an insulating layer. We established that process some years ago, using facilities in CFN. Unfortunately, as CFN has become busier, the cleanliness of the process chambers we use has deteriorated. We have had several compromised sensor fabrication runs which we attribute to contamination incurred during the plasma-enhanced chemical vapor deposition (PECVD) of silicon dioxide, our preferred inter-metal dielectric. Such facilities require a silane-capable cleanroom. We have discovered a non-silane process which can grow SiO2 films, though not polysilicon. That makes it viable for us to acquire a PECVD machine for this purpose and install it in an existing cleanroom. Both IXS and ISS detectors rely on this two-metal process, so it is becoming critical that we arrive at a stable, reproducible process. The inability to deposit polysilicon would be disappointing, but we have begun testing polysilicon deposited at the Cornell Nanofabrication Facility, and perhaps this will prove satisfactory.

The other process which we are developing is that of indium bump-bonding. That process is well-developed elsewhere and we feel it is within our capabilities to realize it at BNL. This will provide us with an alternative interconnect strategy to the wire-bonding we currently use, and result in better performance from some of our systems. The HEXID detector is a bump-bonded design, although the ASICs are not provided with bumps from the foundry, as originally intended, so we need to either learn this process or find a commercial vendor who will work with individual chips, rather than full wafers. A second example is the Maia detector, which is notoriously difficult to wire-bond, and our attempts to find a commercial wire-bonding source has failed. A fairly straightforward re-design of our readout ASICs would allow a bump-bonded solution. For the SDD-Maia project it would also result in improved noise performance due to the reduced interconnect capacitance.

The fabrication of detector systems is a slow, labor-intensive operation. The fabrication of sensors requires a long sequence of process steps, and each step needs to be tested and calibrated before being used on real detector wafers. There is always the possibility of a design error or a processing error which can render an entire run worthless. As an integral part of the detector development, our process of fabrication of Application-Specific Integrated Circuits (ASICs) has relied on the Instrumentation Division at BNL completely for ASIC design support. This has never been entirely satisfactory, since that group has pressures from many sides, but recent developments in personnel within IO should cause us to reconsider this posture. This is potentially a more serious problem than the sensor processing issues since we need the ASICs to use the sensors.

To address these processing infrastructure and staffing challenges, we will develop a sustainable long-term plan in FY17 for the detector program at NSLS-II / BNL, taking into account the evolving future plans for the Instrumentation Division where we currently rely on for the critical process of sensor design and ASIC fabrication, among other essential tasks. We will also work closely with other DOE Laboratories to continue to coordinate our development projects with the overall goal to enable cutting-edge science well-matched to the rapid development of new light sources.

6.5 MULTIMODAL SAMPLE ENVIRONMENTS

The multimodal approach, defined here as utilizing techniques across multiple beamlines at NSLS-II, and/or in combining synchrotron-based techniques with other modalities, such as the electron-based imaging methods at CFN, is an important component of our strategic approach. Multimodal studies are becoming widely used in almost all scientific disciplines ranging from materials physics and engineering to environmental and biosciences. In particular, multimodal experiments are typically required to characterize complex materials systems and hierarchical heterogeneous structures. Understanding process-structure-performance correlation in these systems is of great value in sciences and technologies.

<u>Initial Multimodal Science Drivers.</u> We have identified two scientific cases to use as a starting point to drive the technical development of multimodal experiments.

First, in *energy storage* studies, synchrotron x-ray methods have proven to be powerful ways to characterize energy storage and energy conversion systems, where complex heterogeneous structures exhibit chemical reactions and structural changes across multi-length scales during electrochemical operation. A wide range of *operando* and *ex situ* synchrotron experiments, including imaging, diffraction, scattering and spectroscopic experiments with various length scales, are currently used to study specific aspects of the complex chemical and structural changes correlated with battery functionalities. Developing multimodal approaches that not only illuminate a single aspect of one component but also visualize the impact of these changes on all other components inside the device will provide the critical information, e.g. on how different constituents interact with each other during battery operations, that is currently lacking to optimize the full battery structure and the interaction between species. Such an optimization would lead to potentially very large economic impact.

The following NSLS-II beamlines and techniques have been identified to contribute to the multimodal and in-situ/operando approach in battery studies:

- XRF mapping for elemental distribution evolution: hard x-ray nano/micro probe – HXN, SRX, and XFM and tender x-ray micro probe TES
- Hard x-ray spectroscopy for oxidation states and local structures – bulk: ISS, QAS; spatially resolved: SRX, XFM
- Nano-tomography/spectroscopic imaging for morphological and chemical evolution – FXI, SRX and HXN.
- X-ray diffraction for structure and phase-identification

– average structural investigation at XPD and spatially-resolved diffraction at HXN, XFM and XPD.

- Small angle scattering for longer range structure – SMI, CMS.
- Surface reflectivity for surface structure e.g. solid-electrolyte interface – ISR and SMI
- Soft x-ray spectroscopy (XPS and XAS) at CSX-2 for surface chemical and electronic state information
- Laboratory-based tools including imaging techniques such as electron-based microscopy and infrared microscopy are also critical in characterizing battery materials, providing complimentary information. Electrochemical characterizations performed in laboratories are also essential to ensure the success of synchrotron experiments.

The second science driver is *chemical catalysis*. Catalytic systems typically consist of heterogeneous systems with multiple components in the catalyst in contact with reactants either in gaseous or liquid phase. Under reaction conditions, the dynamic interactions between the catalyst and the reactants result in structural, morphological, chemical, and electronic changes in the catalyst itself both in the bulk and on the surface, as well as the formation of adsorbed chemical species. Multiple experimental probes are required to obtain a coherent picture in terms of understanding the role of active sites, determining the structure-function relationship of the catalyst, and elucidating reaction mechanisms.

One of the major experimental challenges in catalysis research is the necessity to perform experiments under operando conditions. Typically, this means that the experiment is performed at pressures of 1 bar or above, but more importantly, results from synchrotron experiments need to be correlated with the functional characteristics of the catalyst such as activity, selectivity, stability, and turnover frequency. Additional infrastructure needed includes gas handling and delivery system and a support lab for sample preparation. *Operando* cells may need to be designed for x-ray and electron-based techniques separately due to limitations on compatible window materials for 1) XPS/TEM/other electron techniques, and 2) XAS/XES/diffraction/IR/other photon techniques.

The following NSLS-II beamlines and techniques have been identified to contribute to the multimodal and in-situ/operando approach in catalysis studies:

- Soft x-ray spectroscopy (XPS and XAS) at CSX-2 and SST-1/SST-2 yields information on the surface chemical and electronic states of the catalyst and adsorbed species
- Hard x-ray absorption spectroscopy (XANES, EXAFS) at ISS (provides information on bulk chemical and oxidation states as well as local structural information; spatially resolved measurements can be done at XFM and SRX if needed.
- Tender energy XAS at TES to bridge the energy region between soft and hard x-ray spectroscopies
- XES and RIXS at ISS to probe molecular interactions such as between metal and ligand
- XPD to determine long-range ordering (average over the sample, with atomic resolution), average atomic structure
- PDF to determine short range (nm scale) structural studies, local ordering
- X-ray fluorescence imaging and tomography at SRX, XFM and HXN provides morphological information of the catalytic material
- Laboratory-based techniques such as infrared spectroscopy (IRRAS, DRIFTS), TEM, and Raman spectroscopy are commonly used to study catalysis.

Catalysis research, therefore, benefits from multi-modality not only through the combination of different techniques to simultaneously study the same system or sharing the sample environment, but also to correlate a vast amount of data to achieve a unified understanding of the process.

Development Plans. We plan to coordinate the development multimodal capabilities at NSLS-II in two types of sample environments – static and in-situ/operando. For static measurements, the exact same samples need to be measured across different beamlines without physical changes. For these types of measurements, simple and fast sample registration between beamlines and laboratory techniques is critical. We plan to meet these needs by developing common fiducial markers, common sample mounts, data acquisition with automated sample position registration, and data analysis tools for data merging, analysis, and integration. Radiation dose may need to be tracked and addressed to ensure samples truly remain unchanged across beamlines.

Operando/in-situ experiments require measuring samples that are evolving under various conditions, and in some systems, it may not be feasible to measure the same samples across different beamlines because the samples may have evolved after one measurement and cannot be reused. To address this challenge, we plan to develop *in-situ* sample cells that are compatible across different beamlines in order to create the same *operando* conditions for correlative measurements using multiple techniques, and to develop data handling software that provides the ability to align, analyze, correlate, and integrate the *operando* data measured from different beamlines and techniques.

Our specific plans for the development of multimodal/operando capabilities at NSLS-II include both technical and logistic aspects. Technical developments focus both on beamline *hardware*, such as common sample mounts where feasible, fiducial marking and sample registration, standard form factor sample cells, sample environment control, common equipment and stages, and on *software*, such as data storage/retrieval/architecture needed for multi-modal studies, common tools for sample tracking, data acquisition, registration, analysis, visualization, merging and access, and modeling. Logistical developments will include user access features such as multi-beamline proposal submission and review and beamtime allocation, multi-facility proposal system and time allocation, and access to support laboratories and associated user training, education, and outreach.

In FY17, our overall goal is to first establish sample mounting, measurements and analysis across a small number of beamlines, using battery and catalysis standard samples as test cases to establish a baseline. In battery research, we plan to pursue (a) static sample registration with fiducials at SRX, HXN, TES based on XRF microscopy at multiple length-scales, and (b) a common operando cell: for SRX, XPD and ISS based on hard x-ray XRF imaging, diffraction, and spectroscopy. In catalysts, we plan to pursue a common operando cell at CSX-2, ISS, and XPD for both hard X-ray and soft X-ray techniques.

In software, we will evaluate and establish specifications on the data acquisition, management, analysis processes, data architecture, and data policy to ensure compatibility with the multimodal approach. This includes (a) identifying commonalities in data acquisition and analysis processes across beamlines, (b) identifying compatibility of the data acquisition schemes and analysis platform/architecture, and (c) evaluating and establishing a metadata policy on sample information to ensure that can datasets can be retrieved and sorted across different beamlines.

On multi-beamline user access, we plan to develop a number of changes that are required in NSLS-II proposal administration, safety, and scheduling (PASS) system, in proposal reviews, and in beamtime allocations in order to enable multi-beamline access. We will aim to phase in these changes starting in FY17.

On laboratory-based ancillary instrumentation, we will conduct a survey of the user community to evaluate the needs for, and the current availability of, specific ancillary characterization tools such as scanning electron microscopy, transmission electron microscopy, scanning tunneling microscopy, atomic force microscopy, focused-ion-beam/SEM, optical Raman spectroscopy, infrared spectroscopy, and nano-indentation. We will develop a plan to assess such needs, to acquire them as new instruments, or to partner with others for shared usage.

In FY18, our overall goal is to further the multimodal capabilities on both the static and the operando directions, and apply these capabilities over a broader range of science examples. For static samples, we will demonstrate the multimodal approach on three-dimensional techniques by measuring the same sample with different contrast/interaction mechanisms – absorption/spectroscopic nano-tomography (FXI), fluorescence tomography (SRX, HXN), scattering tomography (LIX) and diffraction tomography (XPD). For samples under *operando* conditions, we will broaden the range of compatible beamlines to carry out experiments under common environment, by e.g. including compatible soft X-ray beamlines and techniques.

In software development, we plan to establish the data handling capabilities to be able to load data from multiple beamlines into one analysis process, establish tomographic reconstruction routine and visualization tools for multiple contrast/interaction mechanisms, and set up cascading analysis capabilities to using intermediate outputs from one analysis as inputs to another.

In logistics, we plan to optimize the multi-beamline proposal mechanisms taking into account the lessons learned from our experience to date, initiate a multi-facility, multi-instrument proposal mechanism for NSLS-II and CFN, hold short courses on specific topics, and establish point of contacts in specific scientific areas for multimodal and operando experiments.

In FY19-21, we will continue to mature our multimodal and operando tools at NSLS-II beamlines and in partnership with our collaborators. We expect that multimodal approaches will be carried out in broader scientific areas, beyond energy storage and catalysis, to include such research areas in materials degradation, bio-fuels, porous media, and phase transformations in materials sciences.

6.6 USER LABORATORIES AND EQUIPMENT POOL

User Laboratories. NSLS-II facility operates a number of laboratories in the five Laboratory and Office Buildings LOBs 741-745, in support of the research activities by users and staff. The primary purpose of these support laboratories is to provide staff and users with the space and capability for sample preparation and equipment setup space, as well as workspace for beamline support groups for equipment set-up, maintenance, and repairs. The laboratories are accessible for all staff and users supporting the NSLS-II experimental activities in the experimental hall.

As of second quarter FY17, the user laboratories in Bldg.741 and Bldg.743 have been in operation mode for more than a year. There are sixteen laboratories in use consisting of ten dry labs and six wet labs. All laboratories are based on shared usage for a number of beamlines with common needs and/or for specific science areas where specialized ancillary equipment may be located. Program Managers and Group Leaders have been assigned the responsibility for the overall operations in the laboratories as well as Cognizant Space Managers (CSM) for managing the day-to-day tasks in the laboratories. There is also a Laboratory Space Manager (LSM), working for the Research Operation Support Group, that oversees the entire Lab process including providing support to the CSMs and beamline staff and maintaining consumables and most equipment for these laboratories.

Location	Lab/Function
741 lab 4	Dry Lab for XPD, ESM & CSX
741 lab 5	Dry Lab for FMX, AMX, LiX
741 lab 6	Dry Lab for Beamline Assembly
741 lab 7	Soft & Bio Materials Wet Lab
741 lab 8	Structural Biology Wet Lab
741 lab 9	Condensed Matter Wet Lab
741 lab 10	Infrared Lab
743 lab 1	Dry Lab for HXN, SRX, XFM, FXI
743 lab 2	Dry Lab for ISS, TES, QAS, BMM
743 lab 3	ROS group/ Detectors
743 lab 4	Dry Lab for IXS, SIX, ISR, SST
743 lab 5	Dry Lab for SMI, CMS, CHX
743 lab 6	Beamline Assembly Lab
743 lab 7	Environmental Sciences Wet Lab
743 lab 8	Mesoscale Imaging Wet Lab
743 lab 9	Chemistry Wet Lab

In FY17-18, the user laboratories will continue to be outfitted with standard laboratory equipment as well as equipment and capabilities based on the user and the programmatic needs. Specifically we are equipping the Chemistry lab with much needed EXAFS sample prep equipment (e.g. hydraulic press, sample prep supplies, benchtop spectrometers). We will be setting up battery/electrochemistry capability in the chemistry lab (e.g. Ar glove box, battery cyclers, cell fabricating supplies, vacuum oven) to support in-situ beamline battery & electrochemical-related measurements. This equipment will eventually be moved to the energy & electrochemistry lab in Bldg.744 once the construction of the Bldg.744 laboratories is completed – see plan below. Other planned support laboratory improvements include a new growth chamber for the environmental science laboratory to support bioenergy related research, and a mechanical stretching/heating microscope stage for the complex scattering dry lab.

In FY19-21, we plan to have finished construction of 10 new laboratories in Bldgs. 744 and 745. CSMs will be assigned for each laboratory space and plan to have populated each laboratory with most of the necessary instrumentation. We will continue to outfit all NSLS-II support laboratories based on user/programmatic needs. We plan to establish new capabilities within the support laboratories such as a shared laboratory to support high pressure research and diamond Anvil cell sample prep & pressure calibration.

Location	Lab Program
744 lab 5	Metrology and Instrumentation
744 lab 6	Complex Scattering Dry Lab
744 lab 7	Complex Scattering Wet Lab 1
744 lab 8	Complex Scattering Wet Lab 2
744 lab 9	Energy and Electrochem Wet Lab
745 labs 4-6	Structural Biology wet lab
745 lab 7	Dry Lab for NYX, XFP, FXI
745 lab 8	Dry Lab for FMX, AMX, LIX

Infrared Laboratory (741 Lab 10). In partnership with Consortium for Materials Properties Research in Earth Science (COMPRES), NSLS-II is currently developing an infrared beamline, Frontier Synchrotron Infrared Spectroscopy under Extreme Conditions (FIS), dedicated for infrared spectroscopic studies of materials under extreme pressure and temperature conditions. This beamline is expected available for general users in the summer of 2018 based on current schedule.

To jump start the infrared program for high-pressure studies and to help bridge the gap between former NSLS and the FIS beamline at NSLS-II, we have been working with COMPRES and have established an IR laboratory in Lab 10 of Bldg.741. The core facilities in this Lab include a FTIR spectrometer with conventional sources combined with an IR microscope, a micro-Raman system, and a user-working bench for sample preparations. This facility can be accessed by general users through the regular NSLS-II proposal system. Such general user program started in FY16, allowing users to carry out their experiments under moderate pressures with reasonable sample size. It has significantly minimized the impact to the high pressure IR research community during the NSLS to NSLS-II transition period.

Research Equipment Pool. A new Research Equipment Pool (REP) has been established where the NSLS-II scientific community can use this equipment at the beamlines and laboratories. There are currently over 70 pieces of equipment available consisting of detectors, XAS foils, powder standards, a radiation generating device for alignment and measurements, LN_2 dewars, power supplies, sealed sources, chillers, and more. The equipment list can be viewed from a link on the NSLS-II website.

The Research Operations Support group is responsible for managing this program and will add more items to the Research Equipment Pool and welcome ideas from the scientific community. Improvements are also planned for having online requests and calendars that show real time availability of equipment.

7

INITIATIVES AND PARTNERSHIPS

NSLS-II recognizes that the development of cutting-edge synchrotron beamlines and enabling capabilities is only one of several necessary ingredients of producing discovery-class and high-impact science at NSLS-II. Scientific research in the 21st century has become increasingly interactive and interdisciplinary, and often relies on a larger team of researchers with complementary expertise to achieve the best possible research objectives. As stated in Section 1.1, one of our strategic approaches is to integrate the scientific community interest and expertise in NSLS-II facility operations, facilitating university-industry-government partnerships to catalyze innovation to support the strategic mission of our stakeholders. Here in this Chapter we outline our list of ongoing strategic initiatives to leverage the intellectual power and resources in the community to enhance scientific productivity and impact of NSLS-II.

7.1 PARTNER USERS

NSLS-II has established, and will continue to pursue, an effective Partner User program. The main objective of this program is to leverage the community interest, expertise, and resources in the joint development of new technical capabilities and new scientific programs at NSLS-II. Through this approach, a partner user group may contribute cutting-edge instrumentation and technology, new analysis methods and software, and/or specialized staff expertise to NSLS-II beamlines to bring new scientific capabilities that would otherwise not be present at NSLS-II. This may include the construction and operation of a complete beamline and/or establishment of a brand-new endstation.

Typically, a partner user group proposes a partnership by submitting a partner user (PU) proposal through the NSLS-II proposal system, outlining the science and technical case, the new capability they would bring, and the beam time that is required to develop the new capability and its user program. The PU proposal is peer-reviewed and rated by NSLS-II proposal review panel (PRP), and is additionally reviewed by NSLS-II management and the NSLS-II SAC. Once approved by NSLS-II management, the terms of the partnership are formally captured in an NSLS-II Partner User Agreement that will summarize the partner user group membership, their specific contributions, the beamlines where the program is located, the amount of beam time that will be used for the partnership development, and the roles and responsibilities of the partner user group.

As of March 2017, NSLS-II has twenty-three partner user agreements in place across twenty NSLS-II beamlines that are in operations or in development. These partnerships include:

- *Center for Functional Nanomaterials (CFN):* To jointly promote and support nanoscience at NSLS-II, CFN has established several partner user programs at NSLS-II beamlines, including ambient-pressure photoelectron spectroscopy (AP-PES) at CSX-2, aberration-corrected X-ray photoelectron microscopy (AC-XPEEM) at ESM, and in-situ X-ray scattering program at CMS and SMI.
- *X-ray Scattering group (BNL-CMPMSD)* supported the development of the CSX-1 endstation that enabled coherent soft X-ray scattering studies of strongly correlated materials such as high-Tc superconductors,

with a current focus on the development of soft X-ray ptychography and phasing algorithms to allow real-space visualization of complex correlations in these systems. The group is also working with the SIX beamline group to develop a soft X-ray polarimeter and will contribute to the associated hardware for polarization dependent RIXS studies.

- *Consortium for Materials Properties Research in Earth Science (COMPRES):* To promote and support earth science studies under high-pressure, COMPRES has two partner user programs at NSLS-II – one focuses on using angle-resolved X-ray diffraction under high-pressure at XPD and the other on spectroscopic studies at high-pressures using infrared radiation at FIS.
- *Synchrotron Catalysis Consortium (SCC):* The SCC provides additional specialized expertise and staff support at a suite of X-ray spectroscopy beamlines at NSLS-II. The main object of this partnership is to promote synchrotron catalysis studies at NSLS-II through the joint development of in-situ and operando sample environments that enables characterizations of new catalysts and their associated chemistry under realistic operating conditions.
- *GeoSoilEnviro Center for Advanced Radiation Sources (GSE-CARS):* GSE-CARS is based at University of Chicago and plans to provide additional staffing with relevant scientific and technical expertise to support the operation of the XFM beamline and to promote geo-environmental research in partnership with NSLS-II.
- *New York Structural Biology Center (NYSBC):* NYSBC a consortium of structural biology groups of major institutions in the New York region. It has developed and is currently operating the NYX beamline at NSLS-II. This partnership focuses on cutting-edge instrumentation in structural biology, particularly to enable ab-initio phasing of macromolecules using weak anomalous scattering signals.
- *Case Center for Synchrotron Bioscience (CSB):* The CSB at Case Western Reserve University has developed and is currently operating the XFP beamline at NSLS-II, and has a separate partner user arrangement at the FMX and AMX beamlines. The main objective of the CSB partnership is to promote and support biosciences using a wider range of synchrotron techniques including macromolecular crystallography as well as X-ray spectroscopy and X-ray foot-printing.
- *National Institute of Standards & Technology (NIST):* NIST is in the process of developing three beamlines, SST-1, SST-2, and BMM at NSLS-II, and will be operating these beamlines after completion of their construction. This partnership is joined with IBM, and focuses on supporting the NIST mission of promoting science and technology development for the nation's commerce, through providing cutting-edge materials characterization capabilities at NSLS-II.
- *Rapid Acquisition PDF (Columbia-APAM and BNL-CMPMS):* The PDF group at Applied Physics and Applied Mathematics Department of Columbia University and at the CMPMS Division of BNL has developed a suite of pair distribution function (PDF) data analysis software at the XPD and the PDF beamlines of NSLS-II. This partnership will promote the use of PDF techniques to solve a variety of materials science and engineering problems.
- *Chemistry Consortium (BNL-Chem):* The partnership with this group includes the operation and user support of an In-Operando XAS endstation at the CSX-2 beamline and the development of in-situ/operando capabilities at the XPD beamline at NSLS-II.
- *Tender Energy Microspectroscopy Consortium (Miami University, Ohio):* This consortium contributed a suite of key beamline optical systems and a tender energy X-ray microspectro-scopy endstation to enable and promote tender energy microspectroscopy in climate, environmental, earth and planetary sciences at the TES beamline at NSLS-II.
- *Consortium for real-time studies of thin film growth and surface processing (Vermont/Boston /Stony Brook):* This consortium has developed a cutting-edge X-ray scattering chamber and associated instrumentation to enable and promote at the ISR beamline of NSLS-II the in-situ studies of pulsed laser deposition (PLD) growths of technological relevant thin-film materials systems.
- *Consortium for Physics of Novel Materials (Yale University):* This partnership aims to enhance the capability of the ESM beamline by coupling its photoemission microscopes with a state-of-the-art Molecular Beam Epitaxy (MBE) instrument that is capable of the synthesis of artificial multilayer structures of transition metal oxides with atomic accuracy, leading to research on novel functional electronic properties that include induced superconductivity, magnetism, unusual spin transport, metal insulator transitions, large dielectric constants, and multiferroic behavior.

Overall, this suite of partner user programs leverages the expertise and the resource in the community, significantly enhances the scientific capabilities of NSLS-II beamlines, and expands the user science programs at NSLS-II. We plan to continue to work with the scientific community to develop strong and mutually beneficial partnerships in the next five years.

7.2 MULTISCALE BIO-IMAGING

Many recent advances in medicine, drug development, and biotechnology have been made possible by our ability to study processes at the molecular level. For example, resolving the structure of proteins enabled fundamental insights into the cause of a range of diseases. In addition, the development of a fundamental understanding of genome biology would allow the design, modification, and optimization of plants, microbes, and biomass for beneficial purposes relevant to the DOE missions in energy and the environment. In both these areas, the understanding of complex biological systems and their interactions with the environment require studies across multiple temporal and spatial scales.

NSLS-II is working closely with other BNL departments to establish a world-leading multi-scale bio-imaging institute at BNL for molecular and environmental biosciences. This initiative currently consists of two parts – (a) development of a new cryogenic electron microscopy capability at BNL and (b) establishing coordinated access to a suite of capabilities at NSLS-II for multi-modal and multiscale imaging of bio-environmental systems.

Cryogenic Electron Microscopy. Scientists have long used x-ray crystallography to determine the structure of proteins and deduce their internal workings. Recent advances in cryo-electron microscopy (cryo-EM) have opened up the possibility of resolving the structure of the large multi-protein complexes that perform vital functions within cells. In the future, scientists will combine both techniques in their studies. A complete picture of these complexes is needed to fully understand the vital processes they perform and forms the basis for the development of novel drugs or biotechnology. The U.S. National Institutes of Health (NIH) and the U.S. Department of Energy (DOE) have recognized the transformative opportunities offered by the cryo-EM revolution. In particular, NIH has established funding opportunities for regional cryo-EM user facilities. We plan to develop a funding proposal to attract one of these cryo-EM facilities to BNL.

To provide maximum impact, we plan to combine NSLS-II and its world-leading capabilities in protein structure analysis with a new cryo-EM facility. An investment in cryo-EM would elevate BNL to world-leading prominence in the field of biomolecular science, positioning the lab for additional NIH and DOE investments. Our strategy is to establish an Institute for bio-molecular structure at BNL giving researchers access to the complementary tools of state-of-the-art cryo-EM and state-of-the-art x-ray diffraction in the same institute for the first time thus creating a major national user facility with tremendous impact in bioscience research.

There would be several advantages to establishing a bio-imaging facility at BNL. First, NSLS-II has enabling world-leading imaging performance for samples of nanometer to millimeter size, including a suite of experimental facilities enabling high-fidelity diffraction data to be obtained from the smallest, most fragile macromolecule crystal samples. The combination of world-class x-ray and cryo-EM facilities will provide unique opportunities to understand biological systems of physiological relevance and generate breakthroughs in biotechnology. Second, CFN has world-leading programs in electron microscopy and protein assembly, further enhancing the impact of the Institute through tight integration with these sample preparation and handling programs. Third, BNL's computational capability is the key to managing the data volume, analysis, and integration challenges associated with these microscopes. Fourth, BNL has a strong program in novel electron-detection devices, enabling us to push the state-of-the-art in cryo-EM beyond what is available anywhere in the world today. Finally, BNL has long experience in operating user facilities and the support infrastructure necessary for the Institute.

We plan to employ a phased approach to developing the bio-imaging facility. In FY17, as a first step of our initiative, we plan to procure funding through NY State and Science Foundations, such as the Moore Foundation, to purchase and install two electron microscopes at NSLS-II experimental floor. The first microscope will be optimized for high-resolution 3D imaging of proteins and macromolecular assemblies. Access to this instrument will be possible for scientists physically at BNL and for others through remote access from their home institutions. The second microscope will include an automated cryogenic sample exchange system for bio-sample handling at liquid nitrogen temperatures. This microscope will be primarily dedicated to high-resolution 3D imaging of proteins and macromolecular assemblies, but can also perform 3D cellular reconstructions.

In addition, we plan to work with the relevant community and submit a grant application in response to the NIH funding call for cryo-EM user facilities. This grant proposal, if successful, will allow for additional four cryo-EM microscopes as well as the operating funds to operate the facility and support users. We anticipate this facility will be developed in FY18-19 and operated with the input of the scientific partner groups. User access will follow a similar mechanism as in the NSLS-II proposal system – through peer reviewed proposals including both general users and possible partner user arrangements.

In FY20-21, we anticipate constructing a building to house up to eight microscopes and ten research groups together with a sample preparation laboratory, biomolecular laboratory and complementary imaging techniques including super-resolution light microscopes, scattering instruments, etc. This will build the institute that would aim to speed the rate of fundamental understanding of biomolecular processes by several orders of magnitude through advances in crystallization, in state-of-the-art beamlines, in cryo-EM sample preparation and data analysis, and by tight integration of research groups in the same facility. Realizing this vision would place BNL on the world map for biomolecular imaging.

Multimodal Multiscale Imaging of Bio-environmental Systems. The spatial and temporal resolution available from NSLS-II photon beams will enable unprecedented characterization and imaging of interactions between plants, microbes, and the environment from sub-nanometer to millimeter length scales and over dimensions of time that range from picoseconds to seconds. The capability to provide molecular fingerprints and mechanistic and dynamic understanding of *in-situ* ecosystem processes would impact a range of science focus areas.

NSLS-II provides a suite of beamlines uniquely formed to allow for the investigation of these systems from the atomic level details as revealed by spectroscopy (ISS, QAS, XFP), through to full field imaging (FXI). In addition the elemental and molecular specific information from our micro- and nano-probes will offer unrivaled sensitivity and spatial resolution (TES, SRX, XFM & HXN).

NSLS-II will allow for multi-modal research by allowing coordinated access to this suite of instruments. The further integration of complementary techniques is an opportunity with the integration of cryo-electron microscopy and tomography (cryo-EM/ET) augmenting the imaging capabilities of the lightsource. In addition the traditional structural biology infrastructure described previously will be strengthened through single particle characterization capabilities enabled by the electron microscopes.

Achieving the potential of this facility will require the training of scientists who are not "traditional" lightsource users for their science. When this is combined with active outreach activities, the potential for growth in the user community is high. Benefiting from the information rich data sets emerging from measurements at multiple instruments the NSLS-II program will utilize the BNL initiative in computer science, linking cutting-edge computing capabilities for advanced data analysis and modeling. In all of these areas, the cross fertilization between different DOE facilities and techniques is essential. This area offers another opportunity for effective national stewardship through DOE-BER and NIH coordination. We plan to work closely with the community to develop an agenda for a predictive biology initiative at BNL with such integrative research topics as:

- promoting research from atomic to molecular to cellular and meso-scales,
- increasing bioscience support for imaging in addition to structural biology,
- multimodal research drawing together many types of investigations,
- developing molecular tags to help with the localization of molecules and organelles in cells,
- studies of dynamics of processes using optimization of measurement for time-lapse experiments, and
- multi-spectra imaging for plant science.

Understanding complex biological and environmental systems requires us to be able to bring together measurements across many temporal and spatial scales. Further, complete knowledge will also require merging these data with theoretical models of processes, links to field observations and genetic analysis. To meet these goals, measurements will be made on realistic samples - leading to complex experiments examining highly heterogeneous, opaque samples.

7.3 ENERGY SCIENCE

Catalysis Research: Catalysis is a critical technology for modern society, central to current worldwide trillion dollar industries in fuels, chemicals and pharmaceuticals production. Catalysis advances are critical to enable future chemical and fuel pathways that can incorporate new feedstocks such as abundant natural gas or renewable-energy driven fuels and chemicals production. Catalysis plays an important role in the DOE mission, both in applied energy and basic science programs.

An overarching catalysis challenge is to enable a transition from trial-and-error based catalyst development toward catalysis-by-design. Catalysis science strives to establish principles that can guide the design and application of improved catalysts by elucidating the structure and function of catalysts – materials that accelerate and direct chemical reactions toward desired products. Progress requires understanding complex materials operating in harsh environments. Specific challenges include: i) characterizing complex, multi-scale, multiphase powder or microporous materials; ii) distinguishing relevant surface structures - that activate catalysis at the gas-solid or liquid-solid interface – from dominant bulk structures; iii) capturing dynamic catalyst atomic and electronic structure *in situ* at the pressure, temperatures and reaction conditions relevant to an industrial process; iv) characterizing both the catalyst and the associated chemical pathway, including chemical intermediates, in a complex environment.

Catalysis science is therefore a broad discipline that must understand multi-scale structure and function from the atom scale of the reactive site to the many meter scale of large catalytic reactors. It requires a multi-disciplinary and multi-technique approach to both simplified model systems and complex, realistic reactor environments. It is active in academia, national labs and industry.

Synchrotron methods have been increasingly important in catalysis over the past four decades both to meet the need for information on well-defined model surfaces and interfaces and to enable *in situ* or *operando* studies of complex catalyst powders within reactor cells [14]. Key synchrotron catalysis science trends include: 1) *in situ* or *operando* -increasingly sophisticated cells and methods to probe industry-relevant processes with working catalysts at controlled temperatures and pressures; 2) *multi-technique* – simultaneous (in the same experiment) or consecutive (using portable reactor approach – see **Figure 23**) application of multiple techniques to characterize multi-scale catalyst structure and progress of chemical reaction; 3) *time-resolved* – faster characterization techniques that follow reaction changes to sub-second timescales; 4) *high energy resolution* – X-ray based absorption and emission methods that rely on unique spectroscopic features for distinguishing between effects of adsorbates and support on the catalyst; 5) *imaging* – bright X-ray sources and imaging and tomographic methods to characterize microstructure and composition down to single catalytic particles.

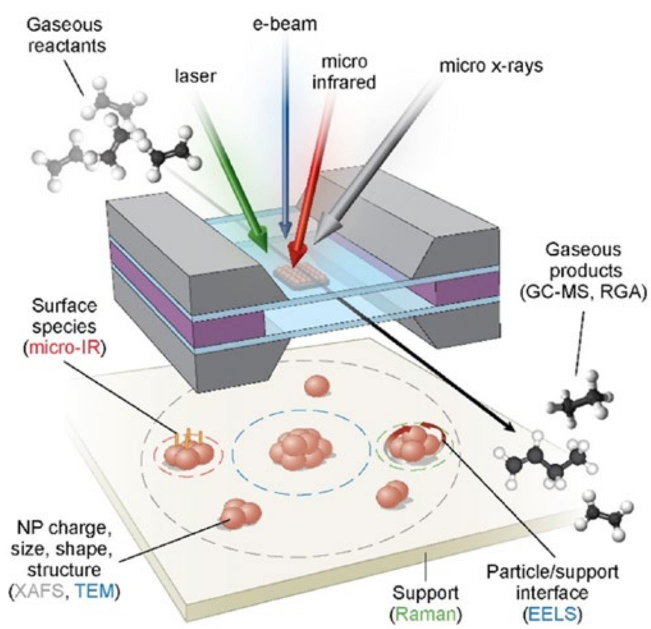


Figure 23: *Integration of photon and electron probes using a micro-reactor platform for multi-modal characteriza-tion of working catalysts [15].*

NSLS-II is uniquely positioned to take a leading role in U.S. and world catalysis science. It inherits an active catalysis science user community from NSLS, including both BNL core programs and effective outreach through the Synchrotron Catalysis Consortium (SCC). Its capabilities of high flux and world-leading brightness across a substantial energy range are ideal, and unique in the U.S., to address the time-resolved, multi-technique, and imaging needs of advanced catalysis science. It has an initial set of beamlines whose development has been informed by the needs of catalysis science in diffraction and spectroscopy, including special capabilities such as gas handling systems.

NSLS-II has developed a three-fold plan to develop and promote catalysis research – (a) develop cutting-edge beamline capabilities for catalysis research including hazardous gas handling and exhaust, (b) attract scientific staff with catalysis research interests and experience, and (c) leverage and integrate community expertise and interest to form partnerships that enhance catalysis research at NSLS-II. The first points are already described previously, and here we focus only on the partnerships that we plan to establish in the area of catalysis science.

We are currently working in partnership with three research groups in catalysis research to develop and utilize the unique capabilities at NSLS-II in the area of in situ and operando catalysis science.

The BNL Chemistry Division's *Catalysis Reactivity and Structure* (CRS) Group was a leader with in situ methods at NSLS, and will be a partner user at the XPD and CSX-2 beamlines. These partnerships aim to establish world leading capability for the user community to carry out high impact research in catalysis while furthering the next generation of tools that rely on use of XRD and soft X-rays to study the structure and electronic properties of catalyst materials during chemical transformations critical to meet energy demands. A central theme is to advance the development of *in situ* catalysis science methods at NSLS-II towards *Operando* conditions. One example is the AP-XAS endstation at the CSX-2 beamline, which enables surface chemical analysis via x-ray absorption spectroscopy at gas pressures up to ~ 1 atm and sample temperatures up to 500 °C. Another example is the structural characterization of working catalysts by X-ray scattering methods. Here the partnership will enable new tools such as *in situ* PDF, combined DRIFTS+XRD and MED measurements of catalytic processes. We expect that these partnerships will be implemented at CSX-2 and at XPD starting in FY18, with mature operations in the FY19-21 timeframe.

The CFN *Interface Science and Catalysis* (ISC) group focuses on AP-XPS and LEEM/PEEM surface studies relevant to catalysis, and is a partner user on the CSX-2 beamline. CFN provided the AP-PES endstation for the CSX-2 beamline, under a partner user agreement. Both CFN and NSLS-II users may access these instruments through the respective proposal systems. Applications include in-operando studies of surface chemistry, catalysis, and energy storage processes. In addition, another partner user agreement is being developed to allow CFN to operate its aberration-corrected low-energy electron microscope / photoemission electron microscope (AC-LEEM/PEEM) at the ESM beamline at

NSLS-II which is currently under commissioning. In FY17, the ISC group will commission the LEEM/PEEM endstation at the ESM beamline, and will upgrade the AP-PES endstation at CSX-2 by implementing an IR spectrometer in the AP-PES endstaton. In FY18 and beyond, the ISC group will participate in the development of catalysis capabilities at new beamlines such as INF, in addition to operating user support programs at CSX-2 and ESM.

The *Synchrotron Catalysis Consortium* (SCC) enables research opportunities for scientists working in catalysis and electrocatalysis fields. This consortium has enabled, since its inception in 2005, advancement of our understandings of catalytic materials and phenomena through the utilization of the state-of-the-art synchrotron techniques under *in-situ* and *operando* conditions. In 2016, the SCC submitted a partner user proposal to the suite of spectroscopy beamlines (ISS, TES and QAS) at NSLS-II. Under this proposal the SCC will provide a wide range of expertise and resources in surface science, catalysis, electrocatalysis, beamline science and instrumentation to existing and new General Users. In FY17, the SCC partnership will work with the NSLS-II to establish *in-operando* catalysis research capabilities at ISS and will start operating user support programs at ISS and TES in FY18, with the plan to expand such program to QAS beamline in the FY19-21 outer years.

Energy Storage: Developing electrochemical energy storage materials for specific applications requires fundamental understanding of the relationship between the structural changes and performance of these materials under different functional conditions. These studies are critical for the understanding of current systems and the development of next generation systems and materials especially under in situ and operando conditions. The diagnostic techniques require a combination of spectroscopic and imaging techniques, sometimes through both electron and x-ray photon probes.

As battery systems operate material phase transitions and particle morphology changes take place during battery discharge and charge cycling. Beyond the targeted electrochemical cell reactions, some side reactions, such as electrode surface passivation, and electrode material dissolution and re-deposition, could also occur in parallel. To understand the fundamental mechanisms associated with the cell reactions and the side reactions, NSLS-II will provide a powerful suite of tools to address many of these questions. *In-situ* and *in-operando* capabilities will be developed at several NSLS-II beamlines to probe energy storage systems, and these are described below.

Spatially resolved chemical states. The Submicron Resolution X-ray Spectroscopy (SRX, 5-ID) at NSLS-II provides the capability of measuring 2D X-ray fluorescence maps at sub-micron (with future plans for sub -100nm) 2D spatial resolution. The unique ability of SRX is to collect X-ray absorption near edge structure (XANES) spectra to facilitate spatially resolved studies of oxidation states within a sample. This type of capability is crucial for battery research, as the electrochemical reaction can be directly probed across active particles/agglomerates within an electrode. This can be accomplished with carefully executed *ex situ* samples, or *in situ* electrochemical cell characterization, where an active electrochemical system is placed in the beamline and directly measured. Recently, the feasibility of EXAFS has also been demonstrated at SRX; this will be used to provide structural information as well as oxidation state.

The HXN beamline will be explored for operando study of battery related materials. Specifically, high resolution mapping at a single energy can be done to assess the progress and homogeneity of an electrochemical reaction. HXN aims to enable x-ray experiments at spatial resolutions ranging from 10 to 30 nm with a longer-term goal of ~5 nm.

Metastable structural phase identification. The XPD beamline will be used for characterization of crystalline (XRD) as well as poorly crystalline (PDF) battery materials as prepared and after electrochemical testing. Further, investigation of synthesis reactions of battery materials is underway. In-situ reactors for solvothermal and solid-state synthesis have been designed and are being utilized for tracking the phases bring formed, including the intermediates, short-lived metastable phases and their structural evolution. The results of such studies will enable strategies to 'dial-in" desired phases and properties, opening up a new avenue for synthetic control of the phase, stoichiometry, and morphology – critical, and often limiting parameters for the development of high-capacity cathodes.

Further, operando X-ray Powder Diffraction studies, **Figure 24**, will be conducted, allowing phase changes to be pinpointed. These are used to elucidate the reaction mechanism.

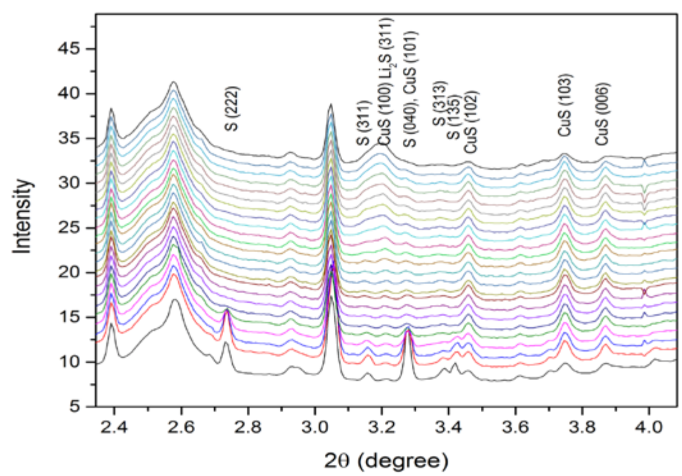


Figure 24: *XPD operando study of phase change in a battery electrode.*

The following programs are envisioned over the next 3-5 years. In FY17, we will continue work on SRX/HXN/XPD, expanding the *in-situ* and *operando* capabilities and extending our work to *in-operando* spectroscopy at ISS. In FY18, microstructural chemical analysis of electrodes will be conducted with enhanced spatial resolution using the TXM as it returns to NSLS-II. The plan for FY19-21 is to conduct in-operando mapping of reaction fronts in full cells and batteries at the HEX beamline or equivalent.

Specifically, new beamlines will be established at NSLS II for characterization of energy storage materials, components and systems. Transmission x-ray microscope (TXM), was operational at National Synchrotron Light Source (NSLS) and was moved to the Advanced Photon Source at Argonne National Laboratory. The capabilities including non-marker auto-tomography, local tomography and spectroscopic imaging are essential for electrode level characterization and will return to NSLS II with enhanced resolution at the FXI beamline, which is scheduled to start commissioning and operations in FY18.

Cell level characterization for as synthesized cells can be accomplished through Energy Dispersive X-ray Diffraction (ED-XRD). This system was operational at former National Synchrotron Light Source and was moved to the Advanced Photon Source at Argonne National Laboratory. The HEX beamline will replace this with operations starting at NSLS-II in the FY21 timeframe. This technique enables the characterization of as manufactured cells including those of large size to gain accurate insight into the function with the systems in an unmodified environment.

As a broad set of capabilities becoming available at NSLS-II beamlines, the capability for imaging and spectroscopy (XRD, XAS, and PDF) with very fast data collection capability will enable dynamic studies under very high rate charging and discharging. Techniques to probe a matrix of samples at similar operating conditions in a short time are needed along with automated data mining software to analyze the huge amount of data collected. Further, these types of studies need to be extended from the material level to the component (electrode and interface), device (full cell or half-cell) level, and even the multi-cell pack-level.

NSLS II is poised to provide a suite of capabilities that would be attractive for energy storage scientists from academic institutions as well as from the government and private sectors. The wide-range of high-flux synchrotron photons will enable unprecedented resolution at very fast time frames enabling real time data acquisition during functional operation of battery systems.

7.4 NANOSCIENCE PARTNERSHIP WITH CFN

For several years, the CFN has been investing resources in partnership with NSLS-II to design and build nanoscience capabilities leveraging this unique X-ray resource. Taking advantage of the brightness, coherence, and focusing at the new light source, these joint ventures will establish world-leading nanoscience capabilities in X-ray scattering, photoelectron microscopy, and operando spectroscopy.

During the 2016–18 period, CFN and NSLS-II will complete critical build-outs of the four partner instruments, bringing them to full operations and building highly productive User populations. This is only the initial phase of a larger plan that includes partnering with NSLS-II to develop additional instruments for nanoscience, as well as upgrading these first ones during the years 2018–20. The CFN will also acquire and enhance a set of complementary laboratory-based instruments that will expand the user program, by providing screening platforms for nanomaterial development.

AP-PES Upgrade. The CFN strategy for developing operando capabilities for catalysis and energy storage, leveraging the unique capabilities of NSLS-II, relies on performing photoelectron spectroscopy at pressures approaching one Bar. An ambient pressure photoelectron spectroscopy (AP-XPS) endstation used for the past three years at NSLS was transferred to the new CSX-2 beamline at NSLS-II, where it is currently operating and supporting Users.

The CFN plans to invest in a next-generation AP-PES endstation (including AP-XPS and AP-NEXAFS) with enhanced capabilities compared to the existing instrument, including operation over an extended pressure range, and in-situ access to infrared spectroscopy. In a first stage, a FTIR spectrometer with a globar source will be coupled into the new chamber. In a second stage, IR light from the proposed new adjacent beamline (INF) will be used. This instrument will allow the study of surfaces of interest to catalysis for energy applications as well as environmental and atmospheric chemistry. The extended pressure range and combination with vibrational spectroscopy will provide unprecedented details for chemical transformations carried out in catalysts model systems that can provide, in turn, the guiding principles for improvements of catalytic processes and design of new tailored catalysts.

AC-LEEM Upgrade. From 2008–2014, the undulator beamline U5UA at NSLS hosted the CFN's commercial low-energy electron microscope (Elmitec LEEM III) equipped with an electron energy analyzer for operation as a x-ray photoemission electron microscope (XPEEM) operating in ultrahigh vacuum (UHV). The LEEM-XPEEM system was a powerful tool for studying the dynamic and static properties of surfaces and thin films, including growth and decay, phase transitions, reactions, surface electronic structure and morphology.

In 2015, the CFN acquired and operated a new state of the art aberration corrected instrument AC-LEEM/XPEEM, with a spatial resolution better than 3 nm in LEEM and 8 nm in XPEEM mode. Besides the imaging modes, it also provides micro-diffraction and micro-spectroscopy capabilities. In 2016, this AC-LEEM system was moved to the new Electron Spectro-Microscopy (ESM) beamline at NSLS-II, and science commissioning experiments will begin in FY17.

Proposed future upgrades to the AC-LEEM/XPEEM instrument include: (1) a state-of-the-art solid-state detector, which will replace the current multi-channel plate setup; and (2) closed-cell sample environment for operation at significantly increased gas pressures, currently being developed at the CFN. The photon energy range offered by the ESM beamline at NSLS-II (15-1500 eV) will be ideal for the implementation of nanoscale XPEEM in closed cells, thus providing world- leading capabilities for operando spectro-microscopy at high gas pressure and in liquids. We will also closely collaborate with the NSLS-II ESM beamline staff towards the tight integration of the two beamline endstations, including the development of common sample preparation facilities and standardized sample transfer systems.

X-ray Scattering Upgrades. The CFN is partnering with NSLS-II to develop a world-class nanoscience X-ray scattering program leveraging two beamlines: the Complex Materials Scattering (CMS, 11-BM) and Soft Matter Interfaces (SMI, 12-ID) endstations. These instruments provide complementary capabilities for structural studies of complex materials, including hierarchical, hybrid and bioinspired nanomaterials, with CMS providing the versatility and automation to rapidly and efficiently explore parameter spaces for materials discovery, and SMI providing the high-performance necessary for frontier measurements. The CFN is enhancing the CMS beamline by developing and deploying automation hardware and software, including coding data pipelines for automated analysis.

Simultaneously, the CFN is acquiring, for installation at SMI, a one-of-a-kind x-ray detector featuring a through-hole. This will greatly broaden the q-space that SMI can access, providing the ability for simultaneous small, medium, and wide-angle measurements of complete (uninterrupted) scattering arcs. These beamlines will begin general user operations in FY18. As partner user, the CFN is curating a high-impact nanoscience user program; the CFN is committed to supporting a substantial fraction of the beamtime on these beamlines for nanoscience general users. This user community is pursuing advanced research in nanomaterials synthesis and functional characterization, including materials for catalysis, batteries, energy processing, light manipulation and sensing.

This X-ray scattering program is strongly tied to the CFN's scientific strategic plan, where X-ray methods are crucial to ongoing studies of self-assembling materials, and multi-functional nano-architectures. The CFN has a strong history of X-ray scattering method development, which will be continued on the CMS and SMI beamlines. In particular, the CFN is developing: (1) correlation methods for quantifying the complex three-dimensional order—and defectivity—of modern nanomaterials; and (2) algorithms and code for autonomous experimentation. These development activities will have impact for a broad range of synchrotron users. The CFN program is strongly engaged across the NSLS-II Complex Scattering program, with CFN research projects counted among the first user experiments at the CHX beamline. The CFN plans to remain engaged with research activities and partnerships across a range of NSLS-II beamlines, and will invest in targeted beamline upgrades and the development of novel end-station capabilities as part of its ongoing commitment to this program.

Nano-IR instrument. CFN and NSLS-II scientists have proposed an infrared spectroscopy (IR) beamline at NSLS-II that will include three simultaneously operating branches: (1) an infrared near field nanoscopy (INF) instrument dedicated to condensed matter physics; (2) a second INF instrument installed by the CFN and setup to carry out first of its kind experiments in controlled environments from UHV to ambient conditions; and (3) direct synchrotron IR light to combine photoelastic modulation infrared reflection absorption spectroscopy (PM-IRRAS) with AP-PES at the CFN-partner endstation CSX-2. The system will be setup to carry out INF experiments in controlled environments, a capability that currently does not exist anywhere in the world. The NSLS-II plan to develop the INF beamline is described in Section 4.2.7.

As part of this project, we would acquire a new apertureless near-field microscope (known as a scattering-type scanning near-field optical microscopy, s-SNOM) that combines atomic force microscopy with optical imaging and spectroscopy at the nanoscale. The system will operate with mid-IR laser based sources at the CFN with a spatial resolution of ~10 nm. As a laboratory-based instrument, we expect it to serve a significant User community, e.g., in research directed to the characterization of mesoscale hybrid organic/inorganic structures. In addition, the instrument will serve as a proving ground to design and develop a modified system to carry experiments in controlled environments (from UHV to ambient pressures) and variable temperatures. This new capability would ultimately be moved to the new IR INF beamline at NSLS-II, where a world record target spatial resolution in spectroscopic mode of less than one nm is expected with extended spectral IR operation.

Staffing Plans. The CFN investments in developing new nanoscience capabilities at NSLS-II must be accompanied by corresponding addition of technical staff to support their operation. In support of these efforts, the CFN will hire in 2017 an Assistant Scientist with expertise in X-ray scattering, who will augment significant strengths in this area (Yager, Gang) and whose research and User interactions will be based at the CFN partnerships at the CMS and SMI scattering beamlines at NSLS-II. Additional CFN staff with this expertise will be important for planned instrument upgrades in 2020. In 2017–18, we plan to hire a scientist to support planned upgrades to CFN partner AP-PES and AC-LEEM/X-PEEM instruments at NSLS-II.

Complementary laboratory-based instruments for screening and materials development. The CFN will acquire and/or upgrade its lab-based instruments for X-ray scattering, LEEM, ambient-pressure XPS, and IR spectroscopy to complement the portfolio of synchrotron-based partner instruments at NSLS-II. These facilities will allow Users and staff to screen samples and experimental conditions prior to scheduled NSLS-II beamtime, maximizing productivity of synchrotron-based instruments by increasing throughput and increasing the total number of supported Users.

7.5 INDUSTRIAL RESEARCH

Industrial research is an essential and integral part of the research program portfolio at NSLS-II. Establishing a vibrant industry research program is a key component of the NSLS-II mission. Further, this program (a) promotes interactions and partnership along the discovery to deployment research pipeline, and (b) provides immediate connection and relevance to the general public.

A Workshop on Industrial Research at NSLS-II was held in May 2014 before NSLS-II began operations, to introduce this world-lead light source to industry and to explore the best way to continue the tradition of industry research from NSLS and further enhance the industrial engagement at NSLS-II. Workshop participants identified three key areas where NSLS-II could do to strengthen industrial research: 1) enhanced support for industry users, 2) flexible and timely access to beam time, and 3) common protocols among National Laboratory facilities.

To promote the industrial research partnership and add to industry perspectives, representative scientists from industry have been included in the NSLS-II proposal review panels and on the NSLS-II science advisory committee. Proprietary research policy and procedure has been established to guide proprietary research. In addition, proprietary users can submit proposals at any time during a given cycle through rapid access to take advantage of up to 10% beam time set aside for rapid access proposals at NSLS-II beamlines.

Based on the discussions at the Workshop and other industrial engagement and interactions, we plan to continue the development of a strong industrial research program along several directions. Our development plan in the next five years includes the following elements:

- Continue developing scientific capabilities at NSLS-II beamlines tailored to industrial applications, particularly in the areas of *in-situ* and *in-operando* capabilities with automated specimen handling in industry-relevant conditions, for example, gas handling systems.
- Promoting closer research partnerships with participations of industry partners, for example, collaborating with beamline staff, participating in the beamline programs through partner user proposals, and pursuing SBIR/STTR funding.
- Developing and implementing flexible and timely access modes to accommodate industry needs within the framework of the NSLS-II User Access Policy, including mail-in, remote control, and paid service.
- Enhancing staff support to industrial users by forming a dedicated group with scientific staff, user support admin, budget and outreach support to provide not only data but also solutions. We plan to establish a new mechanism of work-for-others to allow NSLS-II staff to contribute to industry experiments and associated data analysis directly as early as in the FY18 timeframe.
- Enhancing communications and outreach to the industrial community about NSLS-II capabilities, strategies, research opportunities and solutions for industrial research with a dedicated industry webpage, targeted workshops, training, and conferences and meetings of interest to various types of industrial users, as well as reaching out to other industrial liaison offices of universities and organizations.
- Tracking industrial research by user statistics, publications, funding sources, and corporate impact statement to better understand industry users' needs and identify the impact of NSLS-II.
- Seeking funding opportunities to grow the industry research program to strengthen industry engagement, for example, working with industry to help them to apply or jointly apply SBIR/STTR grants from DoE, DoD, NSF, NIH funding agencies.
- Coordinating with other DOE facilities on common protocols for industry access to user facilities.

7.6 NEW INITIATIVES

Being the newest and most advanced synchrotron in the US, NSLS-II seeks to attract interests from segments of the scientific community that have not traditionally been associated with synchrotron light sources. NSLS-II plans to work with these communities to broaden the usage of synchrotron techniques and increase the scientific as well as the societal impact of NSLS-II. Current initiatives in this area are described below.

Materials in Radiation Environments. Nuclear materials, including nuclear fuels and structural materials for nuclear containment systems, are of critical importance for the next-generation nuclear reactors and the nation's overall energy production landscape. These materials and material systems are traditionally difficult to study experimentally, largely due to the extreme complexity of the interplay between radioactivity and radiochemistry at multiple length scales – from atomic to millimeter or centimeter scales (**Figure 25**). Furthermore, it is very challenging to characterize these systems in-situ, beyond what can be done today typically using electron microscopy which is often destructive, in order to obtain accurate information about naturally occurring radiochemistry and structural degradations that may happen in real nuclear systems.

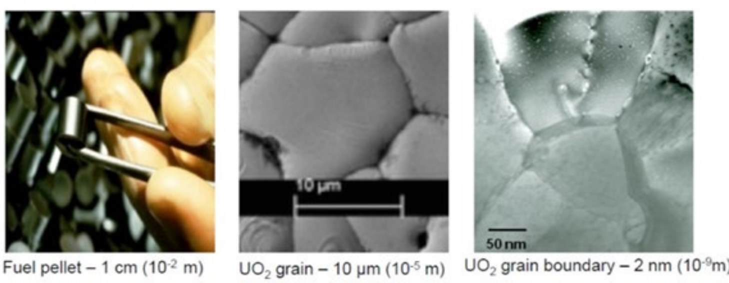


Figure 25: *A picture of a typical nuclear fuel pellet (left) and its micro-grain structures and grain boundaries (right two images) as imaged by electron microscope*

NSLS-II plans to work with the nuclear energy community and DOE Nuclear Energy to address these critical challenges in the nuclear materials and systems. Specifically, in collaboration with the BNL Department of Nuclear Science and Technology (NST) and in partnership with Idaho National Laboratory (INL), NSLS-II proposes developing a dedicated Materials in Radiation Environments (MRE) beamline based on a superconducting wiggler to enable *in-situ* multiscale imaging of radiochemistry and radiation-induced structural changes and degradation in a wide range of nuclear fuel and nuclear structural materials.

This unique facility would house three hard X-ray endstations – X-ray diffraction and diffraction tomography, X-ray spectromicroscopy, and full-field X-ray imaging in an external building of ~17,000 sq. ft. The external building will allow a self-contained secure environment to enable research on hot nuclear materials – from segments of actual fuel pellet to highly radioactive materials due to irradiation. In addition, the facility will house an ion accelerator to enable studies of these and other materials while they are being irradiated by ion radiation. Finally, discussions are ongoing with National Nuclear Security Administration (NNSA) to allow synchrotron studies of a special class of materials in a high-security experimental hutch that will be contained in the external building.

The current timeline for developing the MRE beamline is as follows. In FY17, we plan to

- Work with NST Department and establish a pilot partnership with Nuclear Science User Facility at INL to enable nuclear structural materials studies at the XPD beamline at NSLS-II. These studies will be conducted through an approved Partner User program with BNL/NST and INL/NSUF, and will be restricted to materials with no or minute radioactivity as allowed within the current NSLS-II safety envelope
- Participate in a research needs workshop in collaboration with INL to further refine the science case and define a few key science examples to showcase the MRE potential and support the MRE science case
- Advance the MRE scope definition and conceptual design, and mature cost and schedule estimates
- Work with INL and BNL-NST to present the MRE science case and seek CD-0 equivalent funding decision from DOE-NE.

In FY18, we plan to

- Implement and commission the NST partnership-supported XRD tomography set-up at the XPD beamline. Start science commissioning of this new capability. Develop and implement software tools to allow user-ready algorithms for 3D reconstructure and analysis.
- Complete the MRE conceptual design, and develop a refined cost and schedule in support of the potential CD-1 equivalent funding decision.
- Work with INL and BNL/NST to seek CD-1 equivalent decision from DOE-NE.
- Hold a community workshop on MRE to strengthen community support for the MRE beamline. This will be done in coordination with INL and DOE-NE.

In FY19-21, we anticipate to

- Start full general user operations on the XRD tomography at XPD. Fully operate the NSLS-II/NST/NSUF partnership including the XRD–tomography capability.

- Assuming go-ahead funding from DOE-NE, formally launch the MRE construction project, with CD-2 equivalent decision and CD-3a construction start for the external building by end of FY19.
- Progress MRE construction through FY21, with final design review of the technical beamline in FY20, the beneficial occupancy of the MRE external building in FY21, and start of technical installation in early FY22. Possible project completion by end of FY23.
- Hold an Early Science workshop in FY21 to prepare the nuclear materials community to plan first science experiments at MRE.

Interagency Advanced Manufacturing Initiative. Advanced Manufacturing is an interagency national program primarily funded by the DoE, DoD, DoC, NSF, and NASA. So far DoE, DoD, and DoC have supported 14 National Network of Manufacturing Innovation (NNMI) Centers. 12 of these Centers are located in the East. NNMI Center topics relevant to soft and bio-nanomaterials include: fibers, polymer composites, flexible electronics, sensors, and bio-fabrication. 8 NNMI Centers were sponsored by the DoD, 5 by the DoE, and 1 by DoC (NIST). The 10-year goal in the initial Advanced Manufacturing proposal was 45 NNMI Centers. Each NNMI center involves ~$70M funding agency investment with matching funding from the center members.

As described in section 4.1.3, NSLS-II has a full complement of beamlines with techniques optimized to probe the structure and processing kinetics of the soft and biomaterials that are currently being additively manufactured into devices by the NNMI soft material centers. Moreover, BNL staff has been pursuing additive manufacturing relevant research. Specifically, NSLS-II staff have carried out in-situ X-ray characterization of solvent and gas-phase 2D printing, solvent annealing of cast films, and microfluidic flow dynamics while CFN researchers have pioneered approaches to direct the self-assembly of block-copolymers as well as selective infiltration synthesis approaches to transfer nanoscale polymer structures to inorganic materials (see **Figure 26**, and figure in Section 4.1.3). The CFN has also enhanced its additive fabrication capabilities with the installation of a *Nanoscribe* 3D laser printer that utilizes two-photon polymerization to rapidly fabricate nanostructures with optical quality surfaces and ~100 nm feature size. The complementary capabilities for fabrication, synthesis, and characterization offered by NSLS-II and CFN position BNL to be a key participant in the development of next-generation advanced manufacturing.

In order to realize this potential and explore ways for BNL to contribute to the National NNMI Program, NSLS-II partnered with NIST and AFRL to host an April 2016 round-table discussion with industrial participants from Kodak, IBM, Lockheed-Martin, Boeing, GE, Dow, and Dupont to identify what was needed for NSLS-II/CFN to impact one of the NNMI thrusts; namely, the manufacturing of flex hybrid electronics (FHE), the focus of a recently established DoD NextFlex NNMI center. A three-phase plan was developed and summarized in a meeting Report. The Report was endorsed by the industrial participants and will be submitted for inclusion on the *manufacturingusa.com* web site. Although the focus of the round-table discussions was FHE, the three-phase impact plan was structured to be more widely applicable to advanced manufacturing and forms the basis for our 5-year plan.

In FY17, we have pursued or plan to pursue the following:

- Identify and plan collaborative FHE thin film and 3d printing experiments with colleagues from NIST and the AFRL, and other round-table participants. The intent is to produce examples of how synchrotron techniques can be effectively applied to advanced manufacturing problems.
- In order to establish research teams, NSLS-II staff will visit NIST, the AFRL, and universities with advanced manufacturing centers with reciprocal visits to NSLS-II by potential team members. The AFRL group visited the NSLS-II in December 2016 and Pindak visited the AFRL in January 2017. The goal of these visits is collaborative advanced manufacturing proposals for NSLS-II beam time as well as to identify possible

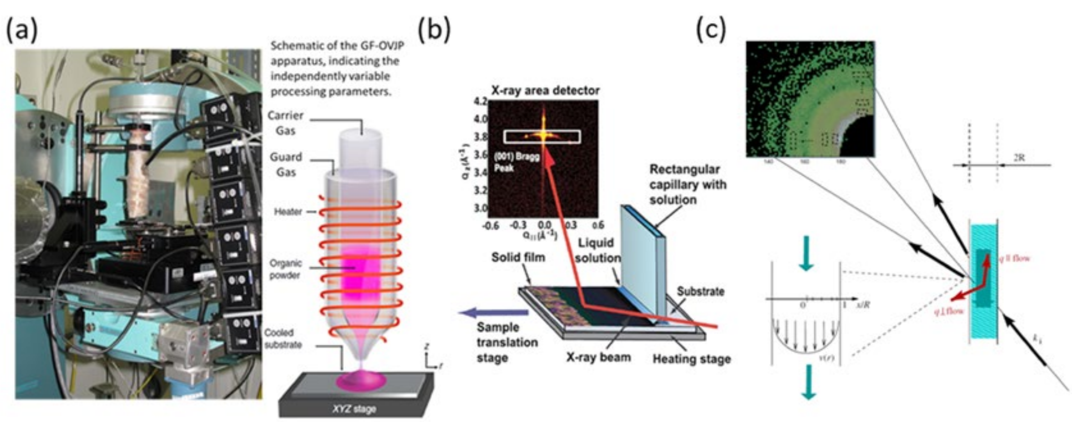


Figure 26: *In-situ X-ray studies of organic thin film processing and microfluidic flow: (a) Guard flow-enhanced organic vapor jet printing of pentacene [16]. (b) Capillary printing of TIPS-pentacene / toluene solution [17]. (c) Dynamics and rheology under continuous shear flow studied by x-ray photon correlation spectroscopy [18].*

jointly funded endstation upgrades justified by their potential advanced manufacturing impact. As a result of these visits, 7 AFRL proposals were submitted for beam time on 7 different NSLS-II beamlines and peer-reviewed with above-threshold proposal ratings. The proposed experiments will be carried out in the 2017-2 cycle. A similar visit is being planned to NIST prior to the next, May 31, NSLS-II proposal deadline. Successful collaborative projects and relevant in-house projects will be summarized on the NSLS-II Industrial Web Page and used in outreach presentations. They will also provide the foundation for future research proposals to the agencies supporting the advanced manufacturing initiative by demonstrating the potential impact of synchrotron measurements on advanced manufacturing.

- NSLS-II staff have attended a NextFlex consortium workshop and technical working group (TWG) meeting. TWG meetings are an opportunity to engage participants from small- and mid-size companies and to identify roadblocks to commercialization that occur when operating prototype manufacturing systems in a *production* environment that might be surmounted by in-situ studies on *laboratory* scale processing platforms at a synchrotron beamline. This will contribute to the ability of NSLS-II staff to write impactful proposals and optimize beamlines for industrial use and applied research.
- At the invitation of the Energy & Photon Sciences Directorate ALD, an Advanced Maunfacturing Working Group was established with Chuck Black (CFN) and Ron Pindak (NSLS-II) as co-chairs. The Advanced Manufacturing Working Group has equal representation from the NSLS-II and CFN and is initially charged with preparing a Report by April 1, 2017 that develops a research plan and identifies growth and funding opportunities for BNL in this area.

In FY 18, we plan to establish a BNL Advanced Manufacturing *Virtual Center* that will:

- Coordinate activities and provide advanced manufacturing industry a single point-of-contact.
- Promote the formation of teams of academic, industry, and government researchers to address issues in advanced manufacturing using existing funds and capabilities.
- Using expertise established from FY17 collaborative and in-house projects, develop processing platforms that can be installed on multiple beamlines for in-situ characterization during processing of soft materials.
- Evaluate the benefits and feasibility of a 'fee-based' consortium that supports activities with a clear return on investment to industry members with respect to information, education, experimental access and support. Use 'lessons learned' from the NIST nSOFT industrial consortium.
- Invite directors of other NNMIs to a workshop and present a case for the potential impact of synchrotron studies on advanced manufacturing.

In FY 19-21 we envision the following activities:

- Research teams will submit proposals to supporting agencies for additional endstation processing instrumentation and staffing for on-going and new advanced manufacturing beamline activities.
- The BNL advanced manufacturing *Virtual Center* membership will determine, based on experience in using the NSLS-II facility, a 5 year vision to advocate for critical capabilities. Critical capabilities might include a *dedicated* beamline for processing such as the Processing and Liquids Scattering (PLS) beamline described in section 4.2.2.
- The *Virtual Center* leadership will develop a white paper concept for management to engage respective funding agencies to structure an NNMI center call that is consistent with the establishment of an Advanced Manufacturing Center *adjacent to a synchrotron source* so relevant beamlines can be extended into a space adequate to accommodate prototype manufacturing systems in a *production* environment.

National Security. Advances in materials science and technology are a critical driving force that supports many areas of a strong national security. In recent years, there has been increasing interest in utilizing synchrotron light sources to help develop cutting-edge and multifunctional materials for sensing hazardous agents and for production of better suits to better protect our soldiers. The Defense Threat Reduction Agency (DTRA) has identified, as one of the R&D needs in chemical warfare agents, the better understanding of synthesis and in-situ characterization of multifunctional materials for the filtration, conversion, and decontamination of chemical agents and other battlefield contaminants under ambient conditions (**Figure 27**). Such research are often pre-classified R&D on e.g. chemical simulants, and thus can be and is being pursued by the broader scientific community.

Advanced characterization capabilities at NSLS-II match well with the DTRA research and development needs. For example, the in-situ/operando diffraction, spectroscopy, and ambient pressure photoemission capabilities at NSLS-II will allow study of novel materials & chemical conversion processes for chemical agents or simulants of interest, and the in-situ X-ray scattering capabilities can be used to monitor structure and morphology evolution during polymer synthesis with active-additives. In addition, DTRA research

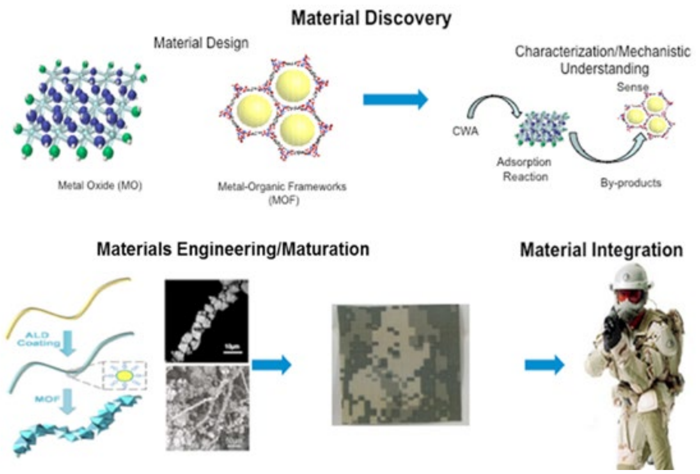


Figure 27: *Schematic illustration showing the R&D needs of making 'smart' protection suites for soldiers – able to absorb and neutralize chemical warfare agents – in addition to protection against weather elements (Figure courtesy of Chris Kawaski of Edgewood Chemical and Biological Center).*

needs in other areas, such as environmental and operational toxicology, aerosol and forensic science, enzymatic biological agents, shock-wave induced dynamics, etc., may be met with other NSLS-II capabilities in nanoprobe and microprobe fluorescence imaging, structural biology, and full-field X-ray imaging.

Recognizing this potential growth area of user science, NSLS-II plans to develop a partnership with DTRA and possibly with other Department of Defense service laboratories such as Naval Research Lab (NRL) and Army Research Lab (ARL) to enable and encourage defense related open research at NSLS-II. Specific activities are planned in a phased approach, as listed below.

In FY17 we plan to

- Work with BNL/Chemistry and DTRA Edgewood Chemical and Biological Center (ECBC) to engage the DTRA chemical and biological research community, through participation of DTRA science reviews and workshops, about using the capabilities and doing research at NSLS-II.
- Engage DTRA and ECBC management to discuss and develop a potential DTRA Consortium partnership, where DTRA would station DTRA-funded scientific staff at BNL and NSLS-II to promote defense related research and assist DTRA users to plan and execute synchrotron experiments at NSLS-II.
- Develop a Partner User Proposal for Phase-1 of this DTRA consortium partnership, which would focus on chemical materials research. With this partnership, Consortium member groups would gain access to in-depth, and wide-range of expertise in materials & chemical research using synchrotron techniques and associated analysis, to expertise to help plan, design, and optimize synchrotron experiments, and to beam time on suite of beamlines with range of capabilities (spectroscopy, diffraction, photoemission) through partner user agreement and general user access.
- Hold a community workshop to engage the broader community to discuss in detail the Phase-1 partnership, as well as potential enhancement of the partnership by expanding to include other capabilities.

In FY18, we plan to

- Implement Phase-1 DTRA partner user arrangement at the suite of spectroscopy beamlines (QAS, ISS, TES) and at XPD and CSX-2 AP-PES as needed.
- Working with DTRA/ECBC to expand the potential DTRA partnership to include structural biology beamlines at NSLS-II.
- Hold a second community workshop to focus on the molecular structural studies of biological agents using synchrotron X-rays.
- Work with DTRA to explore further interests in DoD service laboratories on using synchrotrons for their research, and identify a path forward to include these in the DTRA consortium.

In FY19-21, we will

- Continue to operate the two DTRA consortia at NSLS-II – one of chemical simulants and the other on biological simulants.
- Engage all DoD and possibly NNSA labs to discuss the potential for a large-scale, dedicated, secure research facility at NSLS-II for conducting defense-related research in a secure environment.

NASA Sample Characterization. In 2020, NASA will launch its next rover to Mars. Amongst other missions, this rover will collect soil samples for potential return to Earth. These samples will be amongst the most valuable scientific samples ever. They will be contained in Ti6Al4V alloy tubes, 0.52 mm thick (**Figure 28**). It will be imperative to understand as much as one can about the contents of those tubes, including chemical, elemental, morphological, crystallographic and biological mapping with as high a resolution

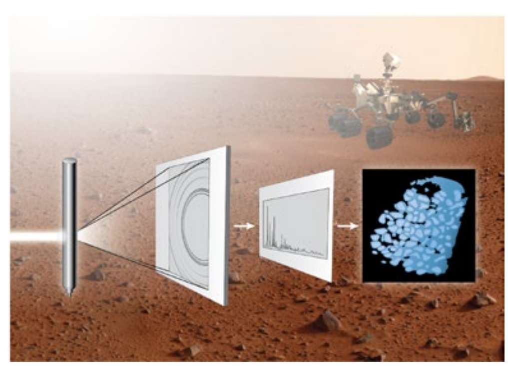


Figure 28: *Background; The Mars2020 rover collecting samples on the surface of Mars. Foreground; schematic of in-situ x-ray tomography experiments*

and sensitivity as possible, *without* opening them. The tubes will have to be contained in a very secure environment to prevent contamination from Earth-based compounds and to prevent anything biologically active escapting. There is a potential opportunity here for NSLS-II to build a unique facility for studying extra-terrestrial samples returned to Earth. Scientific interest in these samples would be almost unparalleled. The x-ray capabilities for studying these samples would be enabled by a high energy superconducting wiggler source and a remote endstation in a satellite building to contain the samples in a secure environment. We plan to work with key members of the community in this area to develop demonstration experiments and engage NASA to discuss this concept. Specific plans include the following:

In FY17-18, we plan to conduct test experiments on similar samples of NASA interest, including differential phase-contrast and phase contrast imaging. In addition, we will begin to develop x-ray Raman spectroscopy (XRS) for soft x-ray edges with hard x-ray photon energies and phase contrast imaging of biological cells *in-situ*; These will be demonstration experiments to form the basis for a LARS proposal. We will then develop a more detailed phased approach and outreach to NASA, concerning our strategy and approach.

In FY19, we anticipate to submit a proposal for NASA to obtain funding to contribute to an endstation (STXM). This may be followed in FY20 by a proposal for a Phase-1 NASA beamline (inside the ring building) that provides the key capabilities without the need for remote building, e.g. for comet and asteroid return missions. If funding application is successful, such a beamline would take four years to build.

Finally, in the 5-10 year timeframe, if the early steps are successful, we would anticipate submitting a proposal to NASA for a full-scale facility for the NASA mission.

Puerto Rico/Caribbean Regional Alliance at NSLS-II. There exists an increasingly active scientific community in the Caribbean region that is interested in accessing synchrotrons for their research. Led by several institutions in the US territories – University of Puerto Rico and University of Virgin Island, and potentially by Cuban institutions in the near future, their research interests are well aligned with NSLS-II strategic directions, in energy science, chemical catalysis, materials synthesis, environmental science, and molecular and pharmaceutical biology. Due to historical and sociogeographical ties, this community has close connections to the eastern US, and NSLS-II is well positioned to benefit from these connections that will bring resources and diverse research projects and enrich the research environment at NSLS-II.

An initial effort to establish a Puerto Rico – BNL/NSLS-II Alliance is underway through University of Puerto Rico (UPR), and may expand to other Caribbean countries if successful. The alliance aims to facilitate access to the expertise and the beamline facilities at NSLS-II to allow Puerto-Rican scientists in academia and industry to use the synchrotron for their research in drug discovery, structural elucidation of proteins, and characterization of nanomaterials at the nanoscale level. As part of this proposed Alliance, Puerto Rico will identify and recruit a Puerto Rico scientist to be stationed at NSLS-II in the area of structural biology. This resident scientist will be fully integrated into the Life Science and Biomedical Technology Research Center at NSLS-II (LSBR) and will assist Puerto Rico users in proposal writing, experiment planning and execution, as well as data analysis and outreach activities.

It is expected that a new funding proposal for the Alliance will be submitted in FY17-18 to Puerto Rico science foundation, and if successful, a UPR-funded scientist will start at NSLS-II to start this program. A potential larger workshop for the Alliance may be held at BNL in late FY18 to facilitate discussions of specific research projects among PR researchers and NSLS-II staff, and the executions of these research projects may start after the reviews by the NSLS-II general user proposal review panels.

8 USER SERVICES AND OUTREACH

The NSLS supported over 57,000 users in its lifetime and was built with a tradition of strong partnerships between universities, industries, government agencies. The success of NSLS-II will depend upon a similar tradition of strong relationships with the user community.

8.1 USER ACCESS MODES

A critical element to the success of NSLS-II is a clear, flexible system for user access to the facility. As a new facility, NSLS-II has the opportunity to evaluate success of the more traditional access modes worldwide and to implement new modes of access that are amenable to what scientists need and expect from a synchrotron facility today.

At NSLS-II, two principles underlie all user access to beam time. The first is that it is based on proposals that are subjected to peer review that is fair, clear, and expedient, that is sensitive to the needs of users, and that recognizes contributions that improve the overall scientific program. The second is that all proposals receive a finite amount of beam time for a limited duration that is justified by the need for beam time of the proposed work.

Current modes

Under this policy, NSLS-II currently accepts traditional **General User** proposals with deadlines three times per year. These proposals are valid for one year. The facility also accepts **Partner User** proposals for researchers that will partner with the facility to develop a cutting-edge capability for the user community. Recently, new modes of access including **Rapid Access, Proprietary,** and **Block Allocation Groups (BAGs)** have been implemented. For users with a quick, routine experiment to perform, Rapid Access proposals provide a quick turnaround time (~1-2 weeks). For large groups of users that want to share a small block of beam time (typically >3 groups sharing a few days), BAG proposals provide a means for these groups to manage their time allocation. Proprietary proposals are used by researchers, typically companies, which want to retain the IP rights to their data by paying a full-cost recovery fee for their beam time. More information on the existing modes of user access can be found here.

New modes

But in today's fast-paced, internet-savvy age, users may not want/need to access the facility at all. For this reason, mail-in and remote access proposal types are desirable.

- **Mail-in:** For routine samples and straightforward measurements, users can ship samples to the facility and have data collected by the beamline staff. This will likely require more staff resources, but the efficiency of data collection will clearly be improved. In cases where users require data processing or analysis too, NSLS-II is exploring the use of BNL's new Technical Service Agreement (TSA) as a way to implement this fee-for-service to cover the incremental cost associated with such work.
- **Remote access:** with standard samples and sufficient automation at the beamline, users can control their experiments without traveling to the facility. This has

become an expected mode of operation for structural biology at other facilities, and it can be extended to other techniques (e.g. XAS, XRD) at NSLS-II.

In addition, other modes of user access are being discussed that would be unique to NSLS-II and provide alternative, flexible modes of access for users.

- **Multi-beamline and multi-facility:** Currently, users must write multiple proposals if they wish to access different beamlines (or other facilities such as CFN) for their single project. This new mode of access would allow users to submit one proposal that focuses on their scientific research problem and can propose the use of multiple beamlines/facilities to accomplish the stated goals.
- **Current-cycle access for GUs:** In this mode of operation, a user would submit a proposal that would be reviewed and scored through the traditional GU review process. The proposal would be good for 1 year and have a finite amount of beam time allocated for the work. But the user could submit beam time requests at any time for this proposal, i.e. at the regular proposal deadlines for the next cycle, and/or for the current cycle. The user could also submit more than one BTR for the same cycle.

User Portal

In order to facilitate user access to NSLS-II, we are developing an online User Portal where user can have one-stop access to their proposals, safety approval forms, training information, appointment status, publications, and beamline data. Synchrotrons around the world have already instituted such systems, which are coming to be expected by the user community. At NSLS-II, the Proposal, Allocation, Safety, and Scheduling (PASS) system is currently the electronic mechanism by which users request beam time. The system also includes the feasibility review by the beamline staff, scientific review and allocation by the Proposal Review Panel, and will soon include a rudimentary scheduling function. PASS also includes a fully functional Safety Approval Form system.

However, future improvements to PASS are necessary to make it a state-of-the-art system. Priorities include (1) a scheduling function, (2) links to user appointment status, training, and publications, (3) access to beamline data, (4) accommodation of rapid access (and rapid turnaround), and (5) multi-beamline/facility proposals. All of these improvements will require additional resources and time to establish smooth operations. In order to prioritize these goals and establish a realistic timeline, a PASS Steering Committee has been established.

Joint Access with other Facilities

NSLS-II has recently initiated a joint proposal process with ORNL for combined SAXS/SANS experiments. Users can submit proposals to either facility requesting both techniques. They are reviewed jointly and allocated time at both facilities if deemed appropriate. Similar arrangements may also be made for combined X-ray PDF and neutron PDF studies. We would like to initiate a similar program with the CFN at BNL, utilizing the PASS system. Other opportunities exist with EMSL at PNNL, cryoEM with CSHL, SBU, and/or NYSBC), and the MagLab at Florida State University.

Transition User Program

In order to provide former NSLS users with access to beam time during the build-up of the NSLS-II facility, NSLS-II has been coordinating with other DOE synchrotron facilities to make near-term arrangements, with committed resources and staffing, to support former NSLS users at the appropriate beamlines at these other facilities. Programs that have concluded operations and transitioned to operating NSLS-II beamlines include hard X-ray spectroscopy at SSRL (now at ISS and TES) and Macromolecular Crystallography at SSRL (now at FMX and AMX). Programs that will continue in FY17 include transmission X-ray microscopy at APS (to move to FXI in FY18), energy dispersive X-ray diffraction at APS (to move to HEX in ~FY21), and infrared micro-spectroscopy (no planned destination to date). We anticipate that each of these continuing programs will seize operations when the respective capability becomes available at NSLS-II.

8.2 EDUCATION AND OUTREACH

As a new facility, all users at NSLS-II require significant training, regardless of their experience with synchrotron techniques. Some users are completely new to synchrotron radiation altogether, and others have used other synchrotron facilities and just need to be trained on the NSLS-II equipment. Combined with the sophisticated nature of the NSLS-II beamlines, we will need to enhance our education and training effort to ensure that the new and inexperienced users can make effective use of the allocated beamtime. Specifically, we will enhance our education effort by providing short courses beyond the general introduction of experimental techniques. These courses will target students or researchers who are interested in specific scientific problem, and tailor the training for them. The combination of lecture and hands-on exercises will allow the students or research meet the experts in the field and beamline staff, as well as become familiar with beamline instrumentation.

Outreach to Potential New Communities: NSLS-II will pursue a coordinated effort to outreach to potential new communities that have not been traditional users of synchrotrons. This coordinated effort has two related approaches.

First and foremost, our main strategy is a bottom-up outreach activities by NSLS-II scientific staff. Equipped with the most up-to-date information about our scientific capabilities and broad scientific knowledge about how NSLS-II can help solve problems in research, our staff can best engage in fruitful conversations with potential new users at conferences and meetings and develop relevant collaborations between NSLS-II and the individual users. The best way in this outreach approach is for our scientific staff to attend topical meetings that are *not* focused on synchrotron applications.

Our second approach is to develop strategic engagements with a segment of the scientific community that may have heard about synchrotrons and are interested in learning more about its usage for their research. This type of outreach may occur at the levels of NSLS-II scientific groups or programs or management, and may require more concerted and coordinated efforts and exploration to develop into real research projects. Typically this type of outreach will quickly involve a larger topical workshop that will involve key stakeholders to discuss specific research directions in this segment of the community.

Combining these two approaches is an effective way to reach out to potential new communities. An ongoing example is a discussion with fashion industry. In this area, smart clothing is an emerging research field with topics such as materials for innovative fabrics, wearable sensors, and 3D printed/integrated devices. Research on these new materials and processes can greatly benefit from utilizing synchrotron x-ray methods at NSLS-II. Joint research opportunities between Fashion Institute of Technology, Stony Brook University and Brookhaven National Laboratory are being explored

InCREASE Consortium: The Interdisciplinary Consortium for Research and Educational Access in Science and Engineering (InCREASE) is a consortium of university professors from Minority Serving Institutions and minority professors from other higher Institutions of Learning, whose mission is to promote research and education, especially as regards increasing their utilization of national user facilities, thereby increasing the numbers of women and those from historically underrepresented groups who pursue science and engineering careers and collaborate together in scientific research to expand their research capabilities. NSLS-II has been actively involved in this initiative and has been working with InCREASE and its members to promote research done at the DOE scientific user facilities especially at NSLS-II at BNL.

NSLS-II plans to continue this effort in the next five years, with the following specific tasks. First, NSLS-II will expand the graduate course and lectures on synchrotron science and technology to InCREASE institutions, most likely through live video conferences broadcasted at the participating institutions. Second, NSLS-II will coordinate with InCREASE and other facilities to hold a series of science workshops at NSLS-II and at other DOE light source facilities as a forum to promote discussions InCREASE faculties and NSLS-II beamline scientists. Finally, NSLS-II will continue to leverage other available resources such as the Alliance for Graduate Education and the Professoriate - Transformation (AGEP-T) to attract and host postdocs from under-represented communities to come to NSLS-II and use the state-of-the-art instruments for their research.

Synchrotron Schools/Courses/Lectures: NSLS-II currently has a few small initiatives in education and outreach, but these need to grow as the facility matures in order to attract and train more users. One current program at NSLS-II is a "traveling" one-semester course that has been taught by multiple NSLS-II and CFN staff at Columbia, Yale, and Stony Brook. This course is suitable for graduate students, postdocs, and advanced undergrads in physical sciences and engineering, as well as students in the life sciences who have a relatively strong background in physics. Each class is given by a scientist from NSLS-II or CFN on the topic of his/her expertise. Lectures focus on advanced concepts in synchrotron x-ray and electron-based methodologies for studies of novel materials at the nanometer to atomic scales. Emphasis is on applying fundamental knowledge of these advanced techniques to real-world materials studies in a variety of scientific disciplines. In the upcoming years, we plan to get the course materials online for the entire synchrotron community at large, and also plan to run this school at more neighboring universities each year.

Related to this, Stony Brook University offers several other courses to its students that are interested in synchrotron science. Specifically, the Geosciences department offers a similar course for eight weeks once a year that is targeted to the interests or geoscience students.

NSLS-II will consider holding a school at BNL with hands-on opportunities to use the beamlines. Other synchrotrons currently have similar programs, where the most well-known is probably the 1-month-long HERCULES school in Europe for neutron and synchrotron techniques. All of the U.S. synchrotrons have similar programs focused on certain techniques and/or research areas. NSLS-II is pursuing partnering with the other facilities for this purpose.

High School Teachers and Students: NSLS had a unique program called Introducing Synchrotrons into the Classroom (InSynC) that trained local Long Island high school teachers about synchrotron techniques and offer them and their students the opportunity to perform experiments at the facility through a targeted proposal process. This program trained dozens of teachers and hundreds of students had the opportunity to experience synchrotron experiments either in-person or remotely. Since the inception of InSynC, the trained teachers have formed a network across Long Island and continue to bring in new teachers and projects to the program and there is strong interest in continuing the progam at NSLS-II.

The primary value of this program was to promote community outreach and to train teachers and students for the design and execution of hypothesis-driven experiments. This program required very little beam time (approximately 1 day per cycle on 3 beamlines for "routine" experiments) but can be very time-consuming to the beamline staff who have to dedicate much more time for the experiment design, data collection, data analysis, and interpretation of the results. Thus, to maximize its benefit, the program will use only those routine techniques that involve quick and straightforward data collection and require minimal data analysis, such as X-ray fluorescence microscopy, infrared micro-spectroscopy, X-ray absorption spectroscopy, X-ray powder diffraction, and macromolecular crystallography.

In the summer of FY16, the first workshop for high school teachers was held at BNL. It was jointly hosted by NSLS-II and the Office of Educational Programs. The first beam time proposals from these teachers were received in September 2016 and 3 were awarded beam time in the Jan-Apr 2017 cycle. A second workshop will be held at the 2017 NSLS-II/CFN Users Meeting in order to attract more teachers and school administrators. To date, the program has not been officially "launched" or even advertised. If the program is to be reinitiated at NSLS-II, in FY17 it needs to be formalized as part of the User Access Policy and measurable deliverables for success need to be defined. Related to this, resources need to be set aside and the possibility of outside funding pursued.

8.3 USER AMENITIES

A new user's experience with NSLS-II usually begins through interactions with another scientist, whether it be a collaborator, colleague, or indirectly through a publication or scientific website. But after the interest is sparked, it's our responsibility to ensure that the user's path to successful science is efficient and 100% positive. This begins, first and foremost, by ensuring that NSLS-II can address the question(s) the user needs to answer and how this would best be accomplished. Thus, even before a beam time proposal is written, a new user would discuss his/her experiments with the appropriate scientist(s). Thus, we plan for every beamline to have at least one point of contact for new users. NSLS-II facility will also consider having a "hotline" list of scientific staff that can field questions in particular scientific areas. Then when a "cold call" comes into the Users Office, they will be knowledgeable about where to direct the call. At this stage, it's imperative that the beamline staff know about the beam time proposal process, i.e. the types of proposals, how review is done, beam time allocation, etc.

Once beam time is allocated, the beam time experience should be smooth and satisfying to the user. To date, we have identified several bottlenecks that hinder this experience and have devised plans to address them. These include:

- *The online registration (GIS) form* is cryptic and confusing. Simplification of the form will be our long term goal, and we plan to provide simple web instructions in the short term.
- *Multiple check-ins:* New users currently must stop at the main gate trailer (for temporary badge), Bldg 400 (for actual badge), and NSLS-II User Administration (for key card and TLD) prior to going to the beamline. This process wastes a lot of time for the users and can be streamlined so he/she only needs to make one stop prior to the beamline. NSLS-II is currently developing a plan such that all of the abovementioned functions can be carried out in Bldg 400, and making this happen is a priority for FY17. In addition, since the users will not be stopping at User Admin, the BNL Guests, Users, and Visitors (GUV) center will become familiar with all of the beamline locations at NSLS-II and the front-desk admins at NSLS-II will be educated in welcoming users.
- *User accounts and passwords:* Currently users need 3 different passwords to work at NSLS-II; they need a PASS account for all proposals/safety information and both a BNL domain account and a NSLS-II network account to collect data at a beamline and retrieve/analyze their data in the future. A goal for FY17-18 should be to minimize the number of accounts, ideally to just one.
- *User amenities:* The accommodations and food services at BNL are subpar compared to all other DOE synchrotrons and desperately need to be improved. This should happen with the development of Discovery Park, but this is years away. In the meantime, one noticeable improvement is the opening of the 24-hour Mini Market in the NSLS-II main lobby. This is a self-service market that provides access to sandwiches, soups, salads, microwavable foods, snacks, and drinks. In addition, steps can be taken to improve the amenities we have right now, but we should at least educate users regarding offsite amenities that may be more desirable. There are hotels, restaurants, grocery stores, and shopping malls all within a short distance of BNL, but many of the users are unaware of them.

9 OPERATIONS EXCELLENCE

Creating a vibrant research environment includes having the staff, the support, and the infrastructure necessary for researchers to safely and effectively work at the NSLS-II facility. As an integral of the NSLS-II strategic plan for the next five years, this chapter describes the initiatives and the activities we plan to pursue in the following critical areas in workforce development, environmental safety and health and quality assurance (ESH&QA) programs, facility infrastructure, and communications.

9.1 WORKFORCE DEVELOPMENT

The NSLS-II has programs and processes in place to recruit the best talent and retain our dedicated staff, and to motivate and enable staff to achieve at the highest possible level. Evaluating and planning for the needs in future activities and preparing employees for positions of greater or different responsibilities is essential to the development of our quality workforce. Our programs and processes in workforce development reinforce our values and instill a culture consistent with those values.

Meeting Evolving Needs. As of March 2017, the NSLS-II Department is closing out major beamline construction activities funded by dedicated construction projects, and is starting to focus most of our efforts on ramping up and maturing accelerator operations and user science programs at our beamlines, with a small effort on continuing R&D in advanced accelerator and X-ray technologies as well as on development of future beamlines. This is a very dynamic environment, with significant on-demand staffing flows among different parts of our effort as needs evolve. The workforce and the way it is organized must easily adapt to the different requirements for these evolving endeavors. The Department is organized by divisions with individuals in those divisions matrixing their efforts to both operations and development activities. Updates and adjustments on partitioning of the individuals efforts are discussed and made at periodic staffing meetings. We plan to continue to pursue this approach and proactively monitor the evolving needs and implement necessary changes.

Diversity & Inclusion. NSLS-II recognizes the strength associated with a diverse staff and user population and is committed to create an inclusive environment for people of all backgrounds, gender, and ethnicity. Here we outline initiatives that will support these goals.

(1) *Promote leadership awareness & education:* In collaboration with the laboratory-wide Diversity & Inclusion (D&I) initiative, NSLS-II will be early adopters of the initiative and provided input to the overall strategy. This includes:

- Continue implicit bias education for supervisors and above using short educational videos, talking points and tools from Steve Robbins and Caroline Simard/Clayman Institute. The aim is to reduce unconscious bias as it relates to recruitment, candidate selection, and to improve the environment for women and underrepresented minorities.
- Develop/Implement hiring model incorporating processes and practices from other DOE Laboratories (e.g. SLAC's Smart Hiring Model). We will include the BNL model once developed and approved.

(2) *Increase representation and inclusion of women and underrepresented minorities* in management, scientific and engineering job classifications:

- Human resources manager will provide the NSLS-II management team with semi-annual underutilization workforce demographics, with a view to spotting trends and highlighting problem areas that need attention.
- Human resources manager will provide the NSLS-II management team semi-annual data that monitor hiring, promotional activity, appraisal ratings, and award nominees to ensure that we are fair and inclusive of all employees.
- NSLS-II will require at least *one* D&I goal for Division Directors, Group Leaders, and Program Managers. Examples include how they plan to increase awareness in their groups, or outreach to partner with universities who have a high number of women or underrepresented minorities in a specific scientific program. This could include a specific level of engagement in the BNL-wide initiatives listed above of education/awareness or the structured hiring process.

Career Development. NSLS-II considers its talented and enthusiastic staff as the single most important asset of the facility. As a newly developed synchrotron facility, NSLS-II has been able to attract many high-quality and expert staff to join our facility and the continued career development of our staff as we ramp-up and mature science programs is a critical aspect of NSLS-II facility operations. Recognizing this need of talent management, NSLS-II will implement a staff career development plan that includes the following elements.

- *Leadership Training:* Human resources manager will provide the NSLS-II management team, semi-annually, data on current employee leadership training, including what is available, who has participated, plans for future employee training. NSLS-II management will review this data and will discuss and nominate appropriate staff members to participate in these leadership training opportunities as part of their career development.
- *Scientific Staff Promotions:* Following BNL guidelines for scientific staff promotions, and recognizing the special situations in balancing scientific and support activities, NSLS-II has developed, implemented in FY17, a more optimized scientific staff review (SSR) process. The new SSR process clarified the case for permanent employment at the level of continuing appointment at NSLS-II, before tenure cases are considered. It has the benefit of strengthened employee/supervisor relationships, and better alignments with staff career development needs and with our mission.
- *Cross-training for Professional and Technical Staff:* Evolving programmatic needs require evolving skills set from our technical and professional staff. NSLS-II plans to continue to explore the opportunities for technicians and engineers to work in or to provide project support in other areas within NSLS-II or BNL. The aim is to encourage skill development, expansion, and employee engagement.
- *Mentoring:* BNL has a Laboratory-wide mentoring program that allows a non-supervisory mentor to interact closely with an employee outside the person's management chain. The mentor may provide useful advices to the employee's career development from a more neutral point of view. NSLS-II strongly supports this program. The human resources manager for NSLS-II will provide the NSLS-II management team the details on who has participated in the mentor program, as well as plans for others who should participate in FY17.
- *Exchange Program for Scientific Staff:* NSLS-II scientific staff spend most of their time at a single beamline and become experts in this area. However, most research programs nowadays utilize more than one technique and it would be beneficial to our staff to be knowledgeable across synchrotron techniques, especially those that are commonly used in their research area of interest. Therefore, as a continuing education effort for our staff, and a new way to cross-train staff and users, we will initiate an exchange program that swaps beamline staff for a few months or up to one year. During this time, the staff would get a different perspective on how a beamline is operated, learn a new technique, experience different beamline software and controls, and contribute their own experiences from their beamline. This would be implemented through changes to the staff R2A2 that reflect the new beamline tasks and responsibilities.
- *Postdoc and Graduate Student program:* In order for NSLS-II staff to have time to maintain their own scientific research program, they need help from students and/or postdocs. In addition, training of students and postdocs can provide added hands at the beamline and will help grow the experience workforce of the future. To be successful, the facility should have a reasonable number of students/postdocs so they can interact and learn from each other. The biggest challenge to having a team of students and postdocs is funding. Since this cannot readily come from the operating budget, staff are incentivized to find matching funds from other sources such as collaborators or LDRD. Programs such as this exist at ALS and SSRL and NSLS-II will investigate these programs and adopt and adapt them as appropriate.

Recruitment and Retention. NSLS-II will continue to develop hiring pipelines for areas of high needs. In partnership with historically black colleges and universities (HBCU) and Howard University, NSLS-II is currently discussing development of offering engineering and computing & controls internship opportunities to their students. This will not only help with our current needs but also enable recruitment pipelines for future hires.

We plan to expand outreach activities to attract a diverse applicant pool (see also D&I above), and partner with the BNL Diversity Office to engage in outreach with local universities to hire entry level controls employees. We will continue to develop and participate in the intern/student assistant program for summer 2017, including GEM students. The aim is to hire local students who could continue working during the school year. We are also investigating to expand such outreach effort to include co-op programs.

As discussed previously, we will continue to proactively identify future staffing needs. Currently we see the needs in the following areas:

- Beamline scientists - NSLS-II will continue to need beamline scientists in the three- to five-year timeframe who possess beamline experience at light sources/synchrotrons.
- Computer Scientists/Controls Engineers – Given the need for scientific computing capability to support the anticipated heavy demands for handling and analyzing the large data sets generated, NSLS-II will continue to need computer scientists with light source experience who have the ability to interpret data. The fact that there are a limited number of people having both the science and computing background with relevant experience in the synchrotron community poses a significant recruitment challenge.

Hiring of beamline and computer scientists will remain a major recruitment challenge because of the limited number of candidates with relevant experience and the intense competition for talent among the international synchrotron community. To address these challenges, NSLS-II will employ the following strategies:

- Promote and leverage the opportunity to work at NSLS-II with potential candidates because they will have the opportunity to build and design the beamline/scientific program on which they will want to ultimately conduct their research.
- Utilize incentive plans (sign-on supplements, relocation assistance, performance bonuses, retention bonuses) where appropriate to attract and retain staff.
- Proactively sponsor foreign national scientific staff for permanent residency.
- Support ways in which the controls group can have undergraduates begin working on an as-needed basis to increase conversion rates to regular staff post-degree.

9.2 ESH & QA

Every staff member, contractor, user, and guest has the right to go home at the end of the day without suffering injury or illness due to his or her work activities or the environment in which they perform work here at BNL. We must provide facilities that are designed and operated in accordance with safety and environmental requirements that are protective of people, the environment, property, information, and computing systems. Failure to maintain a safe and secure workplace with minimal environmental impacts can result in the unacceptable consequences of personal injury, illness, or death; property or information loss or damage; and fiscal penalties and criminal enforcement actions. Any of these can quickly and severely erode our ability to pursue and achieve our mission. Operating our facilities in full compliance with safety, environmental and security expectations brings a level of trust and support from our stakeholders that cannot be earned otherwise.

The risks and severity of accidents or environmental contamination are proportional to the nature, scale, and complexity of activities, supporting infrastructure, and the condition of physical facilities. Staff in the department currently engage in complex activities spread out over approximately 800,000 square feet of space which comprises our complex. As we ramp up operations of NSLS-II, we will grow to hosting thousands of users each year who will engage in complex and difficult experiments at our facilities, often under time pressure.

The NSLS-II Department is proud of its safety programs and resulting safety statistics. Accidents or events when they do occur are investigated to understand their cause and to ensure corrective actions not only address the event but also prevent the recurrence of future similar events. All events, no matter how small, are used as learning opportunities and where practical shared with other Laboratory and/or DOE facilities.

Success in ESH necessitates safety and environmental leadership, whereby all management and staff constantly look out for the well-being of their coworkers. In addition, managers and staff must understand the consequences and cost of failing to perform their work in an acceptable manner. Research and operations personnel must develop, own, and execute work in a manner that fully addresses compliance, safety, security, and environmental protection. Systems, processes, and tools for supporting work accomplishment must be designed to integrate the users' needs with clearly established ESH expectations. Rigorous work planning and control processes are key to ensuring all work is appropriately planned, hazards identified and mitigating measures implemented to reduce the potential for injury or environmental insults. The PASS is the tool used to ensure proposed experiments are evaluated and safety practices and controls are established before the users arrive on-site.

We continue to foster a positive and interactive relationship with our stakeholders and continue to exhibit demonstrated safety leadership. We will ensure that ESH competence is embedded within our organization and will create and manage our facilities in a safe, secure and environmentally friendly manner.

As the NSLS-II continues to build-out and mature, a standardized and rigorous Instrument Readiness Review process has been developed to ensure all beamlines or changes to the NSLS-II accelerator facilities have been designed, installed and will be operated safely and in accordance with Laboratory and NSLS-II requirements prior to being approved to move from construction to operations. This process has been developed and refined over the past two years and will be used as we build out the balance of the facility. It is a structured method for comprehensively verifying that the hardware and software, personnel, procedures, and management structures, systems and processes needed for commissioning or operations are ready to permit these activities to be undertaken in a safe, secure and environmentally sound manner. In the event of a significant change to the accelerator systems, the IRR is used to ensure its readiness for an Accelerator Readiness Review.

Integral to ESH is the NSLS-II Quality Assurance (QA) program. The QA program includes:

- Implementing QA procedures;
  - Design, procurement, inspection/test, nonconformance control, calibration, etc.
- Managing QA databases and tracking systems;
  - Family-Action Tracking System, Safety System Verification Recall System, Discrepancy Reporting System, Calibration Recall System, Fabrication/Installation Traveler processes, etc.
- Managing the contractor assurance program including the NSLS-II internal assessment program;
- Maintaining the NSLS-II lessons learned program;
- Maintaining a suspect/counterfeit item program;
- Managing and maintaining a robust document control and records management program to ensure that documents are prepared, reviewed, approved, issued, revised, etc. in accordance with DOE, BNL and NSLS-II records management requirements;

The QA program assures that purchased materials meet technical specifications, are tested in accordance with factory and in-house acceptance testing requirements and that all systems perform to their expected level. The QA program has been key to the build-up of the NSLS-II conventional and experimental facilities. Many of the QA program functions also serve to support the NSLS-II Readiness processes including the IRR and ARR processes.

In 2015, the majority of the ESH&Q programs transitioned to the centrally deployed services model with former NSLS-II staff becoming part of the central ESH&Q organizations. This staff was then matrixed back to NSLS-II through the use of Service Level Agreements. The deployed services model provides development opportunities for professional staff through short or long-term assignments with other BNL organizations while providing NSLS-II the ability to level-load resources to overcome slow periods or ramp up resources during busy periods.

Looking ahead to the next five years FY17-21, we anticipate that the needs for ESH & QA effort will stay more or less constant for NSLS-II operations. This expectation is informed by two factors. On the one hand, there are higher demands or needs on ESH &QA during the start-up phase of facility operations because majority of the operating and user activities are completely new to the facility and therefore require more attention, scrutiny, and review. On the other hand, while we expect significantly higher number of operating beamlines and visiting users in the coming years, majority of the cases that require ESH & QA attention would already become routine, allowing the ESH & QA to focus their effort to the small number of new cases that require more thorough ESH & QA reviews. These two factors will roughly balance out, leaving the demands more or less constant.

9.3 FACILITY INFRASTRUCTURE

Infrastructure is broadly defined for the purposes of this Plan to include all of the structures, systems and components needed to execute the NSLS-II mission. The NSLS-II infrastructure falls into two categories; *programmatic* and *conventional*. This section of the Plan will focus on the conventional infrastructure. Aspects of the programmatic infrastructure are covered in the previous sections.

The NSLS-II programmatic infrastructure consists of the accelerator, beamlines, other experimental equipment, and related controls, safety, communications and data systems. It includes conventional building systems that exclusively serve these systems structures and components. Operation, maintenance and modification of the *programmatic* infrastructure is planned, managed, and funded by NSLS-II directly. The conventional infrastructure includes the buildings and building systems, as well as the Laboratory's utilities central plants and associated distribution systems, including telephone service. The data infrastructure is covered separately in Chapter 5. NSLS-II pays for the use of these facilities and services through a monthly charge for space and metered utilities, General and Administrative (G&A) charges, and various allocations.

The overall infrastructure planning goals of the NSLS-II over the planning period are to (a) provide an infrastructure that supports excellence in operations, including best in class ESS&H performance, and world class construction project management performance, (b) ensure all required facilities, utilities, and services are available to support the NSLS-II mission when needed, and (c) maximize NSLS-II mission delivery by optimizing infrastructure life cycle costs, including further footprint reduction and energy conservation.

9.3.1 Conventional Space

The NSLS-II Department infrastructure consists primarily of the "NSLS-II" complex comprised of 9 buildings, Buildings 740-747 and 749. Space in 12 additional buildings is utilized for laboratories, offices, machine shops, assembly and test areas, storage and mechanical spaces at various locations across the Laboratory. Total billable space in use is 264,673 sf. Space not yet billed for by space charge on the B740 experimental floor is billed under a direct charge for maintenance ("Pay by the drink") agreement. Total annual space costs for the NSLS-II Department in FY17 are expected to be $6.9M. Space charges for the experimental floor in Building 740 are based on beamlines authorized for General User Operations and are apportioned based on (approx.) 1/60th of the total floor space ("a slice"). As space charges are added, the Direct Charges (Pay-by-the-drink) are proportionately reduced by a multiplier.

As of March 2017, of the five Lab Office Buildings (LOBs), LOBs 1 and 3 are fully built-out with all office/cubicle/conference/laboratory spaces finished and occupied. LOBs 4 and 5 have office/cubicles/conference spaces finished, but laboratories are shell space only. LOB 2 is all shell space. BNL has plans to buildout the remaining unfinished spaces in LOBs 2, 4 and 5 over the next 7 years through four IGPP projects. The total estimated cost of this effort is expected to be between $25 and $27M.

An FY16-18 IGPP project ($5.9M TEC) currently in design, will build out half the labs in LOB4 and 5. A follow-on project in FY18-20, ($5M) will build out all laboratory spaces in LOB 2. The next project in the sequence will be FY20-22 ($5.9M) and will build out the other half of labs in LOBs 4 and 5 and the final project, planned to start beyond the planning period FY 22-24 ($5.7M) will finish the office/cubicle/conference spaces in LOB2. See **Table 9.3A**.

Additional buildings for experimental facilities have been proposed to be developed adjacent to the Building 740 complex. These include experimental stations for the proposed Materials in Radiation Environment (MRE) and the High-energy Engineering X-ray (HEX) Beamlines and a proposed new building for a Cryogenic Electron Microscopy facility. Impacts on population and workstation demand have been included in this Plan. Other impacts will be evaluated as more information becomes available.

Office Space. The planning for space to support current and evolving mission needs at NSLS-II is focused on ensuring continuing delivery of high performance laboratory space and modern and efficient office space for staff and users as the buildout of NSLS-II continues.

As of the end of FY16, the NSLS-II Department had 417 permanent staff and contractors, a partner-user staff of 22, and a coincident user population of 18 (coincident users

Table 9.3A
IGPP LOB Buildout Program

Project	Scope	TEC	Schedule	Notes
LOB 4 Offices	½ office space and cubicles in LOB4	$3.9M	FY14-16	Completed
LOB 4/5 Labs	½ lab spaces in each building	$5.9M	FY16-18	In progress
LOB 2 Labs	All Lab spaces in LOB2	$5.0M	FY18-20	Storage relocation required Justification for IGPP use required
LOB 4/5 Labs	½ lab spaces in each building	$5.9M	FY20-22	Justification for IGPP use required
LOB 2 Offices	All office spaces in LOB2	$5.7M	FY22-24	Storage relocation required
Total		**$26.4M**		

are defined as the number of users at NSLS-II whenever the accelerator is delivering beam), for a total population of 457. Population is expected to grow over the planning period driven primarily by coincident user numbers that are expected to increase by more than a factor of 4, the addition of authorized beamline staff for new beamlines, and several new staff to support the increase in general user operations. Population in FY21 is expected to reach 557 people. See **Table 9.3B** below. Based on the Laboratory's IGPP program plan, no new office or cubicle space will become available within the planning period; the next expected addition to the workstation inventory will be in FY24 with the completion of the buildout of LOB 2 offices and cubicle space.

With the current population of 491, the office vacancy rate is 6%, with only a few offices open at any given time due to departures and reassignments. By contrast, 40% of cubicles are currently vacant. With offices being the preferred occupancy, it is expected that they will continue to have an occupancy rate of close to 100% throughout the planning period, with cubicle workstations absorbing the growth either by direct assignment of new staff to cubicles or staff being relocated from offices to cubicles to accommodate new staff and users.

For the purposes of this plan, the total population growth of 66 people (491 to 557) from FY17-21 is assumed to be in the B740 complex. Other office occupancies are expected to remain stable. The transition of 22 additional beamlines to General User Operations by FY19 (bringing the total to 28) will cause a rapid rise in the coincident user population, from 18 in FY16 to 84 by FY18. Several new beamline projects will begin in FY20-21.

With office occupancy effectively 100% at present, the total addition workstation need will have to be met by cubicles. The current inventory of vacant cubicles can meet the short term need, but will reduce the vacant cubicle count to 38 by FY21. See **Table 9.3C** below. Demand for additional offices will drive a reprioritization and reassignment of office space, and relocation of some people from offices to cubicles will be expected to be necessary as early as FY19. At an assumed pace of 3 new beamlines entering development each year, there will be a shortfall of workstations by late FY23.

Laboratory Space. NSLS-II has 46 laboratories in 7 buildings on site. See **Table 9.3D**. Currently, there are only 4 vacant laboratories, all located contiguously in the west wing of B703. All of the NSLS-II laboratory spaces are "owned" by the Laboratory and "leased" by NSLS-II. Their utilization is controlled by the BNL ALD for Facilities & Operations under a Facility Use Agreement and they are accessible for use by scientists working on various programs across BNL. NSLS-II staff manage the allocation of space within the laboratories to assure activities are within the Accelerator Safety Envelope for the facility and do not cause vibration issues that impact the accelerator.

Table 9.3B
NSLS-II Population Summary FY17-21

FY	NSLS-II Staff (including contractors)	Partner-Users	New Coincident Users (due to additional Beamlines)	Total Population
17	421	22	48	491
18	407	22	66	495
19	401	22	84	507
20	423	22	84	529
21	451	22	84	557

Table 9.3C
NSLS-II Work Station Demand FY17-24

FY	Workstations in Use (Demand)	Workstations Vacant (Cumulative)
17	420	87
18	435	72
19	439	68
20	451	56
21	469	38
22	483	24
23	502	5
24	522	-15

The IGPP project to build out LOB 2 offices will deliver 150-160 additional offices and cubicles, but not until late FY24 based on the current LOB Buildout plan. See Table 9.3A above. Any delay in the IGPP LOB2 Office Buildout project would require NSLS-II to relocate and expand into other office space at BNL remote from the NSLS-II by late FY23, resulting in significant operational inefficiencies and impacts on users. A smaller IGPP project to build out half of the office/cubicle space in LOB2 should be considered for funding earlier

Table 9.3D
NSLS-II Laboratory Inventory

Building	# Labs
421	4
463	4
535	2
703	14 (4 vacant)
741	10
743	10
832	2
Total	46

Table 9.3E
Incremental Laboratory Demand FY17-21

FY	Lab Needed B740 Complex			Number of Labs			Actions to Manage Shortfall
	Other BNL Scientist	NSLS-II staff & Users	AD Labs	Total Demand For Labs	Available Labs	Shortfall	
17	2	22	4	28	20	8	Secure and activate 10 labs in B703 West Wing and reallocate space
18	2	26	4	32	30	22	Secure 2 additional lab spaces in other directorate facilities (CFN, ISB, CMP)
19	3	30	4	37	40	3	None: 10 Labs added to B740 by IGPP project
20	3	30	4	37	40	3	None
21	3	32	4	39	40	1	None

For the purposes of this Plan, the current utilization of laboratories in other NSLS-II buildings is expected to continue unchanged. As a result, this Plan focuses on the forecasted incremental needs in the B740 complex. With 20 labs in use now, there is a small backlog of demand for laboratories in the LOBs from beamline staff and the Accelerator Division (AD). BNL multi-program scientist (non-NSLS-II) demand, estimated at 2 labs, is expected to increase to 3 by the end of the planning period. The 11 beamlines in General User Operations and the 17 under development or in commissioning are using the remaining 18 labs and that demand is expected to grow as the 17 remaining beamlines transition to receiving general users. That will create a demand for 30 labs by FY19. The Accelerator Division requires 4 lab spaces for assembly and test activities. As new beamlines begin development in FY 20-21, they will add demand for labs. As a result, the total demand for labs in the B740 complex will increase to 39 by FY21, an increase of 15 over present occupancy.

The FY16 LOB 4/5 laboratory buildout project (see **Table 9.3A**) is expected to deliver an additional 10 labs by the Summer of FY18, raising total lab availability in the B740 complex to 30 (and the NSLS-II total to 56). The follow-on IGPP project to build out LOB2 laboratories will further increase the lab inventory to 66 by late FY21. Both of these projects are essential to keep pace with the demand for laboratory spaces. In the interim, however, demand will exceed capacity by as many as 12 labs in FY18. Two options will be evaluated; secure and activate labs in the B703 west wing (10 additional labs) and utilizing available lab space in other directorate facilities. The analysis of laboratory demand and strategies to meet it are summarized in **Table 9.3E**.

Seminar and Conference Rooms. Utilization of NSLS-II conference spaces within the B740 complex is very high and the capacity of individual rooms is limited. There is no seminar room in the complex and one is currently needed. Construction of a new Seminar Room in LOB5 is estimated at $1M and would need to be funded by IGPP. However, current IGPP project priorities are to continue the LOB buildout program, so a Seminar Room project is not likely to be funded during the planning period. In the interim, other seminar spaces on site will need to be used.

Machine Shops. NSLS-II currently operates machine shops in 8 buildings and also routinely has work performed in the Central Fabrication Shop. All NSLS-II machine tools have been upgraded to comply with OSHA standards. Fabrication needs are expected to remain stable over the planning period.

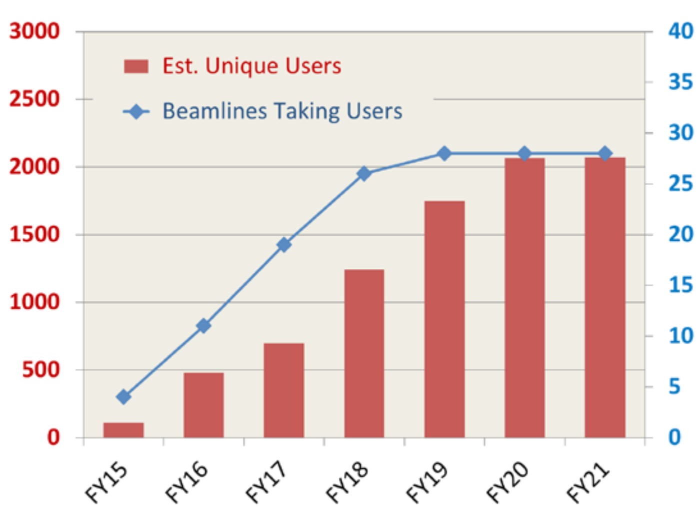
Test/Assembly/Cleaning Space. The Accelerator Division requires laboratory space in the B740 complex for assembly and test labs in LOB 4 (as described above under Laboratory Space). These needs may be accommodated in FY18 through activating the west wing labs in B703 and reallocating lab assignments. The cleaning facility at B945, and the assembly and test space at B832 will be adequate for expected needs through the planning period.

Stockroom and Storage Spaces. There is a dedicated stockroom off the B740 experimental floor that is currently ramping up its inventory. Full inventory should be reached by FY18. The space is marginal, but will suffice for the planning period. Future expansion will be needed in the form of a second stockroom as additional beamlines are built out and inventory quantity and diversity increases.

Storage space is in the process of being consolidated. Inventory in B820 will be reviewed and un-needed, obsolete equipment and materials will be discarded or excessed by the end of FY17. The remainder will be relocated to B729 which is being reconfigured from the Source Development Laboratory (SDL) to a storage and technician shop facility. The B729 conversion will be completed by the end of FY17. The relocation of NSLS-II Special Process Spares from B820 to LOB2 will occur in mid- FY17. Remaining equipment and materials will be relocated from B820 to B729 in late FY17.

User Housing. User housing demand is expected to grow as the coincident user number increases by over a factor of four over the planning period, and will continue beyond the planning period as beamline buildout continues. BNL's housing assets are managed by the Laboratory's Staff Services Division. Current plans are to retain the current housing stock that is predominantly WW-II wood frame structures until sufficient additional commercial capacity is developed as part of Discovery Park. Currently, 125 rental housing units are part of the Discovery Park plan with occupancy in early FY21. The Meadows at Yaphank development being constructed on the west side of William Floyd Parkway has developed rental housing that is already available for long term lease, and is expecting to host an extended-stay hotel with occupancy expected as early as FY18. With BNL maintaining its housing stock well into the middle of the planning period, housing capacity is not expected to be an issue. As commercial units displace BNL's housing stock, quality will improve significantly, but costs will also increase. This will be an issue for some members of the user community.

Table 9.3F
User Growth



User Population is expected to grow by > a factor of 2 over the planning period FY17-21

9.3.2 Utilities

Data. External network connectivity, storage needs, computational capacity and all related matters are discussed under other sections of this Plan. Fiber optic capacity within B740 is sufficient for the planning period and looped via separated routes for redundancy and greater reliability. Adequate data transmission exists between the former NSLS building (B725), which is planned to be converted to a computing center, and NSLS-II (B740) and B515. A planned cable between B725 and B515 has not yet been installed to complete the loop.

Electric Power. NSLS-II presently has a peak demand of 5.9 MW including chilled water loads estimated at 0.75 MW, and an annual consumption of 40,000 MWh. The principal components of demand are the power supplies for the accelerator magnets (1.8MW), RF (1.5MW), and HVAC (0.6MW). Electric power is supplied to the B740 complex by the Laboratory's 13.8kV distribution system. Emergency power is available from two 700kW diesel generators and provides for critical loads including the Control Room, RF building/Cryogenic Plant, sewage ejector pumps, storm water ejector pumps, Service Buildings HVAC, and LOB lighting and door locks. The generators have fuel storage capacity for two days of running. There is no emergency power available for the accelerator or beamlines; the machine would be shut down for the duration of a power failure.

Growth in load and peak demand is projected at approximately 5% per year as beamlines continue to come on line, operating hours rise to 5,000/year, and commissioning hours to 1,400/year by FY19. A 0.5MW step function in demand is expected when the 3rd RF cavity goes operational. This will result in a peak demand of 6.5MW and annual consumption of 59,000 kWh by the end of the planning period.

Power transmission capacity to NSLS-II will be sufficient through the planning period. Power is supplied to NSLS-II at 13.8kV from a dedicated 20/30MVA transformer (OA/FA) and feeder, both installed as part of the NSLS-II project. The feeder is constructed of two paralleled 1000 kcmil cables. For the present NSLS-II operating loads, one of the two cables is sufficient, however both will eventually be required as the load grows. This is not expected to occur during the planning period. Currently, under a fault condition in one of the cables, the paralleled cable could be used and down time would be limited to several hours. Sufficient spare cable and splice kits are on hand (in LOB2) to replace a damaged section of the faulted cable within a manhole or cables that may be damaged between manholes. An escalation in the cost of electric power, driven by a rise in fossil fuel prices, is an operational risk during the planning period.

The BNL Central Chilled Water Facility (CCWF) is fed by two single 30+ year old 13.8kV underground feeders, with no redundancy; capacity of both is required to sustain full operations. A loss of one feeder would significantly reduce chilled water production capacity and require chiller outages that could impact NSLS-II depending on site load at the time. Repair time is estimated to be several hours to several days depending upon the severity of failure.

Chilled Water and Compressed Air. NSLS-II chilled water and compressed air is supplied by the Laboratory's Central Chilled Water Facility (CCWF). The CCWF produces and distributes laboratory quality 125 psig compressed air from 3-750 cfm air compressors. The compressors are substantially underutilized at the present time, with only 1 in service. NSLS-II is supplied by a 4" compressed air service from the CCWF. The NSLS-II project paid for 2,500 tons of new chiller capacity in the CCWF. This capacity is available for current and future NSLS-II loads. The 740 complex also has a capacity of 190 tons of "Free cooling" using its cooling towers. Chilled water is provided to the B740 complex through 24" chilled water supply and return lines.

The NSLS-II cooling load is currently approx. 1,000 tons and is projected to rise to 1,500 tons by the end of the planning period. Providing NSLS-II's chilled water needs from the CCWF ensures "firm capacity" for NSLS-II loads due to the recent expansion of the plant to 11,000 tons, and the addition of a Chilled Water Storage Tank that provides 22,000 ton-hours of cooling. The tank can supply the site for up to 4 hours in the event the plant cannot operate. NSLS-II also has the design capacity to achieve 190 tons through "Free cooling" using its cooling tower, however, operational experience shows this is difficult to achieve under many weather conditions. CCWF capacity can handle all anticipated NSLS-II chilled water and compressed air loads during the planning period, with sufficient reserve/firm capacity.

Steam, Potable Water, Sewage Collection. Steam at 125 psig is provided to the B740 complex and most other NSLS-II Department buildings for heating and hot water generation. Potable water is supplied to all NSLS-II buildings by the Laboratory's water distribution system. Sanitary sewage and storm water collection systems service the NSLS-II complex and other Department facilities. Industrial and hazardous wastes are analyzed for proper disposal pathways and are either discharged into the sewage collection system or collected and packaged as hazardous or radioactive waste. The Laboratory's infrastructure plans will ensure high reliability and sufficient capacity for NSLS-II needs over the planning period.

9.3.3 Roads and Grounds

Access Roads. NSLS-II Department buildings are served by the Laboratory's roadways, primarily laid out in a grid pattern, except in the vicinity of the accelerators and other specialized facilities. The NSLS-II 740 complex is serviced by internal and external ring roads fed off the Laboratory network. The condition of the north access road to LOB2 is very poor. Repaving will be required prior to the completion of LOB2 labs in FY20.

Parking at the B740 complex is provided primarily by parking lots serving the five Lab Office Buildings (LOBs). Total capacity of the LOB lots is 861 spaces. LOB1 has larger parking capacity since its lot was planned to support the Central Office Building that was deleted from the NSLS-II project scope. The other main NSLS-II office space location is Building 703 which is served by a dedicated parking lot with a capacity of 68 parking spaces. Outlying buildings typically have small lots but they are adequate for the limited population of those facilities.

Current observations of parking space utilization correlate well with population numbers. The average utilization ranges from 30-70% for the built out LOBs, and 13% for B703, based on observations over the course of a typical work week. Peak utilization typically occurs during meetings, conferences, and reviews when people from other institutions or BNL organizations utilize the lots and NSLS-II people from other NSLS-II buildings travel to in-briefings and closeouts. Peak utilization which exceeds 100% occurs about 5% of the time and is most acute at B703.

Sufficient aggregate parking capacity exists to support the forecasted 20% population growth over the planning period, but inconvenience will likely be a factor as early as FY19, since the majority of current reserve capacity exists at LOBs 1 and 2. Buildout of labs in LOB2 by FY20 will increase the parking demand at LOB2 lot, but that lot has sufficient reserve capacity. Construction of the Cryo-EM facility will impact the parking lot at LOB5 during construction and may require a temporary lot to be constructed.

Landscaping. A comprehensive Landscaping Plan has been developed by F&O for the B740 complex. The first in a series of landscaping projects was completed at the B740 entry in FY16, co-funded by the NSLS-II Users Committee and F&O. F&O budget reductions may impact their ability to support an annual landscaping project.

9.4 COMMUNICATIONS

As NSLS-II matures, communications and engagement with key internal and external stakeholders will be key as we seek to attract new and returning users and report on the accomplishments of the facility to DOE and other funding agencies, the media, elected officials, policymakers, and the general public. These communications and engagement activities will take multiple forms and will be tailored to these audiences based on best practices and available resources. The primary communication goals at NSLS-II include:

- Raising the profile of NSLS-II and its mission, vision, capabilities, advances, and initiatives among key audiences, including potential visiting researchers, the synchrotron science community, internal stakeholders, and policy makers.
- Communicating to key audiences about NSLS-II's scientific advances, personnel, capabilities, news, and developments through the production of news releases and feature stories; activity and progress reports; periodic internal and external newsletters; web content; and brochures and promotional materials in electronic, web-based, and hard-copy formats.

Existing and new products that will support these goals include:

- Press releases on NSLS-II's high-profile science publications and major milestones to raise awareness of the cutting-edge science funded by DOE and other sponsors.
- Feature articles on NSLS-II's staff and users to attract potential users and make them aware of the in-house expertise, scientific programs, and capabilities available at NSLS-II.
- Brochures, fact sheets, videos, and other materials intended to attract users and provide key information on NSLS-II to elected officials, policymakers, potential collaborators and partners, and the public.
- Web content, news syndication, and site maintenance to ensure pages are current and serving key audiences, both internal and external.
- Newsletters: Bi-monthly internal staff newsletter and quarterly user newsletter to keep staff and users engaged and informed about NSLS-II developments.
- DOE reports/science highlights to keep DOE and other customers informed on the progress of beamlines and science at NSLS-II.
- Major events support: Promoting, coordinating, and reporting on major events including VIP visits (e.g. Secretary of Energy) and key milestones/celebrations.
- Conference messaging: Selection and production of appropriate fact sheets, brochures, and other promotional materials for outreach purposes, including both BNL-hosted conferences and those at external venues.
- Media outreach: Arranging media tours and access for film crews, pitching news stories and responding to media requests, and conducting media training for NSLS-II staff.
- Public outreach: Ensuring NSLS-II is highlighted in the Lab's public outreach programs, including Summer Sundays, PubSci, Science on Screen, National Lab Day, the World Science Festival, and Maker Faire.
- Social media: Showcasing NSLS-II science and scientists (both staff and users) on Brookhaven's social media platforms, including Twitter, Facebook, Instagram, YouTube, and Tumblr.

NSLS-II currently funds one full-time communications position, which is expected to be filled in FY17. This position will focus on Photon Sciences staff and user communications and engagement activities (for existing users), DOE reporting, and outreach to potential users and industrial/ academic/government partners. This position will be augmented by freelance writing support (0.25 FTE), as well as resources within the BNL's Media and Communications Office (focusing on communications to media, the general public, and elected officials).

10 SUMMARY AND OUTLOOK

The next five years will be exciting times for NSLS-II and our community as we ramp up our accelerator and beamline operations, develop and mature our strategic science programs and communities, and conduct innovative research and produce results with high scientific and societal impact. Through all these activities as the first low-emittance storage-ring light source, NSLS-II will play a key leadership role in the synchrotron community in advancing high-brightness synchrotron technology and associated R&D, in pioneering high-brightness science to address challenging problems in the society, and in cultivating and developing the ever evolving scientific community to maximize the scientific impact of high-brightness synchrotrons.

This Five-Year Strategic Plan summarizes our vision, strategy, and approach, our strategic science directions and crosscutting development themes, our facility and beamline development plans to meet the science needs, and our initiatives to facilitate and enhance the impact of NSLS-II.

For the next five years, our strategic goals are:

- Ramp accelerator to full performance of 500 mA and > 95% reliability and continue to develop accelerator to improve brightness and stability for user program
- Develop and mature science programs and associated user communities and partnerships in areas strategic to NSLS-II mission
- Complete the beamlines currently under construction and transition them into user programs
- Begin development of additional beamlines consistent with strategic direction of facility
- Advance R&D critical to meeting the research needs of NSLS-II and the DOE scientific user facilities mission
- Develop data architecture, including analysis, to optimize productivity for the user community
- Achieve operational excellence in all aspects of facility operations.

We look forward to working with our community and stakeholders to make these goals a reality.

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APPENDIX 1

2017 NSLS-II Five Year Strategic Plan — Planning Assumptions

Assumptions for the planning period (FY17-21) for NSLS-II are:

- The accelerator will routinely operate at 350mA by end FY17 assuming new ceramic chambers work. This will continue FY18-19 until overheating issues are resolved. Then operations will deliver 400mA. Full design beam current of 500mA will be routinely delivered by the end of FY20 with a present set of beamlines (28 BLs)
- The third SCRF cavity will be installed and operational by FY20: requires ~$2.2M each year burdened FY17-19 ($6.6M total)
- Ultimately need 4th cavity as a spare (need additional $3M) or as a hot-spare (need utilities and transmitter totaling additional $5M) – timeline should be having this operational by FY22
- 3rd harmonic cavity installed and operational by mid FY19 (requires $1.2M to finish)
- Beamlines authorized for General User operations will increase from 11 currently (March 2017) to 28 by end of FY19
- NYS initiatives for HEX will be approved April 2017 with first fund expected no later than June 2017; HEX begins commissioning/GU operations in FY22 (assuming funding profile FY17 $2.2M, FY18 $1.1M, FY19 $4.8M, FY20 $8M, FY21 $10M)
- Cryo-EM will be in FY18
- MRE Beamline and Experimental End Station Building will be funded by principally DOE/NE (possibly NNSA/FES also) in FY20 and in place by the end of FY24
- Computing demands will increase steadily as additional beamlines support general users.
  - FY21: 30 PB storage needed
  - Central computing facility for NSLS-II will reside in B725.
- For a beamline in general user operations, users on site at any given time while the beamline is taking beam (Coincident user population) will be 3/BL.
- Total unique users will increase from 477 to 2694 over the planning period.
- NSLS-II permanent staff (407 BNL staff in FY17) consists of NSLS-II employees, deployed staff, partner users, and support contractors.
- Permanent staffing level will remain approximately stable, with the addition of several FTEs starting in FY20 to support additional beamline operations.

Total Population growth will be:

- Beamline users require 1 cubicle per beamline (revised from 2 based on operating experience). The balance of beamline users will use workstations at the beamline
- Staging requirements for materials and equipment on the experimental floor and in LOB2 will decline as current beamline construction projects reach completion
- New beamlines will continue to displace cage space on the experimental floor
- NSLS-II electric power demand will grow by 10% in a fairly linear pattern through FY21

The Laboratory has infrastructure plans in place that will support some of the emergent needs of NSLS-II. Institutional level assumptions are:

- Infrastructure investment (CURL) will remain flat (annual growth of 2%) over the planning period
- LOB Build-out projects will continue to receive BNL support and DOE approval
- Discovery Park infrastructure development will begin in FY17-18
- The Science and User Support Center (SUSC) in Discovery Park will be funded in FY18 and completed in 2021
- The Meadows at Yaphank will deliver rental housing options by the end of FY17
- Discovery Park will deliver user housing by 2020
- Bldg.725 SLI project starts in 2018 and complete in 2021
- BNL will demolish most of the wood frame housing stock by the end of the planning period.
- BNL staff will be consolidated from WW-II wood buildings into SUSC and other permanent structures.
- The B725 repurposing as a Computational Science Initiative facility (Core Revitalization Project) will be funded in FY17 – FY21.

- Electric power contracts will be successfully renewed in FY17 and FY20 preserving advantageous electric rates
- Utilities infrastructure renewal and expansion will be supported by Institutional GPP to ensure continued reliability
- A second Utility Energy Services Contract (UESC) will be launched ensuring sufficient central plant capacity and distribution/collection capability for future site needs
- Current support services (Central Fabrication, Laboratory Protection, ES&H and ITD) will remain at current level of availability and associated costs will increase at the rate of inflation.