

Some comments on the BAT report for the NIST beamlines at NSLS-II are inserted in the text below (in red).

## Report from Beamline Advisory Team for SST-1, SST-2 and BMM

### Introduction

The BAT thanks the NIST and NSLS-II staff for the organization and hospitality during the BAT meeting. Overall the BAT was impressed with the detailed planning and progress to date of the three NIST partner beamlines currently under construction at NSLS-II. There is no doubt that these three beamlines will greatly enhance the scientific capability of NSLS-II. In particular, the canted undulator pair SST1-SST-2 combination will provide a world-class capability for advanced spectroscopy of real materials using the NSLS-II source combined with the unique detectors/end stations under development. The capabilities provided by these beamlines fully meet the need identified by NIST, specifically, the “Development and optimization of advanced materials and innovative devices by U.S. industry requires measurement of electronic, chemical, and spatial structure at the nanoscale.” The BAT looks forward to the IRR and commissioning of the beamlines!

NIST has a long history (35 years) as a stakeholder in synchrotron science primarily at NSLS, and also at the APS. The beamlines under review by this BAT continues that tradition, now at NSLS-II. NIST has made a significant financial investment (approx. \$40M) in the design and construction of the three beamlines, and NSLS-II management is strongly encouraged to work with NIST to see completion of the project as soon as reasonable, and to continue this collaboration through the beamline and science commissioning process. The BAT believes that the facilities that will be provided by NIST at NSLS-II will be world-class and enhance the overall scientific mission and visibility of NSLS-II.

The report is organized according to the ten specific questions posed in the charge that was given to the BAT followed by some general comments. This is followed by an Appendix containing the members of the BAT, the Agenda for the meeting, and the Charge.

#### **1. Is the scientific mission for the beamlines clear and appropriate to needs of the community that it is expected to serve?**

The BAT has no concerns regarding the scientific mission. The capabilities that will be provided focus on materials characterization using unique and novel methodologies, and there is a focus on applicability to materials of interest to both the fundamental and to the industrial user community. The capabilities at the undulator lines will be unique and state-of-the-art at NSLS-II and will be of great value to the scientific community. The capabilities provided by BMM will complement the other spectroscopy beamlines at NSLS-II. However, the BAT recommends that the NIST team consider developing a broader portfolio of *in situ* sample environments and perhaps better sample preparation capabilities.

The development of additional in-situ sample environments is limited currently by available funding. We (NIST and NSLS-II teams at BNL) are very aware of the financial situation (strict limit on funds, little contingency and “no more money” to complete the project scope). We are therefore extremely reluctant to use project funds for additional end station equipment; however, we do see opportunities to increase the scope without using project funds;

- Collaborate with other beamlines to borrow and share existing equipment.
- Retain possibility for short lead time procurements late in the project if sufficient funds are retained.
- Develop equipment using operating funds by beamline staff, and/or in collaboration with User groups.
- Use existing equipment such as the cryostat, four channel ion chamber, etc from NSLS.

While the BAT respects the need for a basic diffraction capability at BMM, we encourage the team to develop science narratives that combine it with spectroscopy to demonstrate a unique differentiating capability.

This was listed in the Beamline Development Proposal (BDP). We will send a copy.

## **2. Review progress on the SST and BMM construction projects. Are there adjustments or enhancements that you would advise as scope additions when feasible?**

The amendments to the purchase order with FMB Oxford needs to be the #1 priority of all involved at NIST/NSLS-II and the NIST staff at NSLS-II. The timing of the remainder of the project depends on it. We cannot overemphasize enough how critical this task is to timely completion of the project. Delays can propagate in a nonlinear fashion, with little control.

This has just been promised to be completed by the end of the month (August 2016)! We'll see.

Continuous oxygen cleaning of contamination of optics as is being performed at Diamond and at Soleil. This methodology should be strongly considered now for the SST suite as this may affect construction / design considerations. It is recommended that this method be implemented before first light to preserve optical surfaces from the beginning.

We intend to pursue this. Dan has been in communication with Tien-Lin Lee and has received some useful information (thanks)!

## **3. Do you see any technical complications for the beamline as being constructed? Can you suggest ways to address any such complications?**

The experiences from some of the BAT members suggests that mirror provider has notorious quality issues. This is therefore an enormous risk for this project with little/no contingencies. The BAT strongly recommends that NIST develop plans for mitigation of this risk (e.g. metrology, spot checks,

coordination with Diamond colleagues). We also recommend that NIST integrates the NSLS-II metrology group personnel into vendor discussions.

Several of our mirrors have been rejected, or send back for additional work (to Zeiss, SESO and InSync) to either correct slope errors or coating defects. At present we anticipate all mirrors being delivered on time, and to specification. We have metrology facilities here at BNL and the current workload is not high, so we anticipate being able to measure most, if not all, of the mirrors.

The BAT also strongly recommends involving Ruben in the early commissioning stages if at all possible. Given his involvement in the overall design the BAT believes that his experience will be invaluable during the commissioning phase. This will be especially true regarding any issues with the mirrors and overall optics.

Dan will commence discussions with Ruben with the idea of having him visit BNL for a period of 2+ weeks. Ruben is currently working part time, so this may now be more feasible.

The BAT expresses concern at the simple indirect cooled design for cooling the first crystal on BMM. Beamlines with similar heat loads and power densities are using direct water cooling in small multi-bore channels to good effect. Whilst the FEA showed indirect cooling gave similar slope errors to direct cooling the panel is concerned that the thinness of the direct solution crystal will give other problems due to strain and distortion from clamping and thus the (already large) slope errors will not be achieved. A multi-bore indirect design should be considered, although it is noted that a side clamped indirect cooled design can also give very similar FEA results and would not suffer from clamping distortions.

We believe that this is now closed out satisfactorily following discussions between Joe Woicik and Andy Dent.

As the crystal cage will be rebuilt NIST should ensure they have the latest crystal cage mount and mechanics as it is thought that considerable improvements to stability have been made by the vendor since the monochromator was purchased.

The crystal cage isn't really being rebuilt; the crystal assemblies are being replaced along with significant associated modifications of the primary stage.

#### Comments from FMB-Oxford.

There have been no significant improvements in the crystal cage mounts and mechanics since the BMM DCM was delivered (this also applies to the SST DCM). The design features the unitary trapezoidal flexures that were developed for the Petra III DCMs and which have been deployed in monochromator upgrades in Australia (on PX-2 and SAXS/WAXS beamlines) and at ALBA (on CLAES beamline). Subsequent work on stability is based primarily upon effects from cryogenic cooling and is of little relevance to this DCM. We fully expect that the relative pitch vibration of the DCM crystals over the range 2-1000 Hz will be  $<0.1 \mu\text{rad RMS}$  when holding at a fixed energy.

The overall success of SST relies on the ability to scan the PGM and undulator simultaneously and quickly to allow continuous scanning. The BAT recommends that this issue requires immediate facility attention and coordination, and that appropriate resources are provided by NSLS-II for successful implementation.

The development of continuous scanning of the undulator and monochromator is basically complete and can be performed at the HXN beamline right now (even though this is not a core beamline requirement) and is expected to be complete at SRX beamline within one month (here it is a core requirement). We will certainly utilize this development work.

#### **4. Discuss and recommend priorities for activities within the commissioning plan.**

The BAT agrees that the prioritization for commissioning makes sense as described during the review. For SST the BAT agrees that HAXPES seems to be the ideal first experiment. For BMM it seems that priority be given to the purchase of the appropriate optical table for the experimental hutch so that repeated work of incorporating this into the beamline operation is avoided.

We have arranged to borrow a table as an interim measure before NIST can purchase a table (funding not yet allocated, but will be requested soon).

#### **5. Is the data acquisition plan adequate and a good match to the research program?**

The BAT fully understands and appreciates NIST's desire to "go it alone" and develop a data collection system that it controls and has prior experience with at NSLS. However, the inadequacy of the presented data acquisition, data management, and data analysis plans is the most significant concern of the BAT. Indeed, a data management plan appears nonexistent. The BAT strongly recommends that NIST works with NSLS-II to co-develop software in open source manner, presenting a common interface for users of similar techniques across beamlines. The complexity of the new beamlines with all of the motors and controls is greater than that of U7A and the BAT is not comfortable trusting the development of the software to a single individual. The whole user community will benefit from a beamline control, data acquisition and visualization package that is common across all of the spectroscopy and microscope/probe beamlines.

The work at NSLS-II on a program to control the experiment unfortunately started rather late in the overall build of the facility, however, work is now progressing very quickly on the program "BlueSky" which is in use on all currently operating beamlines at NSLS-II except XPD. XPD had to develop something quickly in order to get going quickly; support is consequently difficult and it is anticipated that migrating to BlueSky will occur in the near future. Several of the early beamlines suffered somewhat from software development in parallel with hosting Users; however the recent installation of BlueSky at SRX was very successful and includes spectroscopy functionality. Currently more than 35% of NSLS-II Users use multiple beamlines and a common User interface is seen as a necessity. Amongst the beamline staff at NSLS-II there is widespread praise for the support provided, and the DAMA group is

currently recruiting staff in order to support additional beamlines (in development and operation). We will continue to review development of the software; incorporating this into the beamlines and end stations will be technically possible and should be done in a phased approach.

We will organize visits to some of the beamlines for NIST staff in the near future so that the recent developments can be understood.

Moreover, teams at NSLS-II working with similar tools such as imaging detectors or electron analyzers should consolidate knowledge and effort into a single extensible, well-annotated package.

Agreed.

The BAT also suggest that NIST should be plan from early stages for remote operation for troubleshooting and also remote data acquisition, visualization, and hopefully also control.

Agreed, and again we hope to benefit from much of the development work already completed, and in progress.

#### **6. Community outreach –is there enough interest in the proposed research capabilities?**

The BAT fully supports the idea of NIST-level liaison connected to relevant technical communities. This is a win-win situation for all involved and will help NIST's synchrotron group achieve greater visibility and impact within the NIST organization and leverage expertise from a larger NIST community (for example, software development for data acquisition/analysis).

Ron Jones, the new NIST liaison, will visit BNL on Sept 28<sup>th</sup>, in order to get started with this.

The BAT recommends using a workshop model to inform the community about the new innovative measurement capabilities and suggest that the workshop is held around the time of first light?

After discussion, we envisage holding a workshop at the Users' Meeting in May 2018 to showcase the beamlines and some of the results from the Scientific Commissioning of the beamlines.

There is significant excitement about the project, and NIST left behind a great legacy of hundreds of users from its beamline at NSLS. Therefore, the BAT suggests that NIST synchrotron group initiates regular communication within NIST and with their extensive user community regarding progress and important milestones.

The BAT applauds the inclusion of IBM as a partner in the diffraction capability of BMM.

#### **7. Do you have any advice for the commissioning and operation of the beamlines, particularly as ongoing efforts in the construction project might be adjusted for beneficial impact? Do you have suggestions for prioritizing construction or commissioning efforts?**

The BAT recommends that Andrew Broadbent continues to be deeply involved in commissioning and early operation phases of the NIST project. His role in connecting the NIST team to the NSLS-II is critical, and will continue to be as the suite is optimized. For example, the BAT cannot fathom how the fast scan capability at SST-1 could be implemented without his advocacy, support, and coordination.

This is under discussion.

The BAT suggest that NIST implement continuous scanning immediately and not delaying its implementation –we recommend tackling this during commissioning of BMM.

We agree with this comment, but this is constrained by available funding. We would hope to be able to procure the necessary hardware so this will become feasible during the commissioning process. The EPICS software for the beamline and BlueSky would support this.

#### **8. Comment on synergy with other beamline programs at NSLS-II.**

The techniques that will be available at the NIST suite of beamlines range from totally unique (imaging XPS, imaging NEXAFS) to more standard XAFS at BMM. There is no obvious duplication with other efforts at NSLS-II.

The BAT recommends that BMM should better coordinate with QAS/ISS/TES, particularly with respect to software suite so that users could easily move between systems. Perhaps NIST also consider connecting to the gas handling system at ISS (goes to our earlier point about in situ capabilities) but the BAT notes that the ISS system is complex and it may be better for NIST to design something that is more flexible and cheaper. In a similar vein, SST should better coordinate with other spectroscopy beamlines such as CSX for software, swappable sample holder, etc.

Klaus's talk discussed this, but probably not in sufficient detail. We will try to organize an "open house" on a rotating basis at each of these beamlines in order for scientists to identify opportunities for improved coordination.

#### **9. Do you have suggestions to improve the beamtime allocation process?**

The BAT fully supports the allocation be such that it allows NIST to pursue NIST's mission driven scientific program in material measurement. The BAT also fully supports the wording of the Draft NIST NSLS-II Partner User Beamtime Allocation Process.

#### **10. Are there any safety concerns that have not been addressed adequately?**

The BAT could not identify any significant concerns regarding radiation safety. The BAT urges beamline personnel to keep housekeeping / trip-and-fall safety in mind, especially with large sample prep / staging area. It is expected that NIST beamline operations implement chemical safety standards in accordance with BNL/NSLS-II guidelines.

## 11. Miscellaneous

The BAT recommends careful consideration of a plan for the open space on the floor. It seems like a missed opportunity not to have a full wet chemistry lab.

A full wet chemistry lab will not be permitted on the experimental floor for various practical reasons, however, Dan Fischer is currently negotiating to secure access to the closest lab within the LOB (currently used for vacuum work). This would be quite suitable and have significant practical (cost) benefits over a lab on the floor.

The BAT is concerned that the current staffing levels when moved to operations might place undue strain on the NIST team. The NSLS-II standard is 3 FTE/beamline. Counting the NIST synchrotron group's permanent scientific staff only they have ~4 FTE and will operate 3 beamlines. Though the BAT realizes that some exemplary additional staff members are hired through contracts, much of these temporary personnel address instrument development rather than user support. NIST should ensure adequate staffing during regular operation so as not to spread the group too thin.

- The staffing of the beamlines is based on NSLS experience operating three beamlines.
- We envisage that increased automation will allow unattended running, eg overnight.
- Several of the staff on contracts have been with the beamlines for many years (20 years in the case of Zugen Fu).
- Conan Weiland (long term contract) is behaving in the same way as a staff member and will provide assistance to Users.
- Ray Browning is the only dedicated instrument developer, and it is anticipated he will take on a support role to help Users in the future.