SPring-8 BL40B2 Review Committee Report on Structural Biology II (BL40B2)

Report for Director General of
Japan Synchrotron Radiation Research Institute

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1. Introduction

The SPring-8 beamline review on the Structural Biology II Beamline (BL40B2) was held at the SPring-8 site on November 4-5, 2004. The following written materials were provided to the committee members;
(1) Beamline Report BL40B2 (Structural Biology),
(2) SPring-8 Overview 2004.
The committe members submitted their individual review reports to the chair prior to the meeting. Four local members attended the meeting. They heard an explanation on SPring-8 from a representative of JASRI, had a beamline tour, heard the detail explanations on the beamline from beamline scientists, and then had a question-and-answer session. Finally, they prepared this review report.

The BL40B2 beamline started as a public beamline with two different purposes; one is for protein crystallography (PX) and the other is for small-angle x-ray scattering on biological materials. The construction of this beamline begun in 1998 and public use started in January, 2001. Since then, the beamline has been expanding its target to include soft materials such as polymers and lipids, and hard materials such as alloys, other than biological materials in the field of small- and medium-angle x-ray scattering. Recently, a powder x-ray diffractometer designed with Guinier geometry has been installed at this beamline for its R&D's using proteins and organic compounds. At present, the BL40B2 beamline is a public beamline used by scientists from many research fields using different techniques.

Taking this situation into account, the beamline review committee evaluated the research activities of the last five years and assessed the future strategies, and then prepared this report.

2. Executive Summary

2.1 Technical achievement of beamline facility and experimental stations

BL40B2 is a bending magnet beamline which accommodates a general-purpose experimental station using x-ray diffraction and scattering techniques for structural biology. This beamline is mainly used in the protein crystallography (PX) mode and the small angle x-ray scattering and diffraction (SX) mode; changing the mode is easily performed by moving up or down the goniometer used in the PX mode. Optics and other factors are well optimized for general-purpose experiments. Both general-purpose and specific-purpose beamlines are useful for x-ray diffraction and scattering experiments.

The beamline employs a standard setup of optics, which consists of a fixed-exit double crystal monochromator and a bent cylindrical mirror. These standard optics meet the conditions for general purpose experiments. In reality, the tunability of x-ray energy enables the conduct of a multi wavelength anomalous diffraction (MAD) experiment for phase determination in the PX mode, and a sufficient angle resolution is available for small-angle x-ray scattering in the SX mode. The beamline enables various levels of experiments from basic measurements to advanced measurements in

each mode. In the SX mode, the target is central in the static measurement since the photon flux is less than that of undulator beamlines. Notably, the camera can cover a wide range of angle of x-ray scattering because of the adustable camera length in the SX mode. In addition, the sufficient space around the sample position widens the scope of application since any sample stage can be used according to the purpose of the experiment.

As the number of users increases, it is increasingly important to decrease the time needed for changing the mode. The experimental station is well equipped and used so as to minimize time loss.

Because of its standardized design, frequent users are familiar with the beamline optics and do not feel any difficulty in performing their experiments. Beginners can carry out their experiments after a short instruction since a well-written manual is provided.

A CCD detector (ADSC: Quantum 4R) is installed for protein crystallography, II+CCD (Hamamatsu Phononics) is for small-angle x-ray scattering and diffraction, and an imaging plate system (RIGAKU: R-AXIS IV++) is for both purposes. Users choose the appropriate x-ray detector according to their experiments.

Because the experimental station was designed for general purpose, the research target is expanding to include the fields of small- and medium-angle x-ray scattering for non-biological materials and those of powder x-ray diffraction.

This beamline allows users to control the beamline equipment via an interface program to meet users' needs for a high level of experiment.

2.2 Results of Research

1) PX mode

In addition to protein structure analyses using the MAD technique, notable results have been obtained from high-resolution structure analyses with a spatial resolution less than 1 angstrom and from the determination of the position of hydrogen. Many studies using this technique have been reported in international journals with a high value of impact factor (56 papers for the last five years), showing the high productivity of the PX mode. Some of the studies in the PX mode have contributed much to the Protein 3000 National Project.

2) SX Mode

Besides the standard experiments of biological materials in solutions, a new type of research, which accurately measures the intensity of x-ray scattering at large angles has been expanding. Analyses of large-angle regions will become more important, and will cover interesting subjects from a theoretical point of view. Besides biological materials, carbon nano tubes and functional polymer materials have been extensively studied using the small-angle x-ray scattering technique, showing that the technique is useful for materials science. Although the number of publications (20 for the past five years) is less than of studies on protein crystallography, a few pioneering works have been carried out. Many proposals have been submitted from various research fields. In addition, the JASRI started an R&D

of a powder diffraction instrument for protein and organic compounds. We expect that the R&D will open new opportunities for these studies using BL40B2.

2.3 User operation and support

The beamline is designed so that users can perform their experiments themselves from tuning the monochromator to taking experimental data. For this purpose an instruction manual is sufficiently provided. The beamline scientists are highly capable of providing high-precision and user-friendly instruments to users. To further strengthen the user support, we recommend that the JASRI should increase the number of staff members at the BL40B2 beamline. The number of proposals is reasonable, and the selection rate is about 70 %. The selected proposals are well balanced among the research fields.

2.4 Future technical and scientific developments

The research in the PX mode has produced sufficient scientific results. However, presently the BL40B2 beamline is behind the other public beamlines for protein crystallography, namely BL38B1 and BL41XU, for automatic measurements with a high throughput. Regarding the SX mode, its target materials are expanding to include functional polymer and carbon nano tube materials, in addition to biological materials. Studies on the powder x-ray diffraction of proteins and organic materials that are the focus of much interest have started. The beamtime for the PX mode experiments has become about 30 % of the total. Beamline operation in the SX and PX modes is inefficient since it takes about 40 shifts a year for changing the mode.

We recommend that the optics, the measurement instruments, and the sample environment should be improved to focus on non crystalline materials with a hot issue. We suggest the following for the experimental station; an extension of the angle range in measurements, the development of a system that can change the camera length easily to deal with various samples, and an introduction of a new platform for easy setting up of the instruments, while improving the flexibility of the sample environment. We expect that the number of publications will increase in the field of non-crystalline materials by converting the BL40B2 beamline into a single SX mode. We also expect an increase in the powder x-ray diffraction experiments in the SX mode. The JASRI is now planning to move experiments in the PX mode to the other beamlines. We consider the plan is reasonable if all of the experiments in the PX-mode were moved to the other beamlines.

3. Summary and Recommendations

The BL40B2 has fulfilled its function as a general-purpose experimental station for x-ray diffraction and scattering of biological materials. One feature of the beamline is that the two different methods, x-ray diffraction of protein single crystals

and small-angle x-ray scattering and diffraction of biological materials, are available at a single beamline. However, considering the growing diversities of research purposes and experimental methods, we recommend that the experiments using each method should be performed at a beamline dedicated to each method. Therefore, we consider it as reasonable that BL40B2 will be a beamline dedicated to small-angle x-ray scattering and diffraction. This will develop the research on non crystalline biological materials in BL40B2. Moreover, the beamline should deal with various developments in small-angle x-ray scattering and diffraction studies of non biological materials. This will increase the number of users in the SX mode, and will improve the beamline performance in the terms of quality and in terms of the number of research outcomes. In addition, to further develop the small-angle x-ray scattering and diffraction research, it is important to develop a reliable, quantitative analysis. Finally, the committee recommend the invitation of a theorist who evaluates the analytical method as well as the increase in the number of beamline staff members.