SPring-8 BL02B2 Review Committee Report on Powder Diffraction Beamline (BL02B2)

Report for Director General of
Japan Synchrotron Radiation Research Institute

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1. Introduction

A meeting of the SPring-8 beamline review committee on the Powder Diffraction Beamline (BL02B2) was held at the SPring-8 site on October 28-29, 2004. The “Beamline Report BL02B2 (Powder Diffraction)” and “SPring-8 Overview” had been posted to the committee members, and a review report from each member was submitted to the chair prior to the meeting.

Four Japanese members attended the above-mentioned committee meeting. On the first day, Prof. Shimomura provided guidance in the beamline review and presented an overview of the SPring-8 facility and organization, and then the committee members visited the BL02B2 beamline. After the beamline tour, the committee heard detailed explanations of the experimental equipment, research results and future plans from a beamline scientist and had a question-and-answer session. On the evening of the first day and the morning of the second day, the domestic committee members put together this report based on their discussion referring to the report from Prof. Rosseinsky.

2. Executive Summary

2.1 Technical achievement of beamline and experimental apparatuses

*Evaluation

The BL02B2 beamline is well-equipped to provide users with opportunities to obtain highly accurate powder diffraction data, and the beamline and experimental apparatuses are appropriately maintained.

(1) Optics: The mirror and monochromator have attained the designed performance.

(2) Debye-Scherrer Camera: The main body of the camera is simply designed without any extra functions, and the camera is of high quality. The technique for correcting the data obtained from the imaging-plate (IP) reader is well-established, and the angle resolution and the shape of the peak profiles obtained by the camera are satisfactory for most of the experiments.

(3) Sample environment: The development of sample preparation methods is highly evaluated. The sample temperature is controlled using different devices according to three ranges of temperature ($15K<T<300K$, $90K<T<400K$, and $300K<T<1000K$). In particular, a new low-temperature device has been fabricated. The gas-flow control and laser-light guidance systems are designed skillfully, and such a positive attitude toward development of a new device for controlling the sample environment is highly evaluated.

(4) Measurement and data-analysis software: On the whole, user-friendly software is provided.

*Recommendation

(1) The incident photon flux should be increased by installing a horizontal focusing mirror, in order to carry out a more efficient measurement.

2.2 Research Activity

*Evaluation:

Publications of findings are highly evaluated in the terms of quality and in terms of the number of papers published.

(1) All of the research studies described in “Scientific Activity” of the beamline report are ranked as high quality. In particular, the following is very impressive: (a) elucidation of the thermoelectricity in Zn4Sb3 through the charge density by MEM, (b) observation of adsorbed oxygen (hydrogen in a recent work, till then it had been difficult to prove) molecules in nano-porous organic conductors, (c) observation of the structural phase transition from a low spin state to a high-spin state induced by photo excitation, (d) encapsulation of organic molecules in single-wall carbon nano-tubes , (e) chemical bonding of hydrogen in MgH2, and (f) observation of a case in $Sc_2@C_{66}$ which violates the isolated-pentagon rule.

(2) These outcomes from many research fields are deserving for our attention.

(3) Most of the users take full advantage of the MEM-Rietvelt method to carry out their research, showing that the method is useful in a wide range of research fields.

(4) In many projects, hot-topic materials in each research field have been investigated. These successful selections of research subjects should be given a high evaluation.

*Recommendations

(1) Maintaining a high level of activity in the future is important.

(2) Large Contributions to basic sciences are highly evaluated. In the future, promoting the use of this technique in industry is necessary.

2.3 User Support

*Evaluation

The user support system is satisfactory.

(1) The selection rate of the proposals is appropriate between 60 and 80 percent, but we have a concern about the decreasing of the average beamtime per proposal.

(2) We appreciate their efforts to invite new users constantly.

(3) The distribution of beam time for each research field is reasonable.
(4) A group in Nagoya University is supporting users' research studies in collaboration with the beamline scientists and other power users.

*Recommendation
(1) Drawing and implementing future plans, as well as maintaining the current level of activity, is very hard because of the shortage of manpower. The committee recommends that the JASRI should increase the beamline staff by two by employing a beamline staff member or inviting a post doctoral fellow.
(2) In order to solve the problem of beam time shortage caused by the increase in the number of new users, the JASRI should provide another beamline dedicated to powder diffraction experiments. The two beamlines should share responsibility for user support; one is for special purposes like time-resolved measurements or measurements with a sample under a special environment (i.e, advanced research accompanying a new technical development), and the other is for high throughput measurements using a rapid and simple system.
(3) Strengthening user support regarding data analysis is important. We think that a virtual school on the net which offers a course on MEM analysis is beneficial to users.
(4) Developing the users' community in Asia and inviting scientists from Asian countries are important.

2.4 Facility Development and Research Direction in Future

*Evaluation

Future plans regarding the development of the beamline facility and experimental techniques are appropriate for maintaining a high level of research.
(1) The present status of the beamline facility is satisfactory. This should be maintained in the future.
(2) Future plans, such as time-resolved measurements, extension of the range of controllable sample temperature, photo-gas reactions at a low temperature, surface diffraction, and development of an easy and rapid measurement system, all meet the current requirements. These directions are appropriate for widening the scope of research.

*Recommendation
(1) The Debye-Scherrer Camera has been working well because of its simple design. The development of an automatic IP reading system and an automatic sample is required for high-throughput experiments in the future.
(2) This report describes the development of new experimental apparatuses and methods in "Strategies for the next five years." The JASRI should prioritize

these developments after clarifying the scientific target for each development.

(3) Regarding the development of a high-temperature device, if the sample temperature could rise up to approximately 1600 K, ceramic materials could be the target of research.

(4) As already mentioned, the construction of a new beamline for powder diffraction is the best option. However, since it is difficult to realize under the current situation, the JASRI should consider other options to provide a new beamline or an experimental station for powder diffraction users by restructuring the current beamline lineup.

3. Summary of Recommendations

The Powder Diffraction Beamline (BL02B2) is one of the most successful beamlines in SPring-8. The research results are excellent in terms of quality and in terms of the number of articles. Maintaining the current level of activity in the future is important. For further development of this beamline, the JASRI should implement a plan which will increase man power and will improve the performance of the beamline equipment in BL02B2.