

Report of SPring-8 Beamline Review Committee, BL02B1

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The review committee was held at SPring-8 on November 25 and 26, 2002. In advance of the Committee the following materials were sent to the member.

- Beamline Report BL02B1 (Crystal Structure Analysis), Supplement (Selected Reprints)
- SPring-8 Overview

The Beamline Report BL02B1 includes the specification, performance and upgrading status of the optics and measurement equipment, scientific activity performed at the BL and the future programs. In addition, the reprints of selected papers are contained in the Supplement. The SPring-8 Overview, on the other hand, consists of the various statistics gathered at SPring-8 and the report of research activities obtained through use of all the beamlines. As far as the BL02B1 is concerned, the number of papers published during the period from 1998 to 2002 totals 41 including papers in press. Before the Committee meeting, the members were requested to review the materials individually and submit their reports to the Review Committee. All the materials were shared by the members.

All the members except Prof. Stephens attended the Committee: they went on a one-hour tour of the BL02B1, and Division Head, Dr. Suematsu gave a general presentation while the detailed explanation was given by Dr. Naoshi Ikeda, beamline scientist of the BL02B1, before discussions and exchange of opinions. As a reference material, the "Interim Report on the Large Synchrotron Radiation Facility (SPring-8) prepared by Subdivision on Research Planning and Evaluation, the Council for Science and Technology, MEXT" was distributed on that day.

The committee members reviewed the current status of the beamline, and prepared the report on the evaluation and recommendations described in the following four subjects.

1. Beamline and experimental equipment

Current status

- The BL02B1 is provided with a bending magnet as its light source, which consists of a front end, collimation mirror, double crystal monochromator, and focusing mirror. A focused and monochromatized X-ray beam is led to two devices in a tandem configuration within the same hutch: (A) 7-circle diffractometer (abbreviated to 7XD) and (B) Low temperature vacuum camera (abbreviated to LTV).
- The main feature of this beamline is its high energy X-ray (<100 keV). Currently the beam size is 0.1mmV x 3.0mmH. Now the improvement of the second sagittal-focusing monochromator is under consideration toward the smaller beam size.

Evaluation and recommendations

- The beamline has achieved the high-level of maturity that commensurate with a third-generation synchrotron radiation light source.
- As for the equipment, (A) 7XD has been operational for five years, and has achieved a satisfactory level of maturity as a multipurpose diffractometer. Furthermore, a variety of the sample environment that covers a wide range of temperature and pressure is highly evaluated. Considering that SPEC, a standard control system is being introduced in addition to an already-completed device control software, the beamline will meet the needs of a wider range of users. (B) LTV was installed with external funds of Dr. Toriumi (Himeji Institute of Technology) and the JASRI's support based on the experience of using the 7XD on camera mode and has been operational since the first half of fiscal 2000. It is highly preferable for both the facility and the user community that JASRI has vigorously supported the introduction of such an experimental device with external funds of public users and provided for public use. It is a unique camera for fine crystals that can achieve a high S/N ratio with a vacuum pumping system. Since the camera is a prototype and in a developmental stage, and it still requires a great deal of skill, it has not reached a point where general users can use it easily.

2. Research activities

Current status

- The present review is intended for equipments with five years of operation since its installation. The 7XD of the beamline needed the overall adjustment and tuning for the first two years (1997 - 1999) and, during the period it was also used on powder diffractometer mode. Then, based on the experience it was developed as a powder diffractometer dedicated for BL02B2. Therefore, the beamline has been fully operational for public use only for most recent three years. The LTV, on the other hand, has been operational for only two and a half years.
- Although the annual user time at SPring-8 amounts to 4,100 hours, it comes short of 5,500 hours/year of ESRF, a similar international large synchrotron radiation facility. The ratio of beam time allocation for the beamline's two equipments in a tandem configuration was 7XD: LTV = 2 : 1 in fiscal 2001.
- Since the main theme of the 7XD is structural studies using single crystals, the selection of the various experimental conditions (wavelength selection, focusing and high harmonic rejection) and various sample environments (temperature and pressure) is necessary. In order to measure a large amount of data with accuracy, each research theme will require more beam time.

Evaluation and recommendations

- Some excellent research results have been published regarding the strongly correlated electron system, in which Japan currently leads the world. Other high-quality research results are also found in the fields of the precision molecular crystallography for a platinum complex and structural analyses with photo-induced excitation. It is noteworthy that the industrial use for the improvement of a turbine blade coating, which makes full use of a high-energy X-ray is now under way. However, the number of published papers is relatively small and many of the research results have not been published. As mentioned in the "current status" above, each proposal will require more beam time. Therefore, it is significant to find out the reasons: (1) whether it is due to the lack of beam time, (2) whether it is the lack of public users' capabilities, (3) whether there is an innate problem in the system of public use. As for (3), let us point out that the current system under which SPring-8 invites proposals every half year is not suited for the structural studies of single crystals that require

a great deal of beam time and especially for challenging and time-consuming research proposals. Despite such a setback, we appreciate the fact that the facility was aware of the problem and introduced on a trial basis a new proposal selection system for the beamline that is valid for one year. The system to support startup activities which will promptly respond to hot topics will lead to building esprit de corps of the beamline and the facility's research groups, so that the efficient use of the reserved beam time of JASRI (20 %) is expected to play an important role. Since users know of the reserved beam time, the facility must do its best so that users cannot complain about the efficient use of its beam time.

- To produce more high-quality, world's leading research results, the facility must take a vigorous and offensive approach not the passive and defensive approach just to support the public use. For that purpose, it is desirable for the facility to contribute to raising the level of science and experimental techniques, while the beamline scientists, who know every inch of the equipment and public users strive to further promote the public use by accepting attractive proposals and by giving priority to important proposals with precise timing.
- The 7XD is an equipment with many uses suited for multipurpose structural studies and the apparatuses for various sample environments can be used for experiments in a wide range of temperature and pressure. In addition, the facility aims to introduce a magnetic field applying device and 2-D detector to promptly search a reciprocal space and we rate this offensive approach highly. Since the installation of the LTV aims at crystallography with photo-induced excitation and it has just started to produce results, we look forward to the future progress.

3. Support for public use

Current status

- SPring-8 invites proposals every half year and the acceptance rate of the proposals using the beamline is approximately 50 %, which is the lowest among all the SPring-8 beamlines. Although the beam time requested among the proposals accepted almost equals to the beam time actually used, most of the research results of the conducted proposals remain unpublished. This means that the public users have failed to complete their research in spite of the fact they have used the beam time requested.
- The beamline scientists (a group of five) for the BL02B1, which has two devices, are also in charge of other two beamlines, so the number of staff per beamline is $5/3\text{BLs}=1.6/\text{BL}$. This figure is less than half of the global standard (cf. $3.9/\text{BL}$ at APS and $3.4/\text{BL}$ at ESRF).

Evaluation and recommendations

- The acceptance rate of the proposals for this beamline, as low as approximately 50 %, is attributed to the careful selection of proposals. However, the facility must clear up the cause of imbalance between the beam time used and the number of papers in order to come up with countermeasures. At the same time, it is desirable to trace the unaccepted proposals, the other 50 %, since the tracking will help the facility to find out whether the unaccepted proposals were submitted again with improvements or whether they ended up with one-time-only proposals. The results of the tracking will provide an indication of the level of users' expectations for SPring-8.
- The 7XD is used mainly for single crystal structural analysis, but such experiments require a great deal of time and the effort of support staff in setting the single crystals, selecting wavelength, focusing, adjusting the higher harmonics suppression device and setting the various sample environments. Since it is inevitable that the staff cannot handle all the work due to the lack of manpower, the laborsaving efforts will be necessary. As for the LTV, it is preferred to assign a researcher from the field related to the crystal chemistry, who can support experiments with this

device.

- In order to facilitate the use of the beamline and to reduce the burden on the staff, it will be important to prepare manuals or make full use of the Web sites. The Web sites having interesting research results obtained at the beamline with simple explanations will attract researchers of different disciplines.

- It will be in the facility's best interest to train not mere operators of apparatuses but researchers or engineers who promote science to be introduced to other facilities in five to ten years time. At the same time, the facility must clarify the roles that the beamline scientists and researchers should play and promote mobility. Considering that SPring-8 is an international public use facility, it is significant to keep firmly in mind that the facility is expected to play a role of a pump to encourage personnel exchanges.

4. Future equipment and R&D

Current status

- As for the 7XD, the introduction of a 2-D detector is under consideration with the CCD in mind for fast data acquisition in reciprocal space.

- The number of the beamline users has been steadily increasing since 2000A (the first half of fiscal 2000) and the research fields available at the beamline are also expanding.

Evaluation and recommendations

- The introduction of the 2-D detector is all well and good, but such a basic component technology should not be introduced to each beamline independently or randomly. Instead, it should be introduced along the SPring-8's program under the system where a technical support such as electronics shops is ensured. It will be better if it is possible make the most of the similar component technologies well-established at other beamlines.

- The current LTV is a prototype designed for structural analysis with photo-induced excitation. Since it is constructed with the external funds, it is crucial to make the best use of the LTV to produce results. Furthermore, based on the experience another prototype should be constructed at a dedicated beamline to open up new research areas of low-molecular-weight organic microcrystals and time-resolved chemical reactions. As a matter of course, if there are devices that meet the specifications (especially for biological structure analysis) at other beamlines, they should be fully utilized. In the final analysis, it is best to consider the complementarity with other public beamlines and their originality from a comprehensive viewpoint.