National Synchrotron Light Source II (NSLS-II)
Science Advisory Committee

Meeting Report – September 20-21, 2018

Attending: Harald Reichert (Chair), Ingrid Pickering (Vice Chair), Bruce Gates, Franz Hennies, Robert Hettel (remote), Stephen Kevan, Eugene Lavely, Anders Madsen, Janet Smith, Esther Takeuchi, Soichi Wakatsuki, Mark Dean (representing UEC)

Regrets: None

Preamble

The Science Advisory Committee (SAC) of the National Synchrotron Light Source II (NSLS-II) met at Brookhaven National Laboratory (BNL) on September 20-21, 2018. The inaugural triennial reviews of beamlines were also held on September 21-22, in conjunction with the SAC meeting, the reports of which accompany this document as appendices.

The SAC wishes to commend the entire NSLS-II team on the progress and achievements of the last six months. It is credit to the entire team that NSLS-II is functioning well, with an engaged and growing user community and many publications produced.

The SAC was provided with charge questions by the management and was asked to provide feedback on two major aspects of the facility, which are detailed in Sections 1 (accelerator) and 2 (beamline controls). Section 3, beamline operations, is largely focused on the results of three early mini reviews of three beamlines. Summaries of the SAC reviews of four beamlines, as well as feedback of the process, are presented in Section 4. Section 5 presents brief comments on new beamline development, along with additional comments from the SAC in Section 6. Suggestions of updates for future meetings are provided in Section 7.

1. Accelerator

General comments

The SAC congratulates the Accelerator Division for continuing to achieve highly reliable high quality operation of the NSLS-II accelerator and for setting goals for better performance going forward. The machine operates with 400 mA now and is scheduled for 500-mA operation in FY20.

The accelerator team's dedication in responding to machine problems (notably the HXN IVU, booster dipole supply, etc.) and the approach for analyzing and mitigating them is commendable.

The team faces 4 main challenges for securing highly reliable operations: system immaturity, threat of insufficient staff, insufficient spares, and insufficient RF redundancy. Subsystems of concern include the SC RF and cryoplant system, pulsed magnets and pulsers, linac klystrons, and the DI water system. The team has launched programs to address each of these challenges and concerns. In particular a

strategic assessment of vulnerabilities has been carried out and an estimated 25 M$ would be needed to fully address them. This includes eventual procurement of costly redundant systems: 4th RF, electron gun, and booster and ring dipole power supplies.

Regarding the reduction in staffing, the Accelerator Division is endeavoring to cross-train support staff, assign controls tasks to accelerator physicists and ensure that essential skills are retained. The SAC approves of the effort to engage support staff from other BNL Directorates where appropriate (such as cryogenic and DI utility support from RHIC) which can improve the overall efficiency of staffing at BNL.

There are many computer control tasks that could be of interest to accelerator physicists, including those already ongoing: diagnostics and related data analysis, feedback systems, beam-based optimization algorithms, etc. So much the better if accelerator physicists learn how to provide general control system support in the process. Machine learning is an emerging area of interest at some other accelerator labs: this technology might be employed to improve accelerator performance for the NSLS-II.

Studies of operating with <10 pm vertical emittance are ongoing. More users are becoming interested in this mode notwithstanding the reduction in lifetime. A 3rd harmonic bunch lengthening cavity will improve lifetime in the future.

In total, 45 accelerator development projects are planned over the next 3 years. These include a 3rd harmonic cavity, improved BPM processors, and ideas for a future lattice conversion. A novel concept using superconducting "complex bend" modules is being studied and funding for a low-energy test of this concept at the ATF has been funded. These development projects are exciting and important for engaging and maintaining a high level of accelerator skills at the NSLS-II and motivating the staff.

Response to charge questions

1.1. Are we on the right track in regard to the heating issues seen at high stored current, in terms of diagnosing the causes and mitigating the effects in order to be ready for 500 mA ops in FY20?

Several components experiencing over-heating due to high beam current have been identified and have been upgraded to mitigate the problem. Still, it seems that the ring remains vulnerable to these problems. A technical review of the 500-mA program held in July addressed several issues besides heating, including collective effects issues. The reviewers urged caution in immediately proceeding with the 3rd harmonic bunch lengthening cavity, which promises to mitigate heating and lifetime issues at 500 mA, until more studies are done.

Recommendation: Make a decision on pursuing the 3rd harmonic cavity implementation and decide whether to do so before going to 500-mA operations.

1.2. Do we have a good handle on the causes of operations downtime and do we have an appropriate program to address the issue?

The Accelerator Division is doing an excellent job of tracking and analyzing the causes of accelerator downtime. A 25-M$ reliability program for addressing issues, including procuring system spares (<5 M$) and costly redundant components has been proposed. There could be some concern about obtaining spares for the Russian-built booster. It is not clear to the SAC whether the elements of the reliability program have been prioritized or placed on a resource-loaded schedule.

Recommendation: Develop a prioritized resource loaded schedule for the reliability program, including the 3rd harmonic cavity.

2. Beamline Controls

Is the controls program on a path to success? Has there been an improvement in the execution of the responsibilities of the Controls Program in the last six months? Are the extant issues (technical and organizational) understood? Is there a clear plan to address these issues going forward? Is that plan executable on a reasonable timeframe with the current resources?

The SAC was happy to see that the controls program continues to receive full attention from the NSLS-II management and welcomed what it perceived as improved understanding of the issues and the willingness to address them. It is our understanding that people from other parts of the organization are involved in the improvement and prioritization efforts, and this we deem essential for success. The SAC fully acknowledges the complexity involved in the Controls and IT systems at any modern facility, the difficulties of staff recruitment and retention in the highly competitive market, and the limited resources that could go into improving controls, data acquisition and analysis.

The head of the controls program presented a number of activities as ways forward in improving the situation. The presented action plans to address the specific recommendations by the SAC and CS review panel; these two plans need to be merged with further focus and prioritization as well as clear timelines. Since the SAC cannot assess whether the action plans are executable within a reasonable timeframe with the materials presented and discussed, we recommend strongly that the NSLS-II Management and the Controls Program head develop a coherent set of action plans with timelines.

Compared to the last SAC meeting, we observed visible progress in some areas, including the PoC definitions, town-hall meetings, and various efforts to prioritize. In all staff interviews, the SAC clearly received more comments that are positive regarding the controls program than the last time. In many areas, on the other hand, frustration continues. It seems clear that there is still a long way to go and that the controls program needs continuous improvement efforts for some time to come. In addition, no overall assessment of the actual amount of work needed to develop the beamline controls has been presented. While this is probably difficult to produce before organizational improvements start to bear fruit, the SAC would like to hear an update from the Controls Group in the next meeting.

We commend the introduction of prioritization meetings with representatives from the beamlines and machine group. We sensed, however, that there were too many different forums that are not fully matured, and that some prioritization is handled differently even from week to week. Therefore, we deem it necessary to lay out and communicate clear pathways for prioritization with clear timelines of work in all parts of the Controls Program including IT, beamlines and accelerator controls.

The PoC flow chart provides a good visual guideline for various aspects of the process, but misses to lay out the process of how PoCs will follow up upon projects to completion. It is not helpful to show a PoC flowchart and to discredit it immediately simply as a symbolic gesture. We also sensed varying levels of commitment by different PoCs, resulting in varying degrees of proper distribution of task assignments and completion. The SAC recommends further developing the PoC role and ways to help developing individuals in this role, including some form of management training and continued attention from the Controls Group head.

Usage of the TRAC system seems to have improved, but its usage as wish lists or even simply bookkeeping of to-do lists should be discouraged. Addressing urgent issues through the TRAC system seems to work much better now, but non-urgent fixes, even small tasks, still seem to take a very long time. Problematic with the latter is that beamline groups seem to have no way of knowing when certain tasks will be performed. We heard from some beamlines that they felt the need to wait until the last minute and create, thus, an “artificial urgency”, in order to get guaranteed controls support even for new, not-so-urgent, tasks.

We commend outsourcing to Central IT, which has been regarded as positive by beamlines and controls teams.

Some beamline groups clearly see a value in the town hall meetings and use them actively by contributing topics, which are subsequently dealt with by the Controls Program. Others, however, seem to have written them off as not relevant after one attendance or without even trying. The SAC strongly encourages all beamline groups to make use of this forum and other occasions to engage with the Controls Program in a collaborative fashion. Beamline groups need to realize that development of controls, DAQ and analysis chains can never be regarded merely as a service, but rather demands active collaboration and commitment from beamline engineers and scientists as well. The SAC wants to urge beamline group managers and the senior management to actively disseminate this message to their group members.

Finally, staff retention and filling of open positions need focused and coordinated efforts across the facility. The NSLS-II management cannot address these issues alone but a lab-wide effort is called for. Hence the SAC recommends strongly that the BNL management, with the active involvement of the Human Resources group, address the slow hiring procedures in mission critical areas such as the IT and controls which need to fight against the most highly competitive market.

3. Beamline Operations

3.1. General Beamline Operations

The SAC congratulates all beamline programs and the experiment development program for the display of activities and achievements from instrumentation to method improvements and enabling early science.

It is difficult to give comments that are more detailed on the individual beamline programs with limited material provided, as was the case for the “early mini-reviews” of BMM, NYX and SIX this meeting. The SAC would encourage NSLS-II to come up with a different scheme for reporting on the beamline programs that allows for a more in-depth discussion of selected areas. The SAC deems including the mini review for SIX, NYX, and BMM as not optimal, since it limits the possibility for follow up questions, especially with no beamline staff members or PIs of the PU program present although in some cases follow-up discussions with staff were held (see below). The SAC would like to propose that at future meetings the mini-reviews return to the old format of 3 beamlines with 15 min each, and that the overall beamline presentation is shortened significantly, addressing mainly cross-cutting issues. According to information from the March 2018 SAC meeting, there are 5 remaining beamlines for mini-reviews: QAS, XFM, FXI, SST-1 and SST-2. Thus, the last 5 mini-reviews (in the form of 15 min presentations by beamline staff at SAC meetings) would be concluded through 2019. From 2020 on, each SAC meeting could focus on two specific beamline programs instead. Thus, every beamline program would be addressed in detail once every 18 months as a SAC mini-review followed by a triennial review 18 months later.

The management presented efforts to improve communication, and these have been recognized by some beamline staff but have not yet had the desired impact. It is evident that these efforts need to be further intensified, and that management must actively and routinely seek the contact (walk the floor, lunches with John, etc.). Keeping an open door or offering a pigeonhole for suggestions may work for some staff, but does not help where staff members feel overlooked. In this context, the SAC sees a need for an active discussion and in many cases individual discussion between staff and management about strategies for developing beamline and individual science activities.

3.2. Early mini-reviews of beamlines

Three beamlines (BMM, NYX, SIX) were presented to the SAC briefly; for each the SAC was asked the following questions: *Are these beamlines on a path to success? If not, are there things we can be doing to ensure successful programs?*

3.3. BMM (Beamline for Materials Measurement, 6-BM)

Paul Zschak's review of the hard X-ray bending magnet beamline BMM presented highly encouraging results, indicating its capability for materials characterization with a small focused beam and high flux, illustrated with fine-grained XAS data obtained with a Pratt & Whitney material incorporating a ceramic thermal barrier coating such as one used in jet engines. The beamline is well suited to XANES, EXAFS, and XRD characterization of thin films and other materials, including reactive materials such as catalysts. First light was July 7, 2017, and a general user program is underway with 14 proposals received and experiments to be run in late 2018; general users are scheduled to receive 50% of the beam time. There is an abundance of detail for users available on the beamline's Wiki. The beamline is designed to be equipped later with on-line analysis capability to facilitate in-operando catalysis experiments. NIST has contributed to this beam line, with highly experienced NIST personnel involved in the start-up and operation. The development of this beamline is proceeding nearly according to the original schedule and is on a positive trajectory. Excellent results are anticipated from this beamline.

In consultation with staff, the following issues were raised. SST has absorbed considerable resources, with little investment in BMM aside from personnel time. Although this is an internal NIST issue, it is negatively impacting progress. The absence of fast scanning implementation is a significant backlog on data collection with 1.47s overhead per data point causing a paralyzing problem. In addition, the XRF detector readout is antiquated and badly in need of an upgrade to provide higher performance.

Overall BMM is a well-functioning beamline on an upward trajectory, on time, and meeting its milestones. It is clearly on a path to success.

3.4. NYX

Commissioning progress for the NYX beamline was summarized by Paul Zschack. NYX is a project of the New York Structural Biology Center (NYSBC). The goal is to be an optimized source for cutting-edge anomalous scattering in macromolecular crystallography by taking advantage of the NSLS-II brightness and improving energy resolution (target $\Delta E/E$ 6×10^{-5}, energy range of 6–18 keV, focused beam size 10 × 10 μm). The NYX instrument readiness review (IRR) occurred nearly two years ago (Nov 2016), and commissioning towards user operations has lagged since then. NYSBC recently appointed Dieter Schneider as lead scientist at NYX, which is positive development given Schneider's success at NSLS and NSLS-II prior to his 2017 retirement.

SAC members met with Dieter Schneider for an update on the status of technical commissioning. A variety of beamline features account for the slow commissioning progress: complexities of the sagittal-focusing double-crystal monochromator (DCM), lack of horizontal white beam slits between the source and the DCM that would enable detailed DCM characterization, lack of beam position monitors upstream of the endstation (3 empty enclosures without controls or feedthroughs), an uncharacterized vertical focusing mirror with passive gravity compensation, and Galil controls that lack the convenient diagnostic tools of EPICS. Schneider outlined an ambitious, accelerated timeline for characterizing the beamline optics. The SAC agrees that his plan should be executed with some urgency, but advises that it be thoroughly vetted with the NSLS-II management, as it relies on facility resources (metrology lab, Controls effort) and collaboration (Lonny Berman and Oleg Chubar for DCM characterization). We

anticipate that with appropriate NSLS-II assistance, the following items could be completed in 12-18 months:

- Definition of an achievable "experimental envelope" that approaches the scientific goal of anomalous scattering with high energy resolution ($\Delta E/E = 6 \times 10^{-5}$)
  - Beam tunability (energy resolution, energy range, speed of tuning, energy stability)
  - Beam size (achievable focus and the associated sacrifice in energy resolution)
  - Flux to the sample
  - Beam positional and intensity stability
- Determination of a range of feasible experiments and appropriate samples for the experimental envelope (sample size, diffracting power, anomalous signal strength)

With an understanding of the technical scope and experimental envelope of the beamline, several critical decisions can be taken:

- Options for continued funding of the beamline
- Options to update outdated aspects of the beamline: detector, sample exchange robot, hardware controls, focusing optics, monitoring systems
- Options to integrate NYX with the NSLS-II facility beamlines for structural biology while retaining the primary NYX scientific goal

The SAC looks forward to hearing an update at our next meeting.

3.5. SIX

The SAC was happy to see that the team has made significant progress over the last one and a half years with commissioning the beamline and the large spectrometer in particular. Installation of mechanics and control for the big spectrometer are finished and first resolution tests have shown that these are working. So far, it was not possible to test the real potential (and limitations) of the optical system due to insufficient optics (refocusing mirror and blazed gratings in mono and spectrometer). It is good to hear that the team will install a mirror with design specifications soon. The SAC supports the decision to start operation with laminar holographic gratings instead of the design gratings, which are mechanically ruled blazed gratings. The SAC fully acknowledges the current difficulties in obtaining high quality gratings.

The SAC however got the impression that more mundane systems at the beamline are still not implemented to a level that will allow for reasonably smooth initial user operation. The status presentation mentions sample transfer to be finalized, but with a deadline that has already passed. Detector readout routines are another example of an important non-optics related system still not fully finalized.

The beamline has made overall slow progress. The well acknowledged difficulties to source quality optics or limited support from the controls program can only account for part of this. With several high-resolution instruments that have recently come up internationally, it would be highly desirable to make SIX available for users as soon as possible.

The SAC congratulates NSLS-II and Valentina Bisogni to her 2018 DOE Early Career Award, and recognizes that other staff at this beamline pursue strong scientific activities as well.

The SAC recommends setting clear priorities and target dates for implementing the most important basic functionality at SIX, in order to give a clear mandate to user science at SIX. Continued development will happen at SIX for a long time to come, but should not further hamper the user program. Installation of the triple rotating flange with associated risks and downtime, for example, or

testing of the next iteration of gratings from Inprentus, needs careful balancing with respect to user operation.

The SAC would have liked to see an analysis of the performance expected with the optics now installed, and what the potential impact on the scientific possibilities at SIX is. In general, the SAC acknowledges that it was difficult to obtain a good picture of the beamline status due to the changed format at this SAC meeting. The SAC welcomes a short update at the next meeting.

4. Triennial beamline reviews of CSX, IOS, HXN and XPD

The inaugural triennial reviews of four beamlines were held in conjunction with the SAC meeting. An executive summary of each beamline review is presented here, together with comments on the format of the reviews (section 0). The complete reports from the four committees are presented as appendices.

The charge for the SAC, in looking at these beamlines is: *1. Is the science program looking healthy for this stage of their development? 2. Are there outstanding issues that require attention?*

4.1. CSX – Coherent Soft X-ray Scattering – 23-ID-1

The mission of the Coherent Soft X-ray Scattering (CSX or 23-ID-1) beamline is to exploit tunable coherent soft X-rays for the study of materials' properties that are accessible at atomic resonances in the range 200-2000 eV. Photon energies tuned at core-electron excitation energies in the soft X-ray regime afford a substantially enhanced contrast not only in terms of element specificity, but also in terms of the chemical state and low-energy electronic properties, such as spatial modulations of charge, spin, and orbital degrees of freedom. In the latter cases, full polarization control of the X-rays provides another essential tool. The energy range of the CSX beamline covers the resonances of *3d* and *4f* transition metals, giving access to several families of quantum and magnetic materials. Carbon, nitrogen, and oxygen K edges, relevant for soft matter studies, are also in this energy range. In addition to the resonant contrast enhancement, the X-ray coherence and full polarization control enabled by the elliptically polarized undulator provides access to the phase information in scattering processes in a straightforward manner.

The overall assessment of the review panel regarding the beamline's mission, performance, staff, and method development is excellent. The past three years have seen substantial development in instrumentation at the beamline to enable experiments along the lines of that mission, rendering CSX at present the world's leading instrument for coherent soft X-ray science with an impressive and rising scientific output in various fields of research. With the methods established and being developed, CSX makes perfect use of NSLS-II as a brilliant, coherent X-ray source. These methods include imaging at the nanoscale to visualize electronic & magnetic textures and studies of static & dynamical electronic symmetry-breaking phenomena as a function of temperature. Materials are primarily represented by transition metal oxides, but other ambitious targets are spintronic devices in operando and soft matter. The scientific program and output showcased during the review conveys the excellent contributions of CSX in the priority area of "quantum and complex materials". A key asset for this success is the exemplary staff (Mazzoli, Wen, Barbour, and Wilkins), who provide dedicated, expert user support while sustaining technical developments based on deep understanding of the scientific context.

With its experimental capabilities, CSX presently defines the standard in coherent soft X-ray science. In order to maintain leadership in this area, the beamline's current broad list of envisaged applications should be prioritized after a reasonable period of exploration. Performance upgrades will be essential to maintain international leadership, expand the accessible materials space, and push for a higher spatial resolution and time-resolved operations. Therefore, the highest possible flux should be realized using the

full length of a large straight section of NSLS-II, i.e., phasing of the two available undulators for the generation of coherent X-rays at higher (3.5x) flux. Further, the NSLS-II management should consider increasing the technical and scientific staffing, either directly or by the appropriate involvement of third parties.

4.2. IOS – In situ and Operando Soft X-ray Spectroscopy – 23-ID-2

IOS shares the cell 23 straight section with CSX in 50:50 equal beamtime sharing. Currently, IOS operates two experimental stations, APPES (ambient pressure photoelectron spectroscopy) and IO-XAS (in situ and operando x-ray absorption spectroscopy), to support the general users' research needs which align with NSLS-II strengths and strategic direction of "Operando Chemistry & Structural Science". The ambient pressure X-ray photoelectron spectroscopy (XPS) capability is world class and supports the research needs to study energy materials and processes in heterogeneous catalysis, fuel cells, photovoltaics, and batteries. IOS staff has been providing exceptional support, especially to the less experienced user groups. There is clearly a rapid increase in the product in the last two years before the challenging situation of the ambient pressure XPS instrument. IOS is currently running a Partner User Agreement (PUA) between with the Interface Science and Catalysis group at the Center for Functional Nanomaterials (CFN), in which CFN receives 23% of the available user time for ambient pressure XPS. The PUA was activated upon the start of GU operation in January, 2016. The PUA stipulates that the CFN receive 23% of the available user time for running their user program as well as their own research, in exchange for an upgraded endstation valued at $800K and some staffing contributions. However, besides the necessary replacements of failing components over the years (for example, detector, pumps, valves), the endstation has not been upgraded since its first construction. The PUA with BNL Chemistry will be activated after the installation of in-situ XAS cells for GU use. Staff research has been demonstrated, is at an appropriate level, aligns with the mission of the beamline, and involves some good collaboration with general users. Staff are appropriately planning a number of incremental upgrades of APPES and IO-XAS to improve the performance and productivity. There are plans to upgrade and replace APPES and IO-XAS to meet the current research trends.

The report is structured according to the specific questions posed in the charge to the Committee in five areas, including Beamline Capabilities, Science Program and Impact, User Support and Labs, Partner Users and Future Plans.

The key findings are listed as follows:

- In-situ chemistry capability at IOS using ambient pressure XPS is established and supported.
- The electron analyzer for ambient pressure XPS has been out of operation since May 2018, which shows significant impact on NSLS-II users' program.
- Some current users require too high a degree of user support due to insufficient experience with handling complex experimental setups at IOS.
- A clear deficiency of the program is the apparent absence of in-operando capabilities.
- Synergy is missing in the PUA involving CFN, in which "partnership" is lost in translation.
- Available shifts on IOS are highly oversubscribed under the current 50:50 beamtime sharing agreement between CSX and IOS.

The recommendations are listed as follows:

- Identify what lessons have been learned from prolonged downtime of the ambient pressure XPS capability to avoid future impact.
- Develop a contingency plan for the ambient pressure XPS capability.
- Move forward with in-operando capabilities and research.
- Find a balance between supporting experienced and non-experienced users to sustain the productivity of IOS.

- Encourage NSLS-II to establish a new relationship under the PUA with CFN in regards to the instrumentation and supporting team.
- Compelling science case was missing for the INSPIRE proposal to replace APPES.
- Encourage the IOS team to have more discussions with CFN and the Department of Chemistry on the uniqueness for the science cases of the new INSPIRE endstation.
- The Committee strongly supports the proposal to increase the canting angle between CSX and IOS to allow independent operation of the two
- Suggest to explore the option of moving the IOS beamline to a dedicated EPU or bending magnet source.

SAC comments on IOS beamline review

The review committee has made a candid and comprehensive assessment of operations and capabilities at the IOS beamline, as well as of operational limitations and development plans. The SAC has nothing to add, but wants to emphasize a few points.

Firstly, the two review panels for CSX and IOS obviously do not come to a coherent conclusion regarding the shared straight section. The CSX panel advocates using the full straight section for generating the highest possible coherent flux, which is incompatible with any scheme that improves independent operation of the two beamlines. The IOS panel accordingly suggests different options that improve IOS operation, and only moving the program to its own port is compatible with CSX needs. The SAC recommends solving this question from a pure strategic point of view. CSX is a flagship coherent beamline, but will only remain attractive with access to the highest coherent flux possible, in other words, the full-length straight section. The demand for IOS is certainly potentially high enough to fill a port of its own.

The situation with the APXPS PUA and setup is worrisome. Although the SAC earlier had received signals that collaboration on this instrument does not work to full mutual satisfaction, it is surprising that it now seems to have completely derailed. The fact that CFN was not present at the review indicates indeed that the “partnership is lost”. This is even more surprising since both partners, CFN and NSLS-II surely realize the strategic importance of this technique for both facilities. CFN has recently done key hiring to strengthen APXPS. The SAC wants to point out that collaborating on APXPS is one area where BNL with CFN and NSLS-II on site has a strong strategic advantage; not capitalizing on this will be of certain disservice for both. The SAC does not know the full context of this situation, and again recommends treating this as a NSLS-II or even BNL strategic question. It seems obvious that some investment, both in instrumentation and commitment, is warranted. Once the potential for future collaboration is established, questions concerning beamtime distribution, in-house research etc, can be addressed. The current situation seems to be of only historical relevance, since no working setup for APXPS is available.

Given the uncertainty about APXPS, as well as simultaneous operation of CSX and IOS, the SAC urges NSLS-II management to be careful about beamtime distribution in the existing and future PUAs, in order to not give away leverage for future developments.

In this context, it is important to point out that improving AP-XAS capabilities towards operando is extremely positive, but cannot replace a development of the APXPS part. Here, internationally, most recently at MAX IV, operando as well as strongly enhanced in-situ capabilities have been developed and will soon be routinely available for users. Personnel at CFN have access to these developments through collaboration. The SAC recommends developing specifications for an APXPS setup based on user community needs for sample preparation and handling as well as advanced in-situ and operando capabilities. In a second step an assessment can be made how such a system could be funded and implemented. Upgrading the old system is probably not worth the effort.

The INSPIRE proposal needs an extremely careful assessment in this context. The beamline review committee pointed out that a compelling scientific case has not been presented. The SAC wants to add that combining RIXS and APXPS in one system will demand that, mildly put, extreme technical challenges be addressed. Such a system risks being very limited, maintenance intense and difficult to operate. NSLS-II should prioritize defining a user-friendly high-throughput specialized APXPS system with operando capabilities routinely offered to users.

The SAC urges NSLS-II and CFN management to sort out these issues and see if a common strategy can be developed. SAC would welcome an update on these developments at the next meeting.

4.3. HXN – Hard X-ray Nanoprobe – 3-ID

The Hard X-ray Nanoprobe (HXN) provides world leading routine nanoscale microscopy with hard x-rays. HXN supports two microscopes, one currently a 50 nm resolution Zone Plate (ZP) optics with long working distance and the other a best-in-world ~10 nm resolution multilayer Laue lens (MLL) based microscope. HXN is used for three focus areas: (i) quantifying trace elemental composition in materials via X-ray Fluorescence Microscopy (XFM); (ii) imaging crystalline ordering or strain with scanning microscopy and ptychography on Bragg peaks; and (iii) structural evolution as a function of in-situ controls using XFM, Differential Phase Contrast (DPC) imaging and ptychography in a single multimodal capability with up to 8 nm spatial resolution.

Currently, materials science and condensed matter users appear to be the community best suited to HXN capabilities; the science program is well aligned and in turn is appropriately driving the technique development. The committee recommends that HXN continues with current improvement and upgrade plans. HXN is encouraged to further expand the user community and the beamline staff is advised to strongly favor potentially high impact 2D work in the near term, while selectively working with users and techniques on 3D capabilities of high scientific impact as they continue to develop.

The beamline staff at HXN is very highly regarded by the user community. We strongly support the addition of a new staff member, to backfill both for the effective reductions caused by reorganization and departure of beamline postdocs in the last year. This additional staff member is intended to focus on in-situ or spectroscopic capabilities at HXN. The support labs at HXN are well maintained by the staff and the plan to upgrade the current scanning electron microscope (SEM) is sensible. Currently there are no Partner Users at HXN. The committee believes this may be a missed opportunity to supplement staffing with on-site expert users and develop new capabilities.

HXN staff have a well thought out upgrade plan going into the future. The renewal of the tomography stage is particularly important to reach routine 3D capabilities. While HXN has become a go-to beamline for optics characterization, the GU program involving optics characterization for other beamlines and light sources is detracting from the science output; HXN should limit beamtime given to other optics developments that will not directly impact HXN performance. The committee recognized that data analysis capabilities and the ability of users to connect the unique data coming out of HXN to their science is sometimes a barrier to publication. The addition of one group-level data analysis support staff is recommended to help develop and maintain codes as well as support users in the post experiment phase. This staff member would help bridge the gap from experiment to publication and improve the output of every beamline in the imaging group.

4.4. XPD – X-ray Powder Diffraction – 28-ID

As one of the NSLS-II's original project beamlines, XPD has served as the foundation of the Diffraction and In-situ Scattering (DISC) program, as the only high energy powder diffraction beamline within the suite of beamlines (ISS, XPD, PDF). The unique properties of XPD provide a distinct advantage in time-dependent, in-situ and operando studies of structure, as the current science program

appropriately emphasizes. The beamline staff have done an excellent job with the optics at the beamline, extracting two powerful, usable beams from the damping wiggler to feed the two parallel end stations/beamlines, XRD and PDF. A major effort has been made in provision of sample environments to support this theme of in-situ and operando experiments (in line with BNL priorities). XPD serves a broad and diverse user community encompassing multiple science areas (from physics, chemistry, and materials science to nuclear engineering, earth science, environmental science and engineering science). In just three years of operation, XPD has ramped up a productive research program and impressive publication rate.

During the review, the XPD Staff presented a comprehensive overview of activities and status of the XPD beamline covering plans for development of beamline capabilities, achievements within the science program including productivity, the breadth of user support activities including training, developing strategic partnerships with the local community, and planning in the context of DISC for the future. The dedicated XPD staff should be commended for their excellent support of users, which is particularly notable considering the breadth of capabilities that are supported. As development of the DISC program moves forward, the XPD should continue to work toward a comprehensive development plan, that has well-defined strategic priorities that are also consistent with staffing levels.

Was the format for the reviews appropriate? For staff? For reviewers? Are there opportunities for improvement?

The SAC review of each beamline involved an expert committee of 4-6 people, including one SAC member and an external chair. A written report was prepared by beamline staff and distributed ahead of the meeting. Presentations by beamline staff and key users, and a tour of the beamline facilities occurred on day 1. On day 2 of the review, which was day 1 of the SAC meeting, the SAC member joined the SAC meeting while the remainder of the committee prepared the report. The review chairs then joined the SAC meeting around midday to make close-out presentations to the SAC.

Generally the SAC felt that overall the process was very successful, especially as this was the first time through. The meeting and travel facilitation and coordination were excellent. The timing was unfortunate for staff as it coincided with beamline start-up after a long shutdown; this should be avoided if possible.

Written materials: Some groups felt that the written document provided by each beamline was very well put together. However, the formats and level of detail varied a lot. We would advise better uniformity and favor brevity. In other cases, the written material provided by the beamline teams was delivered very late – after some reviewers left for the airport.

Talks: More guidance to staff may be needed about the content of the talks. Some of the presentations also focused too much on detail and not enough on the big picture concerning how the staff think the beamline should continue to be developed.

5. New Beamline Development

Is the approach being taken to explore new beamline concepts appropriate?

The process to develop the evolving list of potential new beamlines is good. We encourage *regular, inclusive, bi-directional* discussions with the NSLS-II staff leading to the planned workshop at the spring 2019 user meeting. The SAC looks forward to helping with this process of prioritization.

Does the SAC have any early feedback on the concepts identified?

The six new beamline concepts previously prioritized remain of high quality. The new concepts are interesting and warrant further discussion and prioritization, as noted above.

Does the SAC have any feedback on the prioritization of the next round of beamlines?

Throughout this process, the NSLS-II should consider the evolving landscape at other US and international facilities, particularly for instruments requiring high source brightness. In the hard x-ray regime the NSLS-II will be 10-100x less bright than facilities now being upgraded or built. This is much less true in the soft and tender x-ray regimes, particularly given the accelerator upgrades presently under consideration. To remain competitive in two of its most important research areas, quantum materials and chemical transformations, the NSLS-II should re-evaluate its relatively light investment in soft and tender x-ray tools, as compared to its investment in hard x-ray tools. The prioritization of beamlines planned for the new MIE should be revisited. As noted below, strategic positioning of NSLS-II for the future should be considered, developed, and communicated.

6. Additional Items

6.1. Strategic Plan

The strategic planning of the facility for the period 2019-2023 was presented by Q. Shen. This is part of an ongoing process where the latest plan dates from April 2018. The aim is to have an updated plan by Oct 2018 to comply with the new DOE guidelines. This year there were several initiatives to engage staff in the process, all of which SAC commends, including brainstorming sessions for each of the technical programs, an active outreach to get input from employees on how to improve the facility in a broader sense, and an effort to collect suggestions from the beamline program managers with more concrete ideas for new beamlines. A draft list of new beamline projects was presented to the SAC. To involve the user community, it is expected that several workshops will take place in conjunction with the next User Meeting (May 2019).

The SAC endorses the planning initiatives and recommends to actively engage the user community in the discussions as early as possible. SAC also recommends that management gives feedback and provides regular status updates to all NSLS-II staff engaged in the brainstorming and strategic planning discussions. Some of the beamline projects on the draft list seem to have overlapping scientific aims and/or technical capabilities, also compared with beamlines already in operation. For example, a concept for a new methodology and test beamline was presented, which also could host several of the science programs as end-stations. Studies of additive manufacturing were also mentioned in connection with different projects. Discussions between beamline groups should be undertaken to further streamline the new projects, and SAC looks forward to helping the management with the process of prioritization.

In general, SAC did not observe overarching threads or drivers for planning other than the specification of the three science focus areas. It may be useful in future to clarify further the evolving facility strategy and rationale. For instance, management is recommended to take the rapidly developing landscape of MBA-upgraded facilities in the US into account in the strategic planning, including the 6 beamlines approved in 2016 and the new MIE projects. The relevant question is how NSLS-II remains at the forefront knowing that APS and ALS soon will get significant boosts in performance. SAC believes the answer could be to concentrate on the soft and tender X-ray regimes and techniques that currently are not brightness limited. Additional possible factors for consideration include: (i) the national need (for example, for energy independence); (ii) the overall DOE mission and identification of priorities and challenge areas (for example, those identified in reports posted at

https://science.energy.gov/bes/community-resources/reports/); and (iii) currently funded programs or high-priority initiatives within the DOE and across other agencies that may benefit from NSLS-II capability. Identifying how to fit in and play a role in some of these areas will position NSLS-II for increased relevance, higher visibility, additional funding and collaborative opportunity in diverse, unexpected areas.

The R&D program presented by management supports the strategic planning in several areas, including accelerator development, X-ray optics, data analysis, and modeling of experiments. If priorities are to be set, SAC recommends that a 3rd harmonic bunch lengthening cavity is more important for the facility than a 4th RF cavity and that efforts to achieve 500 mA should not compromise the possibility of a vertical emittance improvement. SAC is of the opinion that NSLS-II can be proactive in shaping its future by further appraising internal capabilities and using this to catalyze new programs, either inter- or intra-agency. A way should be found to empower the immense human talent and potential in the NSLS-II staff and across the lab to participate in strategy and action. Strategic advantage will be gained if the NSLS-II leadership can cajole or inspire cooperation across the BNL campus. SAC encourages leadership to incorporate some of this mindset into the planning, especially with the prospect of limited future resources.

6.2. User Program

The SAC received a brief presentation on the User program at this meeting. The SAC was pleased to see progress in the Single Sign On (SSO) process with the Domain Account now integrated. The SAC looks forward to the milestone of eliminating the need of having a Google account for new user access. Unfortunately, it is clear that proper access to data will need beamline-specific implementation.

The SAC was also enthusiastic to see the progress towards a PASS replacement system, with different options being considered. Working together and sharing experiences across light sources is definitely to be encouraged. The final choice for NSLS-II needs to provide an optimum experience for users, not least because this is often the first window onto the facility, while giving speed and flexibility to the back-end management. The SAC looks forward to updates on progress.

6.3. Staff Development

The long-term success of the NSLS-II is strongly linked to the professional development of its staff, particularly its scientific staff. The staff must be empowered to participate in helping to plan initiatives at NSLS-II and across BNL, on an equal footing with staff from across the lab. The NSLS-II should develop a document that outlines its goals, policies, and procedures related to staff professional development.

The facility should work with the BNL management to end the discriminatory and counterproductive policy that does not allow NSLS-II scientific staff to be “tenured”. At all times, the NSLS-II should represent and champion the unique and valuable combination of expertise found in NSLS-II scientific staff. In particular, the facility should consider including discussion of collaboration with and professional development of beamline staff when new Partner User agreements are negotiated. As the NSLS-II matures, in some cases it will become less important for PUs to bring major instruments to the facility, but it will become increasingly important that PUs establish strong and balanced collaborations with facility staff.

6.4. Communication

There is an on-going need to cultivate good communication between management and staff. Steps taken recently have certainly helped but a continuous effort is needed. The SAC strongly advocates that senior management routinely walk the floor, dropping in on beamlines and chatting with staff and users.

The recommendation is to commit to doing this for a minimum of 1 hour each week. This gesture of reaching out to people on the experimental floor, rather than waiting for people to come to management offices, will be appreciated by those who are encountered and will also benefit members of management through connections made and information received, both on triumphs and challenges.

6.5. Additional feedback from staff

The SAC wants to thank staff for being again available for candid discussions. These discussions are highly valued and comprise the single most important point on the SAC agenda. Most of the comments made by staff have made their way into the respective sections of this report. All staff in these meetings have shown a high awareness of the challenges and conditions under which the facility operates, as well as willingness and ability to contribute to solutions. Communication is desired by the staff and desirable for NSLS-II management. Instilling a sense that staff ideas and comments are seriously considered is important. Any additional investment in further improved communication will directly pay off in form of increased staff motivation and commitment to solutions.

7. Items for Future SAC Meetings

The SAC wishes to receive updates on the following during upcoming meetings:

- Update on the BL controls situation.
- Update on computing/DAMA; status of work with other facilities such as CSI.
- Status of upcoming beamline projects, both in the MIE and beyond.
- Update on issues identified in the beamline triennial and mini-reviews, including a short answer to questions raised above about SIX and IOS.
- Update on undulators – fallout from HXN, early tuning problems. How do they feel now about build vs buy? Seems maybe not a SAC issue.
- Updated strategic plan.
- Continued discussion of communication, employee retention and morale.

Appendices to this document:

Reports from Triennial beamline reviews of CSX, IOS, HXN and XPD