BM01 Beamline Review Panel Report 5-6th Nov 2013

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Introduction

The panel members received a booklet summarising funding and organisational details for the Swiss Norwegian beam line (SNBL) at ESRF. Also included were a technical description of the beamline, an operations report, selected scientific highlights (including reprints), facts and figures and a list of publications.

The panel began in closed session focussing on progress made against the areas highlighted by the last review in 2008. Broadly these were to continue the high quality and volume of output demonstrated in the previous five year period; to give priority in those experiments that would benefit from combining methods; to upgrade instruments and speed up data collection; the preserve HRPD; to put more effort into software for acquisition and analysis; to extend postdoc and student collaborations; to increase off line lab space and to forge collaborations with other beamlines such as DUBBLE.

The panel unanimously agreed that SNBL and its staff had succeeded or had made very significant progress in all of these tasks. The areas of software development and integration are still on-going and there will be new challenges associated with the phase 2 upgrade that are addressed later in this report.

SNBL has produced > 400 papers in the last 4 years with many in journals of the highest impact factor. This productivity places it very highly compared with other beamlines at ESRF or any synchrotron worldwide.

The panel decided to focus on areas of likely strategic importance for beamline development over the next 5 years. The beamline staff gave a series of presentations and gave comprehensive answers to the many questions from the panel.

The panel met before dinner to summarise the afternoons' presentations before reconvening on Wednesday morning to finalise this report.

Main recommendations

Lattice upgrade

Phase 2 of the upgrade, which replaces the present machine with a multi-bend achromat lattice, will eliminate one of the two branches of the SNBL. The panel

concluded that the current space restrictions already severely limit the development of multiphase methods that would utilise larger in-situ experimental cells or analytical apparatus.

There is an opportunity to move one of the branches now to BM 18 and the panel strongly recommends this move be accomplished as a matter of urgency.

There is a very exciting possibility with the lattice upgrade to replace the proposed 'super bend' with a small multipole wiggler. This device could have a magnetic field strength of up to 1.6T. Under these circumstances the beamline would resemble an insertion device in energy range. This would be very attractive for branch B of the SNBL. If the funding were to be made available by SNBL and the space were to be found by ESRF the panel strongly recommends that the beamlines A an B should be rebuilt on separate wigglers tailored to the wavelength ranges of the respective branches.

Software development

The last review panel recommended that more effort was placed on producing software for data acquisition, visualisation and analysis. SNBL has an outstanding track record in developing beamline instrumentation. It was felt by the previous review that SNBL productivity would be significantly enhanced by the development of software to support all aspects of the beamline. SNBL have responded in impressive fashion re-designing the experimental interface with very favourable comments from users. In addition many new areas such as the study of diffuse scattering have been significantly facilitated by writing new codes and developing new algorithms to analyse model and display data.

The panel recommends that the impressive SNBL effort in software development continue and be targeted towards further strengthening the stations capability in visualisation, modelling and interpretive software to help the users, wherever possible, make real time decisions about their experiment.

Experimental integration

The panel heard how SNBL has worked hard to integrate elements such as focusing; temperature control; detector use (CCDs PILATUS); XRD; XRF; XAS; Raman; gas mixing flow control; indexing; refinement and other forms of analysis into a highly efficient, flexible and user friendly system. The panel concluded that SNBL has been very successful in this respect over the past five years. Potential users often request SNBL because of the flexibility, user friendliness and power of the experimental combinations of both stations. The efforts to integrate experimental methods should continue and expand to ensure the continued success of SNBL.

Combined techniques

The panel were presented with a very impressive scientific output with nearly 500 papers published in scientific journals. The panel agreed the selected highlights *of in-*

situ catalysis; modulated diffraction; coupling diffraction with Raman scattering, molecular modelling and *ab initio* calculations; the observation of giant negative compressibility and on the origins of anti-ferroelectricity in $PbZrO_3$ were very impressive. However the panel felt that an even more significant achievement of SNBL was to make complex experiments easy to perform for users. This has taken a very large effort but has been very worthwhile. Rather than concentrating on demonstration experiments as a one off there is real progress in the integration and combination of methods. This enables users and beamline staff to focus on the physics, chemistry and materials science of their samples rather than worry about the operation of the beamline. This is a real strength of SNBL and they should be encouraged to continue this effort unabated.

Other areas

- In satisfying the needs of the Swiss-Norwegian communities the SNBL has created a facility that is in high demand by the world-wide synchrotron community, as evidenced by the healthy oversubscription ratio.
- The panel was highly impressed with the structure of the organisation and the quality and overall performance of the SNBL staff.
- The strong staff collaborations with research groups from the Swiss-Norwegian communities have been very productive.

Summary of recommendations

- Continue with the existing initiative to develop high energy PDF studies.
- Continue the development of experimental capabilities based on the needs of the Swiss-Norwegian user communities. For example diffuse scattering, high pressure research and combined techniques recently developed.
- Flexibility of the CRG to accommodate the in-house research is a particular strength of the beamline and is strongly encouraged to continue.
- The panel recognises the current management approach towards the development of new research concepts and ideas has been very successful and should be continued.
- The panel recommends that the movement to BM 18 be carried out as soon as possible and in such a way as to consider the phase II lattice upgrade in its optical design and to fully exploit the extra space for multi-functional experiments.