Final Report:

Coherent Diffraction Imaging (CDI) beamline

Conceptual Design Review

An account of the deliberations of the ad-hoc review committee for the CDI-Conceptual Design

On-site review October 25th and 26th, 2018

Preliminary Report Date November 13th, 2018

Final Report Date January 14th, 2019

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Executive Summary

The National Synchrotron Light Source II (NSLS-II) is a highly optimized, third-generation synchrotron facility with 21 operating beamlines and 7 more in the commissioning phase. NSLS-II provides world-leading brightness and flux, as well as exceptional beam stability over a broad range of photon energies from infrared to hard X-rays. NSLS-II has room to host several more beamlines. Among new ones NSLS-II proposes to build is a beamline specifically optimized for coherent diffractive imaging (CDI). A team led by Garth Williams at NSLS-II has prepared a Conceptual Design Report (CDR) for the CDI beamline. The CDI beamline proposes to use forward-scattering and Bragg CDI with coherent 5-15 keV X-rays to measure structure, lattice deformation, and fast dynamics in single and polycrystalline materials. Full-field CDI will be used to study crystal sizes up to 10 µm in size at a spatial resolution extending to a few nanometers. Scanning the sample through the x-ray beam will enable studies of much larger samples with the same resolution. The combination of this instrument with the high brightness of NSLS-II will result in a powerful tool for the study of materials systems, particularly real-world functional materials to enable knowledge-directed materials engineering. NSLS-II organized a review of the CDI beamline CDR on October 25-26th, 2018. The purpose of this review was to assess the maturity of the beamline conceptual design and to identify any concerns that could prevent the project from successfully moving forward to the preparation of a preliminary design for the CDI beamline.

Charge to the Review Committee

The purpose of this review was to assess the maturity of the beamline conceptual design and to identify any concerns that could prevent the project from successfully moving forward to preparation of a preliminary design for the beamline. The relative merits of the short (60 m) and long (100m) configurations of the beamline were of particular interest to the NSLS-II management. The charge to the review is given in Appendix A. The membership of the committee is listed in Appendix B.

Review Process and Agenda

The review was held at BNL on October 25-26th, 2018. The CDI beamline team provided information to the review committee in advance of and during an on-site review. The committee evaluated the performance to date on the beamline optical design, endstation design, choice of insertion device, other technical requirements, and cost and schedule.

Documents submitted in advance of the review, in addition to the review charge, agenda and copies of the presentations, included the following:

1. A Coherent Diffractive Imaging Facility at NSLS-II: Conceptual Design Report (October 22nd, 2018).

2. Report of the Beamline Advisory Team of the BCDI beamline First BAT meeting (February 27th, 2018).

3. Response to first CDI BAT report (version 3).

4. Cost and Schedule Summary (October 24th, 2018).

After an introduction by NSLS-II Director John, Hill, the CDI beamline team, led by Garth Williams, presented the main aspects of the project during the first day of the review. Committee members submitted questions and received responses during the presentations. The second morning continued with an additional question and answer period, then the committee convened in a closed session to draft the closeout presentation. The closeout was held prior to lunch with the committee presenting their preliminary results to NSLS-II management and the CDI beamline team. The review agenda is listed in Appendix C.

Review of the Conceptual Design

This section of the report is aligned to the specific charge questions.

1- Do the preferred conceptual design and associated requirements support the CDI beamline scientific objectives, consistent with the properties of the NSLS-II source and facility?

Comments

- Yes. The CDI beamline conceptual design supports the scientific objectives and would provide a unique capability that would set NSLS-II apart from other facilities. The team has done a good job developing a conceptual design to meet these objectives.

- The design supports the objective to perform measurement of Bragg and forward diffraction patterns, or two Bragg diffraction patterns, simultaneously.

- The design supports the objective to perform CDI of few-micron size samples.

- The design is consistent with and exploits the best parameters of the NSLS-II source.

Recommendations

- Consider the possibility of delivering beam size down to 500 nm to the sample.

- Evaluate the possibility of increasing the sample-detector distance up to 10 m, which would enable studying larger samples.

- Update the science case and articulate the most compelling questions that could be addressed with this beamline to make the best case for its unique capabilities internationally as well as domestically. This should be done for both the first experiments envisaged as well as for the 5+ year time scale, taking into account the requirements of strong local user groups, the CFN, participating universities, industry, etc. to deliver the best end-station capabilities.

- Organize a workshop to engage these communities, help guide selection of the technical capabilities, obtain letters of support, and strengthen the overall science case.

2- Please comment on the technical feasibility of the preferred conceptual design. Specific features on which to focus include (but are not limited to) the optical layout and length of the beamline, the size of the experimental hutch, the endstation instrument, detector options, infrastructure provisions, and choice of insertion device. Have appropriate design options and alternative concepts been explored? What are their strengths and weaknesses, in upholding the scientific objectives?

Comments

- The preferred conceptual design for a long (100 m) beamline is technically feasible and meets the main scientific and technical objectives.

- The short (60 m) design is technically feasible and meets many but not all of the objectives. Compared to the 100 m design it will offer less thermal and vibrational stability, working distance, room for complex sample environments, and may limit the detector arm length and angular range. These limitations could impact the scientific scope and future upgrade potential for the beamline.

- The 100 m optics and endstation design will better accommodate various sample environments (high pressure cells, cryostats, magnetic fields, ...) and thereby support the science case better than the 60 m design.

- The choice of a conventional insertion device (warm hybrid in-vacuum undulator, not superconducting) is good. The factor of 2 greater flux that an superconducting undulator could provide does not merit the added risk and potential complexity.

- The choice of horizontally deflecting double-crystal monochromator is best for stability and is adequate for most of the science envisioned, especially the forward scattering case. Temporal coherence could be limiting in BCDI experiments for samples larger than a few microns.

- The double multilayer mirror monochromator offers high flux and broader bandwidth suited to some experiments, such as to follow the evolution of strain in multigrain samples and forward-scattering measurements. However this does not appear to be a high priority for the main CDI science case and adds risk of sample damage.

- The zoom focal system using mirrors is innovative and provides flexibility to deliver spot size and spatial coherence properties matched to a range of sample sizes.

- The conceptual designs for the sample goniometer and detector arms appear feasible.

- Dynamical diffraction is a concern because it could limit the maximum sample sizes that can be studied by BCDI.

Recommendations

- Evaluate whether another insertion device type such as an APPLE device could be used to deliver vertically polarized x-rays to obtain more flux through the monochromator and prevent the diffraction "blind spot" at 90°, while still meeting the requirements of the CDI beamline. The option of a tailored gap ID may also be worthwhile to study for future.

- Explore, e.g. by detailed simulations, partial coherence methods (both spatial and temporal), to study 5-10 µm samples using this beamline.

- Decouple the sample goniometer and detector arms to isolate the sample and detector motions.

- Investigate whether the final focusing optics and sample goniometer can be mounted on the same granite block.

- Evaluate whether mechanical nonlinearity (wobble) of the zoom mechanism will affect the beam properties at the endstation.

- Include the DMM in the design for ray-tracing and radiation safety calculations, but consider implementing it in a later developmental or upgrade phase for the beamline.

3- Does the design present technical risks? Does the design present scientific risks (e.g. may not be able to uphold some scientific objectives)?

Comments

- The design is feasible and does not present significant technical risks.

- Compromises on the planned technical scope, especially for the short (60 m) beamline option which may result in a shorter detector arm length or smaller space for sample environments, would pose risks to the science case. These limitations would compromise the competitiveness of the beamline internationally as well as in the US as the ESRF-EBS and APS-U will be coming online at about the same time.

Recommendations

- Investigate methods to study samples sizes up to 10 µm at energies above 5 keV with this instrument in more detail and quantitatively, e.g. with partial coherence. We suggest starting on this soon.

4- Are there safety concerns related to the installation and operations of the beamline and endstation concepts presented?

Comments

- The installation and operations of the beamline do not pose unknown safety concerns.

- The large mechanical motions required by the detector arms may pose a unique safety concern. Collision sensors may be helpful to prevent equipment damage, while bumper switches should be part of the PPS.

5- Please comment on the future upgrade potential and associated tradeoffs in the beamline design.

Comments

- The large hutch offered by the long (100 m) beamline design provides the greatest upgrade potential for complex sample environments, complementary detection modes such as emission spectroscopy, another diffraction detector, and timing experiments (with associated laser hutch).
- The 60 m design could limit possibilities for further development and upgrades of the beamline.
- Plans for a separate entrance to a dedicated laser hutch would enable more efficient pump-probe and other laser experiments.

6- Is the preferred conceptual design mature enough to proceed to the next (preliminary) stage of engineering design development?

Yes, provided:

- More detailed studies are carried out to see whether sample sizes up to 10 µm at 8 keV could be imaged by CDI with the present beamline design and detector technology. Extension of the accessible sample size to this range would provide a unique capability.
- Realistic simulations of wavefront propagation through the DCM (including heat load) and focusing optics to the sample are performed. The corresponding coherent flux is estimated.
- Provision is made to characterize the quality of the wavefront near to the sample location on a routine basis (especially during commissioning), including its sensitivity to vibrations.

7- Are the cost and schedule estimates presented realistic for this stage in the development of the beamline design?

Comments

- The team has done a good job to evaluate the beamline costs at the conceptual design stage. We have some concern that the labor cost estimates driven by overhead rates are unnecessarily high.
- This is an optimistic schedule based on the best possible funding scenario.
- Timely development of the CDI beamline is important given the new sources and facilities coming online soon.

Appendices

Appendix A – Review Charge

CDI Beamline Conceptual Design Review October 25-26, 2018

Charge to Committee

1. Do the preferred conceptual design and associated requirements support the CDI beamline scientific objectives, consistent with the properties of the NSLS-II source and facility?

2. Please comment on the technical feasibility of the preferred conceptual design. Specific features to focus on include (but are not limited to) the optical layout and length of the beamline, the size of the experimental hutch, the endstation instrument, detector options, infrastructure provisions, and choice of insertion device. Have appropriate design options and alternative concepts been explored? What are their strengths and weaknesses, in upholding the scientific objectives?

3. Does the design present technical risks? Does the design present scientific risks (e.g. may not be able to uphold some scientific objectives)?

4. Are there safety concerns related to the installation and operations of the beamline and endstation concepts presented?

5. Please comment on the future upgrade potential and associated tradeoffs in the beamline design.

6. Is the preferred conceptual design mature enough to proceed to the next (preliminary) stage of engineering design development?

7. Are the cost and schedule estimates presented realistic for this stage in the development of the beamline design?

Appendix B – Review Committee

Member	***e-mail***
Ian McNulty – MAX IV (Chair)	ian.mcnulty@maxiv.lu.se
Andrew Aquila – SLAC	aquila@slac.stanford.edu
Xiaojing Huang – BNL	xjhuang@bnl.gov
Ivan Vartaniants – DESY	ivan.vartaniants@desy.de
Lutz Wiegart – BNL	lwiegart@bnl.gov

Appendix C – Review Agenda

CDI Beamline Conceptual Design Review
October 25-26, 2018
Agenda

Thursday, October 25, 2018 – Bldg. 745, Room 156

08:30 – 09:00 Committee Executive Session
09:00 – 09:30 Welcome and NSLS-II Update ..... J. Hill
09:30 – 10:30 Science at the CDI Beamline ..... G. Williams
10:30 – 10:45 Break
10:45 – 11:45 Source Options and Optical Simulations ..... O. Chubar
11:45 – 12:00 Discussion
12:00 – 01:00 Lunch
01:00 – 02:00 Endstation Requirements ..... G. Williams
02:00 – 02:30 Beamline and Endstation Layouts ..... Y. Zhu
02:30 – 02:45 Break
02:45 – 03:15 Cost and Schedule ..... L. Berman
03:15 – 04:00 Discussion
04:00 – 05:00 Committee Executive Session
05:00 Adjourn
06:00 Dinner

Friday, October 26, 2018 – Bldg. 745, Room 156

09:00 – 10:00 Discussion and Questions/Answers
10:00 – 12:00 Committee Executive Session
12:00 – 01:00 Lunch
01:00 – 01:30 Closeout
01:30 Adjourn