December 2008 BAT Report for the
High Resolution Inelastic X-ray Scattering Beamline

Members present: **Burns**, Cunsolo, Hill, Krisch, Mao, Scopigno, Shapiro, Shvydko
Absent: Chen

The Beamline Advisory Team (BAT) for the High Resolution Inelastic X-ray Scattering Beamline at NSLS-II had its first official meeting on December 5, 2008, with the members listed above present. For this meeting, we were charged with three tasks: 1) review the conceptual design of the beamline (at 50% level of completion), 2) discuss issues raised by the EFAC, and 3) review cost and schedule outlooks for the next 3-6 months. In addition to these charges, the BAT considered a number of other issues as described below.

Our report goes as follows. We begin with a discussion related to the charges to the BAT. Additional questions from the BAT are then considered. We conclude with several recommendations for the beamline and a proposed timeline for early milestones in the R&D.

1) Charge: Review of the conceptual design.

The overall plan for the beamline was described by Yong Cai. Many of the essential features of the design are known. In particular, an understanding of the optics and requirements for the front end, and the optics up to the sample seem well established. The details of the analyzer mechanisms are not as far along, but the mirror which is required for collecting sufficient solid angle appears to be quite feasible. In fact, it appears that commercial vendors are capable of making a device that meets all of the specifications. However, the precise details of some of the analyzer elements, and therefore the exact hutch dimensions remain under study. A final decision requires the completion of ongoing experiments on the optics.

One area of significant concern is the fact that the insertion devices for the beamline have not been chosen. Since this technique involves experiments with very low count rates, the flux per meV is a critical parameter. The "baseline" device for this beamline, the U20-3m device actually delivers about 20% less flux than the minimum believed adequate. Other devices (such as the U-17 5.5 m) deliver about twice the flux of the U-20-3 m. However, NONE of the potential sources, not even the "baseline" device are currently approved by the accelerator engineers. We strongly suggest working with the accelerator systems team to find the source that provides the maximum flux allowable within machine parameters, and, indeed, to push these limits as much as is practical. With a flux limited technique, a factor of two improvement will greatly improve the scientific output of the beamline.

Another issue of importance is the question of the length of the beamline. It was pointed out that certain sections of the ring which are designed for long beamlines also allow for an extended beamline (but still within the ring building), since the vibration isolation joint can be extended out to the external wall. This idea should be evaluated in detail, but especially considering the fact that the R&D for this project is not complete,

the BAT recommends keeping this possibility open in the event that it turns out to be necessary.

Consistent with the EFAC recommendations, we suggest that further refinement of the beamline design wait until the results of the tests of optical components are done. Key decisions about beamline details require real experimental proof of the design before proceeding much further.

In conclusion, the committee feels that the beamline layout is at the required level of completion for this stage in the project, but that further refinement should await the ongoing optics development work.

2) Charge: Response to EFAC Comments

There were several comments from the EFAC (excerpted below in italics) which were addressed as described below.

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1) *We recommend (1) that every effort be made to test critical optical components on a time scale compatible with the beamline design decisions and, (2) that decisions about how to proceed with this beamline be delayed until those optics have been tested. We suggest that count-rate estimates be made in some expected experimental conditions, including, for definitiveness, ideal calculated optical throughput and energy resolution, the effect of sample thickness/transmission/ environment, and desired momentum resolution. As for testing the optics, while finally this will require a third generation source, the work to implement first tests at NSLS seems a step in the right direction. NSLS-II should consider making a semi-permanent installation at NSLS to do this.*
    1) The BAT agrees that detailed testing of the critical optical components should be carried out as soon as possible, and indeed such work is already underway. Preliminary tests of beamline optics have been carried out. The project decision to establish a beamline (X16A) for optics testing at the NSLS is extremely encouraging and is just what the EFAC requested. The project team has also come up with a series of target dates for testing critical components which will allow final decisions about the beamline to be made within the time available. In particular, the BAT feels that a demonstration of the sharp resolution function (at 1 meV) is especially important. If the resolution function is shown to be as good as has been calculated, it means that the instrument will have a unique capability to do groundbreaking science even if it does not (immediately) meet the ultimate resolution goal of 0.1 meV.
    2) The beamline team, working together with the BAT, will also carry out accurate estimates of count rates on several sample systems as indicated below. The BAT agrees with the importance of having such calculations in hand in making science-driven beamline decisions.

2) *In this context, the decision not to pursue our previous recommendation for a medium (~50 meV) resolution setup, being both technically feasible, and scientifically extremely interesting, is regarded with some concern.*

1) While the BAT admits that the 0.1 meV spectrometer is a challenge, a 1 meV or sub 1 meV spectrometer with an excellent resolution function and high flux seems quite feasible and very interesting scientifically. However, the question of a 50 meV option (for example as a back-up) is outside the scope of the BAT. This BAT was assembled to push scientific programs which require very high energy resolution, and our program is incompatible with a 50 meV spectrometer. Essentially, this backup plan is equivalent to creating a different beamline to carry out a different science agenda. It was felt this would be a distraction to the beamline team to pursue this in parallel with the 0.1 meV instrument which has a very different science agenda and very different optics schemes. So while such a plan (to create a second beamline for IXS with 50 meV resolution) may be a good idea from the point of view of NSLS-II, it is a management decision outside the scope of this team, and if it is to be pursued should be done so by another group.

3) *Finally, having looked at the present beamline design, we make the following comments: (1) the "comb-crystal" sounds relatively hard, (2) the 1 meV followed by channel-cut to 0.1 meV sounded relatively promising, (3) the step from a "CDW" backscattering scheme to a "CDDW" in-line scheme seems a technically difficult one, with large impact on BL design, and should be tested relatively soon, and, (4) some scheme for simultaneous collection of several momentum transfers (e.g. using an area detector, as suggested by Baron for the February meeting) should be considered.*

Responses to the individual suggestion are below.

1) Tests to evaluate the comb crystal idea are underway and should determine its feasibility. While the implementation is certainly difficult, it does solve some other major problems for the beamline and the BAT agrees with the project team that the idea should be pursued.
2) The 1 meV followed by a channel cut to 0.1 meV scheme is part of the beamline design plan, and indeed was in the original CDR design.
3) The shift from CDW to CDDW may indeed be difficult, and a timetable for testing of this scheme has been proposed (below).
4) The BAT recommends, and the project team has agreed to begin looking into possibilities of simultaneous detection of several momenta.

3) Charge: Cost and Schedule Outlooks for the Next 3-6 months

The beamline team will have several hires coming up over this period, and also appears to have a detailed timeline for beamline elements. A detailed budget plan has been made by the design team, with what seem to be reasonable cost outlooks for the next 6 months or so. A series of early critical milestones was discussed at the meeting and are shown below.

Due to the especially innovative nature of this beamline, accurate cost estimates for all the components are likely to be difficult, so we suggest that the budgeting be done

with this in mind. Similarly, critical milestones need to be scheduled and pursued early in case of delays.

Additional comments from the BAT

The BAT discussed at length a strategy in which the beamline initially would come up in a commissioning phase with a 0.5 - 1 meV spectrometer, and then bring online a 0.1 meV spectrometer a year or two into the life of the operating facility (when for example the machine currently would be approaching its design goal of 500 mA and the 0.1 meV instrument should have sufficient flux to permit realistic experiments). In this case the first instrument on the floor would have a somewhat lower resolution, with an upgrade path to the higher (0.1 meV) instrument. This seems prudent; since the entire instrument is the first of its kind, it seems reasonable to first make a lower resolution instrument which is more forgiving for the various tolerances and will allow a design "shake down" before building the final instrument. Note such an instrument would be best in class in terms of resolution, and with far more flux on the sample than the final (0.1 meV) instrument. Going straight for the highest resolution increases the risk of an unexpected "show-stopper" arising, or perhaps more likely an unproductive beamline being built with the required resolution, but insufficient flux to carry out many desired experiments.

Note, if adopted, such a strategy should not change the focus of the present R+D which would still be dedicated towards demonstrating the feasibility, and practicality of achieving 0.1 meV instruments, which remains the goal of this beamline and this BAT.

While the committee was generally in favor of this idea, it was decided to delay a final decision until the next BAT meeting when more experimental testing of the optical components will have been carried out, and more information will be available with which to make a decision.

BAT Recommendations

In addition to the points noted above, the BAT has the following recommendations for the project:

1) Work with the accelerator division and push for highest flux undulator possible. This is extremely critical.
    a. Both initial undulator choice and a plan for future upgrades are needed.
2) Explore the possibility of using a Be compound refractive lens at the front of the beamline to reduce divergence.
3) Additional calculations are needed for some features of the spectrometer.
    a. What is the limiting *q*-resolution depending on the initial divergence and how does this effect beamline design parameters (such as length)?
    b. What are the limits on sample sizes at various *q* and energy resolutions values?
    c. What is the scheme for the analyzer – are options for a position sensitive detector (PSD) possible?

d. Make realistic estimates of count rates for several experiments of interest (possible first experiments). The BAT will work with the project team in these calculations, which we are asking be complete by March 2009.
    i. v-SiO_2
    ii. H_2O
    iii. Phonons in cuprates
    iv. High pressure N_2 or O_2 crystal
e. Sketch out a means for employing multiple analyzers to ensure that final design is compatible with such an upgrade path.

4) Accurately measure the resolution function of the asymmetric optics.
5) Final tests for a working spectrometer will require access to a third generation x-ray source (such as the APS). Plans for where and how these tests will take place should be developed soon, with the expectation that a Partner User Proposal (PUP) would be submitted to the APS well in advance of when the beamtime would actually be needed. In a related issue, ongoing collaborations between NSLS-II and APS teams working in this area should be continued and strengthened if possible. The BAT was unsure as to how well these were working currently. It is recommended that more attention be paid in this area.
6) Finally, it is important to establish a timeline for all R&D milestones and critical decisions. A timeline for some of the critical initial steps, based on discussions at the meeting, is below.

Timeline milestones

At the BAT meeting the following milestones were prepared, in discussion with the project. The BAT recommends that these be incorporated into the formal project schedule and that progress be tracked against them.

March 2009	Realistic count rate estimates for 4 key experiments completed.
June 2009	Actual measurement of the resolution function for CDW scheme be performed.
Sept 2009	Fabrication and testing of first comb crystal cut for 1 meV. Energy resolution and efficiency measured.
Sept 2009	Fabrication and testing of multilayer mirror. Demonstrate required specs can be met.
Nov 2009	Demonstration of the CDDW/CDDW scheme (beam passed through all optics).
Sept 2010	Demonstration experiment at 1 meV with a standard sample (Plexiglas).

Summary

The BAT feels that the project team has been making excellent progress developing the beamline. First tests of optical elements have been carried out, and a beamline devoted to optics testing at NSLS-II has been chosen and is under development. Staffing issues are being addressed, the beamline design is progressing, and a budget/schedule has been developed. The next crucial step is creating and verifying the optics, and the BAT encourages the project team to continue to push forward hard on this work. Additional team members will be hired soon and should allow the project to progress rapidly on the development. We look forward to hearing the progress at our next meeting, which we request be scheduled in the July 2009 timeframe.