2018 SAC Review of the NSLS-II Beamlines

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

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1. Executive Summary

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.

2. Beamline Capabilities

With a soft X-ray coherent flux of 10^{13} photons/sec, the CSX beamline exceeds by far the specifications of existing peer facilities. As coherent resonant X-ray scattering mainly suffers from an inherently low cross-section, this high flux is a most important characteristic. The design of the insertion devices with full polarization control (linear and circular) matches the scientific problems to be tackled. Tunable polarization provides an essential means of contrast and selectivity, considering the scattering factors have a tensorial character at resonances. The beamline is further equipped with a KB mirror system that can move the focal point along the beam direction by a few meters, providing flexibility to add end stations downstream from the main experimental chamber.

With the high coherent flux available from the beamline, various methods and techniques are pursued that take advantage of the beam characteristics and that currently are at different stages of development:

- X-ray Photon Correlation Spectroscopy (XPCS)
- Holography
- Ptychography
- Bragg Diffraction Coherent Imaging (BCDI)

Two more methods were presented during the review, which also are essential tools for the study of complex materials, and which instead take advantage of the brilliance of the X-ray source:

- Nanodiffraction
- Surface diffraction

For the experiments, the versatile end station TARDIS allows for soft X-ray scattering and diffraction. For adjusting the incident beam properties, two independent XYZ nanopositioners (piezo actuators) are located upstream of the sample. They are designed for accommodating various optics, like pinholes or Fresnel zone plates and the related order sorting aperture. In the former case, a variable beam diameter of 5 to 20 μm can be delivered to the sample. Using the latter, a sub-100 nm beam footprint (at focus) has been achieved. The instrument is equipped with a fast CCD detector with maximum frame rates of 100 Hz at Megapixel detection. This detector is a comparably new development with a substantial improvement compared to more conventional CCDs having frame rates of the order of seconds. The fCCD gives the CSX beamline additional unique capability and utility for a variety of experiments. The design of TARDIS allows for efficient cryogenic sample cooling with base temperatures down to 4 K (15 K, when total electron yield is to be measured). The cryogenic manipulator has motorized XYZ translations and theta angle rotation, all using external drives. The combination of these capabilities renders TARDIS a worldwide unique instrument for fast coherent soft X-ray experiments at the lowest temperatures. Recently, a second end station dedicated to transmission geometry holography was built and is about to start commissioning and operation. Its main feature regarding sample environment is an in-vacuum magnetic field (~1 Tesla, custom-designed) and current bias capabilities that will enable full-field imaging of magnetic nanoscale phenomena, like domain (walls) and skyrmions.

Both TARDIS and the new end station efficiently utilize the photon beam provided by NSLS-II in terms of brilliance and coherence. Ongoing technical developments and improvements are essential to serve a broad pool of users and increase participation in the X-ray science enabled by CSX. Therefore they are encouraged. The current operation mode (50:50) with the sister beamline IOS works well, for the time being, to support these developments.

3. Science Program and Impact

The scientific program of the beamline is very well matched to the technical specifications and the techniques available at CSX. The resulting high-impact scientific output reflects important contributions to the NSLS-II strategic program of "quantum and complex materials". This has been convincingly conveyed by the staff's and users' presentations and is reflected in the publications that result from experiments at the beamline. The scientific topics (grouped by technique) that have been covered so far include:

- X-ray Photon Correlation Spectroscopy (XPCS)
    - Charge density wave dynamics and memory effects in superconducting cuprates
    - Domain wall motion in nanomagnets
    - Organic liquid crystals
    - Fluctuations of antiferromagnetic domains in transition metal oxides
- Holography
    - Magnetic textures and dynamics
- Ptychography
    - Crystallization in biominerals
- Bragg Diffraction Coherent Imaging (BCDI)
    - Artificial spin ice & nanomagnets
- Nanodiffraction
    - Antiferromagnetic domain texture in transition metal oxides

These scientific activities produced excellent output so far (2x PRL, 1x PRB, 1x Nat. Comm.), while six more papers are under review. The review panel clearly understands that the complexity of the experiments and their data analysis does not lend itself to high-throughput publications. In the beginning, special analytical tools even had to be developed to make use of the massive amounts of data produced by the experimental station. The performance of the beamline is in line with these expectations: A relatively low number of papers in the first year is understandable and is now growing at an impressive rate. Future high performance can be anticipated from the number of presently submitted papers. With the unique capabilities of CSX, a high impact of the results must be anticipated. Moreover, essentially all publications appear in high-tier journals with an average impact factor of ~ 8.5.

The very ambitious scientific program has attracted several user groups on very different fronts with a core user community specialized in the study of electronic and quantum materials. While this has been very successful, now it is the most crucial time to expand their user base. The efforts of the staff towards organizing workshops and conferences are very well received by the panel, see section 4 (User Support and Labs). In this context, science commissioning beamtimes are also an effective vehicle to engage external groups and establish long-term collaborations involving sharing of personnel. This approach and related programs (director's postdoc, resident doctoral student) should be encouraged and expanded as much as possible.

4. User Support and Labs

User support at CSX is at an extremely high level. It is based on the expertise and the dedication of the beamline staff who have provided outstanding service to users. It has to be noted that such a level of engagement is required for the technically and methodologically complex experiments at the beamline. The staff further pursues a strong program in developing and educating their user community, e.g., by organizing regular workshops at user meetings and even international conferences such as REXS 19.

While the scientific staffing of the order of 2 FTE's is commensurate with current efforts, it is right at the limit to sustain both excellent user service and technical development. Accordingly, the performance would substantially benefit from adding personnel resources. An increase of staff, while highly desirable, may be difficult to realize; therefore other schemes, like, e.g., via shared postdocs is highly recommended, possibly in connection with the Partner User program.

Because of the technical complexity of user experiments at CSX, additional support for customization of the experimental setup to address specific scientific cases would significantly accelerate scientific output. Achieving optimal use of the precious beamline operating shifts enables higher research productivity and higher turnover of external users. However, technical support for the beamline has been mostly inadequate, especially in the last 18 months. This has impacted user operations: Problems that needed last-minute troubleshooting such as during GU shifts could have been prevented with dedicated technical staff that would remove less demanding beamline maintenance & commissioning tasks from the scientific staff. The operation of the beamline would undoubtedly benefit from more dedicated technical resources; our panel recommends 1 FTE technician for beamline CSX.

A particular issue, at least in the past, has been identified in the BlueSky software control environment: The learning barrier for users is very high and frequent reconfiguration of the software add to the difficulties in executing script-based beamline operations in the absence of stable APIs. Reliable software controls would make CSX more user-friendly and increase data throughput. Also, future challenges in data management and access have to be considered: while data storage is currently not an issue, server capacity limits may appear sooner than anticipated due to increasing data streams, taking, e.g., the fast CCD detector into account. On a related front, remote access to data and data transfer have been problematic and should be streamlined to further support the users.

Access to support labs at NSLS-II has been highly beneficial for user operations, enabling special preparation of samples or beamline components. To further enhance auxiliary sample preparation activities, a more formal involvement of the Center for Functional Nanomaterials (CFN) could be considered to alleviate the burden on users for highly complex coherent X-ray scattering experiments, notably holography which relies on sophisticated and very precise nanopatterning of sample templates. Here, the capabilities of the CFN might be of substantial benefit. In general, a common NSLS-II / CFN proposal format to leverage advanced sample preparation capabilities at CFN may be valuable both for complex materials and for engagement of the user community.

5. Partner Users

The Partner Users Program (PUP) is considered a very important and useful scheme to both acquire additional resources and ensure the long-term involvement of strong scientific groups. CSX has maintained a very successful collaboration with the X-ray scattering group of the Condensed Matter Physics & Materials Science Department (CMPMSD) at Brookhaven National Laboratory. This is a great opportunity to join forces with a local group of experts that can boost productivity and support technical developments.

The initial PUP agreement involved a loan of the TARDIS diffractometer, that was originally designed and assembled by the CMPMSD at NSLS, to beamline CSX. Additionally (but this may have been unofficial), a staff member (X. Chen) of the CMPMSD X-ray scattering group participated in the CSX beamline activities and duties. In exchange, CMPMSD was granted ~ 10% of the user shifts available at CSX. This original arrangement has led to a fruitful and prolific collaboration between NSLS-II and CMPMSD groups. The very positive benefits on the scientific output are reflected by the fact that the initial core publications of CSX were borne out of this PU group.

Thus, the PUP has been a highly valuable initiative and one that has supported the early scientific productivity of CSX. This panel appreciates the historical circumstances and the underlying changes of affiliations that accompanied the TARDIS transition from NSLS to NSLS-II, but still, we must register that the partnership does not appear to be fully reciprocal in its current iteration. For this reason, we recommend that the terms of the agreement be carefully reviewed by the NSLS-II, particularly given that the primary user operations at CSX rely on the TARDIS diffractometer, which however is not officially owned by the beamline or NSLS-II. We strongly recommend that, if the PUP with BNL-CMPMSD is renewed for three years, the NSLS-II management negotiates what CSX gets in exchange for the 10% beamtime in the partnership (capital investment, involved beamline staff, dedicated postdoc, or else), also considering the depreciation of TARDIS which suggests that the PUP share should otherwise taper down over time. In the long run, it is imperative that NSLS-II resolve the issue of the permanent ownership of the TARDIS chamber.

6. Future Plans

The plans presented during the review meeting are very ambitious. Presently, six major lines of experimental capabilities are considered as already listed in section 2 (Beamline Capabilities). This list involves several methods that each represent an ambitious program, given the complexity of the individual experiments and corresponding data analysis. Nevertheless, all the methods present a straightforward and optimal use the properties of the beam delivered by NSLS-II. This applies to the coherent experiments as well as nanodiffraction and surface diffraction that rely on the brilliance of the source. Given the finite resources of the beamline in terms of scientist staff, technical support, and, eventually, the beamtime available to users, pursuing all these methods is undoubtedly too ambitious. In the long run, scientific and technical priorities will have to be defined in order to maintain a leadership status worldwide.

Nevertheless, at this early stage of operation, the beamline can and should be ambitious and get engaged in development activities to survey the parameter space and identify priorities. This must be performed in concert with the user community to assess the external demand. The review panel supports the beamline's pursuit of a variety of experimental methods to address many scientific cases to intercept a broad user base.

XPCS is already at a rather a mature stage, with three published papers. Other methods are catching up. With the installation of a separate holography chamber, an important new setup for imaging will become available, and the next 1-2 years will be important to capitalize on emerging opportunities. While ptychography, BDCI, and nanodiffraction are highly promising to pursue, surface X-ray diffraction seems to have a somewhat less impactful perspective on a reasonable timescale. Generally, separation of the methods through dedicated end stations that complement the more versatile TARDIS chamber may be a successful approach.

The review panel focused much time and attention on the proposed recanting of the shared undulators with 23-ID-2, both in the presentations and discussion with beamline staff. The availability of in-line undulator operation with a flux enhancement by a factor of 3.5-4 is crucial to maintain the leadership in coherent soft X-ray science and remain competitive as other facilities upgrade to low-emittance operations (Max IV, ESRF-U, APS-U, proposed ALS-U). The idea of matching the two undulators by inserting a phasing magnet is very well received by the review committee and is highly recommended. Consequently, increasing the canting angle to further separate IOS and CSX, while technically possible, would hinder future flux improvements and compromise the competitiveness and leadership of the beamline. *We strongly advise against this canting option*. It is critical to avoid compromising the competitive edge of CSX internationally.

The current scheme of shift sharing with the IOS beamline (50:50) is working well, but this share should be revisited as the situation, and user load evolves over time. The current oversubscription ratio (~ 2) is a good target, but the overall number of proposals remains on the low side. Therefore, it is imperative to expedite commissioning of additional capabilities to expand the user base. Parasitic time with IOS (23-ID-2) could also be used productively to screen samples or test proposed scientific cases or special experimental geometries. Dedicated technical support will be critical here.