2018 SAC Review of the NSLS-II Beamlines

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XPD – X-ray Powder Diffraction – 28-ID

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1. Executive Summary

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.

2. Beamline Capabilities

- An impactful effort has been made in provision and development of sample environments to support the theme of *in-situ* and *operando* experiments, in line with NSLS-II priorities. Hutch D is an asset to develop large complex experiments.
- XPD has proven itself to be versatile, supporting a broad program set. However, the program runs the risk of becoming too strained without the concomitant technical and scientific staffing effort necessary to support such a broad program set.
- Continued planning toward new beamlines offers the potential for spinning off nascent programs from XPD.
- ***The high resolution powder diffraction capability using analyzer crystals has not been put into service, though with the opening of the PDF beamline this should be done.***

3. Science Program and Impact

- ***The scientific productivity of XPD is excellent (>30 publications in 2018) and indicative of high impact for a beamline operating for only three years.***
- Scientific productivity ramped up fast and should be commended.
- The program is broad, as XPD matures it will be critical that strategic scientific directions are identified and appropriately supported.
- There is a need to support an in-house research program and use it to leverage the development of new capabilities.
- For the future, striking the right balance between user and staff research could benefit the productivity and impact of the beamline in the longer term. This could drive coalescence of new user communities.
- Careful scheduling between XPD and PDF will be necessary to exploit the range of sample environments available, but also ensure that each program develops unique streamlined capabilities.

4. User Support and Laboratories

- The support of users at XPD has been exemplary and their impact on experiments is significant, however there is a risk that staff will become overworked. Moving forward, the number of supported experiments/users will need to be balanced with available staff.
- There should be consideration to efficiently train new users. This should include both training to conduct experiments at the beamline, as well as active support and guidance for data analysis.
- ***There should be a continued goal to provide seamless support between beamline controls, data acquisition and management, and sample environments.***
- Consideration should be given for the support (maintenance, installation, service support) of standard sample environments. Could this be done by a central sample environment laboratory?
- Considering the current subscription, its diverse needs, and the proposed future plans the committee is concerned about the sustainability of the high levels of productivity achieved by the beamline in a short span of three years. Lack of adequate technical and scientific support could prove limiting for the proposed commissioning of new capabilities and meeting the demands for new scientific developments.

5. Partner Users

- XPD has three Partner User groups that are active at the beamline at different stages of maturity
    - Columbia/Billinge- Established PU (3 years tenure), provided the foundational software necessary for data control and acquisition; the partnership was instrumental for the early success of the beamline and features an outstanding science productivity.

  - Stony Brook/Weidner- Emerging effort in Large Volume High Pressure experiments, providing significant instrumentation, staff effort, and established expertise. Significant potential for future impact.
  - BNL/Ecker- Partnership with Nuclear Materials community providing enabling capabilities for radioactive materials research. Potential for impact within the nuclear community.

- ***Management should ensure PU's are aligned with overall strategy.***

6. Future Plans

- XPD should continue to work toward a comprehensive development plan that has defined strategic priorities.
- New capabilities will only be successful with appropriate investment and additional support. This should be considered when external collaboration is driving developments.
- Expert staff is necessary for the CT development. Strong support from the data management group will be critical to enable the CT capability to move forward.
- Modernizing detectors is necessary. Replacing the existing Perkin-Elmer flat panel detector by state-of-the-art pixel detectors should be considered a priority, especially in light of the microCT development.