

Report on the SPring-8 Beamline, BL41XU by the Beamline Review Committee

1. Present Status of the Beamline

The beamline, BL41XU, has the basic configuration, equipment and performance required for protein crystallography at the third generation synchrotron radiation facility. It would appear that, in the course of beamline construction, the diffractometer including detector was not constructed as the initial design. However, after the development and improvement, the beamline provides a sufficiently high flux and a very narrow beam of light where experiments of Multiple-wavelength Anomalous Diffraction (MAD) technique can be easily conducted and is presently user-friendly so that users can carry out their experiments as the laboratory.

For the most part, the beamline has achieved the required performance. We rate the beamline facility highly, shortening the time required to change wavelength with the automatic operation and for lowering the level of skills necessary for operation.

The focusing beam size (0.2 mm x 0.2 mm) collimated by mirrors seems to be still too big for diffraction experiments of small crystals, and we call for continuous efforts to improve the focus size. It is indispensable for users to be able to optimize the aperture size of slits easily whenever it is necessary according to the size of crystals.

A higher level of user-friendliness for operation and data processing at the experimental station will ease the burden on the beamline scientists to support users and improve the throughput of experiments. As pointed out by the beamline scientists, the higher level of user-friendliness remains to be a top priority.

Since many of the problems can be solved by helping users accustomed to the experimental equipment, it is necessary to come up with concrete measures to do so and carry them out. Considering that the level of user-friendliness and the user support required vary for users, who are not so experienced but accustomed to conducting diffraction experiments or are absolute beginners, it is important to figure out what level of user-friendliness is actually required. In this respect also, there is a need to arrange a scheme to reflect the demand and opinions of users vigorously and to exchange opinions with the beamline scientists.

Since the operation manual, online manual and instructional materials for the software products are essential to conduct experiments, the efforts to prepare those materials should be further promoted.

As mentioned above, the beamline has already been equipped with necessary basic configuration, equipment and performance, and it is significant to vigorously provide users to carry out experiments with high performance and a quick turnaround.

2. Research Activity

There have been a number of users submitting applications to use the beamline, BL41XU. The average beamtime allocated is recently three shifts. The results have been steadily increasing in the past few years and some of them were highly evaluated. We expect that the results will further

increase.

In most cases, the number of significant results provides an indication of achievements in the review of beamline activity. But our view is that it is more important to review in light of how the beamline contributed to obtaining the results. Considering that in most cases the characteristics of samples prepared for user experiments, the significance of the research and the users' past experience were reflected in the results, there are a lot of distinctive and outstanding results, and the number is increasing. It will be in the facility's best interest that users and beamline scientists cooperate closely with each other to upgrade the beamline toward even smoother process of experiments since an excellent beamline can attract many appealing proposals.

High level of activities is asked for both of the experiments for structural analyses of the high throughput and those that are quite challenging due to the accuracy and the high level of skills necessary for preparing samples. What is significant for the facility is to enhance the level of activities while keeping a balance between these two.

In the materials provided by the facility for the review of the beamline, we found that not a few results came from the experiments using other beamline or other facility such as Photon Factory together with BL41XU. It reflects the fact that users conducted their experiments in other facility before BL41XU was constructed. Judging from the maturity of the beamline, BL41XU, it is expected that the contribution of BL41XU increases. Presently, the beamline, BL41XU, is understood as the only one public beamline in Japan with high performance for macromolecular crystallography with insertion device source, and is indispensable for structural biology research. With the continuous maintenance and upgrading of the beamline, BL41XU remains in an position of high level of contribution. The beamline is an exclusive public beamline, designated for macromolecular crystallography and continuous development is requested to keep the level of the maturity for future success.

3. User support system

Presently, at the BL41XU, three shifts of beam time are allocated on the average and the adoption rate has been steadily high for the past few years. The upgrading of the functions of the experimental station, such as the introduction of a CCD detector, has shortened the time required for data collection. In addition, users have become more experienced and accustomed to the beamline. We believe that the throughput will be improved and it will be possible to conduct more experiments by contriving better ways to make the most of user support system (including user-friendliness) by the beamline scientists and by improving the beamtime allocation system that reduced the period of application and experiments. Such efforts will make it possible to conduct more experiments and also supplemental experiments in their former run. These effort will lead to increase the number of results.

It is greatly appreciated that it has become possible to conduct timely experiments by introducing the reserved beamtime system in addition to the normal operation. By using the reserved beamtime, users can start their experiment within two weeks after application at the shortest.

It is requested that preparatory procedures as storage, picking up and mounting crystals, and data analyses during/after experiments must be supported to carry out experiments smoothly. It will also be desirable to establish a system and to improve the devices for user support so that users can

reflect each step of their experiments on the measurements. The prerequisite for analyses is to be able to reduce diffraction intensities from the measured pattern. However, it is presumable that further support will be necessary for beginners.

4. Future development

Although the updating of the monochromator system to enhance the intensity flux at the beamline and other minor improvements are conceivable, there seems little need for drastic improvements unless serious impediments or problems can be found. Presently, the beam pipe is not evacuated inside the experimental hutch. In the review it was pointed out that the flux will be enhanced significantly for X-rays with energies less than 10 keV by replacing the air path with a vacuum path.

The problem to be solved in the near future at the beamline is the damage on crystals resulting from the high flux X-ray irradiation. A systematic study is necessary to solve this problem and the committee calls for efforts to consider the definite plans and concrete measures to be implemented.

The research and development program of the diffraction from small crystals is also the issue that requires the definite plan and concrete measures.

The user-friendliness and the analysis of sample damage and its countermeasures, though regarded as priorities, are also included in the areas where there is little need for drastic improvements.

It will be significant and essential for users to switch an imaging plate detector and a CCD detector for their experiments anytime they want. There has also been a call for the reduction in the readout time of CCD detectors. The upgrading of the detectors, the preparation of backup devices, and the improvements of the crystal control system and diffractometer are, as a matter of course, indispensable and should be continuously carried on. Since the continued efforts are effective enough to address the difficulties in handling the small crystals and the crystal damages, the drastic improvements won't be necessary.

The robotics of crystal mount is effective, for example, in reducing the loss of time attendant on changing and in selecting crystals with excellent diffraction performance as long as effectiveness and cost performance are ensured and its practical introduction is highly recommended. One thing to note is that it is necessary to standardize the crystal holder on a global level as well as on a national level and to provide users with the holders for its introduction.

Our view is that the beamline scientists' efforts to promote the research theme closely related to the beamline will be of great importance for the future upgrading of the facility. For that purpose, the facility must demonstrate a clear vision and effective programs for the upgrading and management of the beamline and for the "Future Research Promotion Scheme for Staff." Since SPring-8 has other beamline intended for macromolecular crystallography and structural biology, the continued consideration should be given to the assignment of staff, the cooperation and separation of roles among the beamline and its staff members in conducting experiments and the development in the future plans including the higher throughput in conjunction and in parallel with other beamline and their staff.

5. Conclusion

Up to now, we rate highly the maturity of the apparatuses in the beamline facility, the activities and the results on the whole. We call for efforts to keep up the good work and enhance the level of maturity and activities for further development.

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* This report was prepared by the Japanese reviewers listed above incorporating the comments on the review of the beamline that Dr. Peter F. Lindley and Dr. Matthias Wilmanns sent to the review committee.