The First Official NSLS-II Powder Diffraction Beamline Advisory Team Meeting

Date: Monday November 24th, 2008.

Present: Simon Billinge (Columbia Univ), Peter Chupas, Lars Ehm, Jon Hanson, Jim Kaduk, John Parise, Qun Shen, Andy Broadbent, Konstantine Kaznacheev

Charges:

1. Review conceptual layout and design of the beamline (at level of 50% completion)
2. Discuss issues raised by the EFAC
3. Cost and schedule outlook for the next 3-6 months

A summary report of the meeting from the BAT Spokesperson is expected within 3 weeks of the meeting.

NSLS-II entrance

Draft Agenda:

08:30-09:00	Light breakfast and informal discussion.
09:00-09:45	Qun Shen, XFD Director: Welcome and introductory remarks. Project update, schedule and staffing. Role of the BAT and project staff.
09:45-10:30	Andy Broadbent: Update on current beamline conceptual design, as well as any other issues. (Zhong Zhong & Lonny Berman have been invited).
10:30-11:00	Coffee break
11:00-11:30	Andy Broadbent: Initial and mature scope of the beamline. Beamline design schedule outlook, beamline budget discussion (see attached spreadsheet).
11:30-13:00	BAT Spokesperson. Working lunch from 12:00. • Discussion of issues (e.g. issues raised by EFAC): • Scientific mission and priorities. • Design requirements • Interface with user community. • Technical developments and challenges.
13:00-14:00	Signing ceremony (Steve Dierker and BAT Spokesperson), and any questions for the NSLS-II Project Director.
14:00-15:00	Discussion of beamline capabilities: Day 1 experiments, hardware (lead by John Parise) and software (lead by Simon Billinge). (Bob Dalesio invited, Peter Siddons is likely to be off-site).
15:00-15:30	MaDiS (Materials Diffraction Suite) discussion
15:30-16:00	BAT Spokesperson – Close-out summary on items discussed, and report assignment. (30mins)

Project update:

The meeting began with Qun Shen presenting a summary of the overviw and status of the NSLS-II project. The project just completed its reviews for CD3. The overall impression is that no obvious roadblocks emerged from these reviews, though the reports are not available yet. The main building has been enlarged providing much needed extra floorspace, in response to feedback at earlier meetings, with no change in overall project budget. This is good news.

- Qun noted that if our design requires it, we can have beams going outside the building but it is better if they know that before they pour the concrete for the building floor as there has to be an underpass built so a tall person (e.g., Jim Kaduk) can pass under without bumping his head. This is much cheaper before the floor is laid. This info was note but this is not currently in our plans.
- Call for LOI's for new beamline concepts will take place in 2009 after a facility scientific action plan is completed. This is important from the point of view of MaDiS (Materials Diffraction Suite) and the members of PINGBAT hope to contribute leadership in a broader materials instrument suite.

- Qun summarized the hiring activities for a PING beamline scientist. Eight people have been interviewed with one more to go. PINGBAT is involved in this, with Jon Hanson managing to attend all the interview talks and other BAT members such as Peter Stephens attending certain talks. The sense was that none of the early interviewees were suitable, however, there was optimism about the last two interviewees who both look very strong and highly qualified. PINGBAT members provided feedback.
- Qun laid out future hiring plan for the beamlines, which includes 4.5 FTE's at full capacity under operations: two scientists, two techs and 0.5 engineer.
- Comments of the Lehman committee specifically regarding PING were shared:
    - The Committee strongly agreed that the powder beamline should be sited on a damping wiggler beam port.
    - The beamline proposed should provide a world-class facility for high-energy powder diffraction and PDF experiments on materials science samples.
    - The energies chosen for the beamline, 50 and 80 keV, are obtainable with the optics proposed and are suitable to the scientific mission of the beamline.
    - Continued detector development with Peter Siddons' group at NSLS for the curved 7000 element Ge strip array detector is strongly encouraged to exploit the potential of this beamline to the ultimate extent.
    - The concept suggested for the high-resolution analyzer based on work of Peter Siddons at NSLS should be further tested either at NSLS or preferably at a high-energy beamline on a third generation source.
    - The beamline layout uses optics concepts proven at NSLS and APS and should provide high flux in a reasonably small spot size (50 µm x 50 µm).
    - The use of compound refractive lenses for vertical focusing has been successfully employed at beamlines at ESRF and the APS.
    - The heat load strategy of employing heavy filtering and a restricted aperture appears to allow a conventionally cooled monochromator design (water cooled).
    - The beamline layout is reasonable and allows a future fixed angle side branch beamline to be built in the same experimental floor area.

Conceptual Design:
Andy Broadbent presented a talk that summarized the scientific goals of the beamline and the design solutions and issues arising from that.
From January User Workshop (>50 attendees) / LOI:

Concentrate on the high energies (50keV, 80keV).

Main beamline:

- first station for high energy PD studies;
- second (large) station for long set-up time experiments;

- high resolution powder diffraction is top priority.

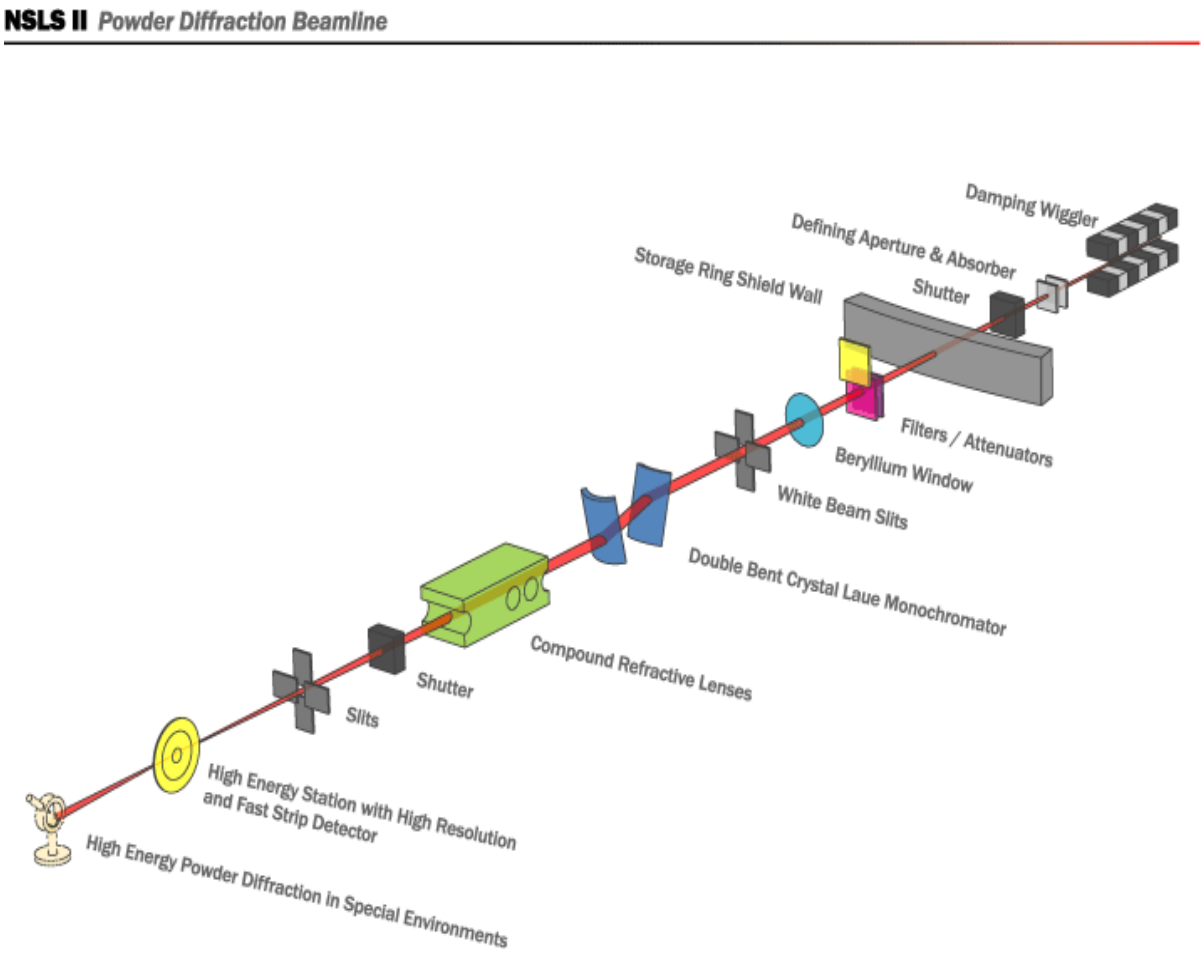
Branchline:

- optimise for PDF studies at high energies;
- focus in both H&V to give a small spot size, target ~50microns.

Sample environments critical.
Beamline would enable classes of experiments that are difficult elsewhere.

Design:

Detailed design work has been carried out by independent contractor, ACCEL. A schematic summarizing the current conceptual design is below.



- Full 7m damping wiggler length
- Selective aperturing:
  - central part of the fan has higher energies,
  - restrict aperture to ~1mrad (H) x 0.1mrad (V),
  - still leaves almost 6kW!

- Concentrating on the high energies allows extreme filtering:
  - multistage C (5mm total) and Al (8mm total) filtering leaves just 280W, of which 21W is absorbed in the 0.5mm Si crystal;
- the cost is some loss of useful flux:
  - lose 64% of flux at 50 keV, and
  - lose 46% of flux at 80 keV.

Quantitative details of the design and design parameters, including flux estimates, can be found in the appendix which contains highlights from the talk of Andrew Broadbent. The main conclusions are:

- Revised beamline design is:
  - feasible, and does not require extensive component development,
  - makes use of both commercial experience and in-house expertise,
  - does not contain any budget or schedule surprises,
- BAT confident that this design will deliver required performance.
- We can make use of the next few years to try some ideas!
- Great progress made.
- Met design maturity requirements for CD-3 approval.
- No remaining design issues for construction start of Conventional Facilities.
- Ready for project CD-3 approval.

Finally, design issues and questions raised by Andy Broadbent were discussed by the BAT and useful and timely advice was passed on to the design team.

Discussion of concerns raised by the EFAC:

The comments of the EFAC were based on the LOI, the Materials White Paper, and on presentations to the committee from Simon Billinge and John Parise. Overall, the EFAC's comments were very positive. They summarized the proposed scientific case as follows:

"The science proposed is exciting, interesting and varied, covering four focus areas:

Complexity on the nanoscale
Extreme environments
Time-resolved studies
Total structure studies.

The BAT will utilize hard X-rays and PDF techniques to examine the behavior of materials under extreme conditions of pressure, temperature, magnetic field, etc.
Their approach is based on the premise that no single technique is adequate to provide all the needed information, and that complimentary techniques must be utilized to fully characterize

materials. While this broad approach poses the potential for lack of focus of the BAT efforts, it offers the prospect of exploiting the virtues of many beamlines at the NSLS-II, including but not limited to those proposed as part of PING. "

There were also some concerns expressed in these reports. These are presented below with a summary of discussions that took place at the meeting

The most significant of these concerned the "fixed energy Pair Distribution Function side station, which all the referees drew attention to. There was general concern that the need for this endstation was not fully justified in light of the existence of similar endstations at the APS and the fixed energy nature of the proposed capability, which limits the available contrast mechanisms likely to be so important in such studies. The project will look into this in detail in the coming year as to whether this should be included in the initial scope of the beamline and looks forward to working with the BAT to further make the scientific case for such an endstation."

- The scientific case for this side-station is well documented in the materials white paper and is a high priority for the PINGBAT. In particular, we consider that the greatest growth in powder diffraction over the next 5 years will take place in the area of PDF studies of nanomaterials, making the side-station an essential component of the suite of instruments for materials studies. Having said this, the side-station is currently part of the mature scope for the PING project.

"We also note the referees' concerns in regard to the requirements for high efficiency high-energy detectors and looks forward to hearing your advice as to the best route forward in this regard."

- We are also actively interested in any developments that occur in this direction and will work closely with the Project to help in any way we can, including seeking external funding for such developments.

"Concerns were raised by the EFAC about this "holistic" approach and the ability of a single BAT to oversee such a broad spectrum of activities as planned in the MaDiS program. We also have concerns about the modes by which the NSLS-II will support such a broad spectrum of activities."

- It is not the role of the PINGBAT to oversee the MaDiS program which is a much broader community activity. However, individual members of the PINGBAT have been pushing different aspects of the integration of different methods to solve difficult problems in nano-material structure. It is therefore maybe not so surprising that leadership of this effort is being taken up by members of the BAT. PINGBAT recommends that this effort gels around a separate entity that is recognized by NSLS-II (Materials Advisory Team?) to ensure that the roles and responsibilities of the two activities are differentiated. Excellent communication

and a tight coupling of the PING and MaDiS efforts are clearly important, however, as well as a tight coupling to other beamlines such as hard-materials spectroscopy, nanoprobe, coherent scattering, and so on.
- In agreement with the EFAC, PINGBAT urges NSLS-II to consider how such an integrated "holistic" approach will be handled from an organizational standpoint.

"The EFAC is uncertain about the relationship of the BAT proposing PING to that proposing the High-Pressure, High-Energy X-ray Beamline [HiPHEX]. We recommend that these two communities engage in cooperative discussions if such discussions are not already underway."

- The efforts of HiPHEX and PING are separate, but there is excellent communication because of the presence of Lars Ehm and Johs Parise on PINGBAT. Lars' and John's research includes scattering experiments under high pressure and they are an integral part of the high pressure community that is responsible for HiPHEX.
- The main issue for HiPHEX is matching the beam characteristics with highly specialized special environments making those beamlines, and the ancillary equipment, tightly coupled. In that sense, there is little overlap between the high pressure and PING beamlines, except that a high pressure component of a broader materials study making use of PING may be carried out at HiPHEX.

"Both the reviewers and EFAC concluded that there was a high probability of the BAT reaching their scientific objectives with these PING beamlines. Some questioned the desirability/necessity of combining the powder diffraction program with the PDF experiments, especially as 80 keV may be too high for the former studies. Others queried whether the DW was the best/right source for such studies; a superconducting wiggler might be better [Note: as of this date, no provision has been made for a superconducting wiggler beamline to be available at NSLS-II on Day #1, although there have been discussions and proposals to move the SCW beamline X17 from the NSLS to NSLS-II early in the operations phase]."

- There may be some confusion here as it is not anticipated that regular, high resolution powder measurements will be carried out at 80 keV, except in rare circumstances where 80 keV is preferable for some reason (for example, an impenetrable special environment). 80 keV is used for the PDF side-station to get wide ranges of reciprocal-space in the forward scattering direction and allow time-resolved PDF studies. Most regular powder diffraction will be carried out at and below 50 keV, which is still high by conventional standards.
- Flux calculations from the damping wiggler presented by Andy Broadbent clearly show that the damping wiggler provides excellent flux characteristics both for the reciprocal-space and PDF measurements. It is far from apparent that the putative SCW would have better characteristics for reaching the scientific objctives.

While some reviewers [e.g, Rev #1] say that the need for high-resolution PDF studies is not well-defended in the LOI, some members of EFAC view the DW as an excellent opportunity to pursue powder diffraction studies, with the PDF work as an extra [free] bonus.

- We agree with the EFAC view. However, beyond that we feel that the absence of a high energy high flux PDF line from the suite of instruments available in MaDiS would be disastrous and would certainly prevent members the materials community reaching its scientific goals, especially as they increasingly evolve towards more complex heterogeneous and nanostructured materials over the next 7 – 10 years.

Note: Although there are some doubts as to whether the PING beamlines will be "best-in-class," there is widespread agreement that there is a high probability that the PING beamlines will allow the user community to achieve their important scientific objectives.

- The PING lines will be best in class because of the high fluxes and small beams with focusing in the horizontal and the vertical directions and ~50 micron spot size in the 50 - 80 keV range. Coupled with the proposed integration of different beamlines envisaged in the MaDiS concept, there will be nowhere in the world where it wil be better to carry out complex material diffraction.

"…work done by Peter Siddons at the NSLS…is highly advantageous for the outcome [of the PING beamlines]…partnership of Siddons and the PING team has the possibility to leapfrog the state-of-the-art."

- We recognize this opportunity. We already have some of Peter Siddons' innovations as probably components in the beamline design (pending testing). We will work closely with Peter Siddons over the upcoming years, especially with respect to fast, efficient, high energy strip detectors, and incorporate advances into our designs where possible.

MaDiS discussions:

John Parise presented a plan for realizing the MaDiS concept and this was discussed by the BAT. The plan involves placing a number of instruments at NSLS over the next few years, with the idea of prototyping and trouble-shooting the integration of different experiments. Beamlines at NSLS can then be transferred to NSLS-II in 2012 ready for operation close to day-1 of the facility. We will be seeking external funding for this project. Details can be found in the appendix containing John's talk. Members of the BAT will also explore the possibility of making this effort part of JPSI developments at Brookhaven.

Closing remarks

PINGBAT would like to thank Qun Shen and the NSLS project for supporting the meeting, and especially Lydia Rogers for her help in taking care of details of the meeting, and Andy Broadbent for the help with the many organizational aspects of the meeting (and for great work on the design of PING!). We are very excited about the developments and we are looking forward to the exciting next few years as this project moves forward.