

SPring-8 BL28B2 Review Committee Report
on
White Beam X-ray Diffraction
(BL28B2)

Report for Director General of
Japan Synchrotron Radiation Research Institute

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1. Introduction

The SPring-8 beamline review committee meeting on the White Beam X-ray Diffraction Beamline (BL28B2) was held at the SPring-8 site on November 15-16, 2004. The following written materials were provided to the committee members:

- (1) Beamline Report BL28B2 (White Beam X-ray Diffraction),
- (2) SPring-8 Overview 2004.

The committee members submitted their individual review reports to the chairperson prior to the meeting. Four Japanese committee members attended this meeting. They heard JASRI's explanation on SPring-8, had a beamline tour, heard the detailed explanation on the beamline, research results, and future plans from beamline scientists, and then had a question-and-answer session. This review report was put together based on the discussion among the Japanese members, referring to the report from Professor Baruchel.

The construction of this beamline began in 1999 and public use started in 2000 for white X-ray topography. Energy-dispersive XAFS (DXAFS), micro angiography, and high-temperature and high-pressure studies started in 2002. At present, four different experiments are performed at two experimental stations. Because micro angiography activities should be reviewed in all SPring-8 beamlines, and the high-temperature and high-pressure experiments have been performed by a single group, this committee has reviewed mainly the white X-ray topography and DXAFS research activities.

2. Executive Summary

2.1 Technical Achievement of Beamline Facility and Experimental Stations

The distinct feature of this beamline is the use of high-brilliance and high-energy white X-rays from a bending magnet in the SPring-8 storage ring. The experimental instruments meet the conditions for high-brilliance and high-energy white X-rays, and are suitable for the third-generation synchrotron radiation facility.

1) White X-ray Topography

The experimental station meets the needs of users and is sufficiently competitive. This is a simple beamline consisting of an absorber, a shutter, and a diffractometer. The diffractometer meets the conditions for high-brilliance X-rays at the third-generation synchrotron radiation facility. Standard instruments are installed for low- and high-temperature measurements. As X-ray detectors, a flat-panel sensor and a CCD are used in various experiments, and well-written manuals are provided for users.

2) DXAFS

The instrument for DXAFS has achieved a world-class performance. Using a Laue-type polychromator, it has successfully measured the high-energy DXAFS at the Pd edge. The detector system, which consists of a fluorescent plate and a CCD, works well and has achieved a time resolution of 6 ms. It has also achieved a high

energy resolution for energy-dispersive EXAFS.

On the other hand, its shortcomings are as follows:

- (a) The DXAFS system is unable to measure the spectrum in a low-energy region since the mirror does not work well. The vertical beam size is large since a focusing mirror is not installed.
- (b) The imperfect bending of the analyzer produces an aberration. Instead of the current bending system, a guide system should be employed to form the curvature of the analyzer.
- (c) The sample environment is unsuitable, particularly for a gas-handling system.

3) Micro Angiography

A combination of a one-bounce monochromator and a high-speed shutter has achieved a high timing resolution. Real-time imaging with such a high timing resolution is an advantage of this experimental setup.

4) High-temperature and High-pressure Experiments

The instrument for the study of expanded fluids was moved from the BL04B1 beamline. A new sample cell was fabricated by the users' group.

2.2 Research Activities

Publications from each field except for white X-ray topography are limited in terms of the number of papers published. We encourage more publications from the fields.

1) X-ray Topography

Compared to other beamlines constructed simultaneously, the number of publications from the BL28B2 beamline is few. This is due to the limited number of materials that the X-ray topography instrument can measure, a small number of users' groups, and a small number of staff for white X-ray topography. Since the instrument is a world-class one, the staff members and users should advertise the usefulness and uniqueness of this technique for materials science, and should invite new users' groups to this beamline to broaden the scope of research.

Research results are rather ordinary in terms of the quality and number of articles. They lack new information to improve this field. In the future, it will be required to investigate more challenging problems to produce results that can draw considerable attention. It will also be required to extend research toward industrial applications.

Comments on some results are as follows:

- (1) Spectroscattering topography is a new promising technique for investigating multicomponent materials. The development of a quantitative analysis method will develop this technique to a great degree. In the future, it is important to broaden the range of applications.
- (2) It has been considered that white X-ray topography is difficult to perform because of the large heat load on a sample. However, we expect that this technique will be improved by taking advantage of high-energy X-rays.

(3) The topography of protein and organic crystals has been drawing attention as a new research field. We expect further improvement in research in this field since the stable observations of protein and organic crystals have been realized. The observation of dislocations in the protein crystal is intensively evaluated. For further improvement, we suggest the use of monochromatic X-ray topography in parallel with white X-ray topography since improving the spatial resolution is indispensable in the future.

(4) The three-dimensional mapping of dislocations in single crystals makes the most of the advantages of synchrotron-based topography. We expect a broader range of applications for this technique.

2) DXAFS

Several results on the behavior of Pd atoms in perovskite ceramics, the structural change of Pd clusters in zeolite, and interesting phenomena related to catalysis obtained by this technique have been reported. It is much better if it could determine an intermediate structure in a catalytic reaction, since the structure is accessible only to the time-resolved XFAS measurement at present.

3) Microtomography

Sequential images of coronary arteries have been successfully obtained, showing that the technical level at this beamline is high. A study of the effect of vasoactive agents on coronary arteries is in progress. This is expected to result in the study of artery regenerative treatment. A study of cerebral angiography in rats is also in progress.

2.3 User Support

The number of submitted proposals and their selection rates are average for the five-year-old beamline. The number of users gradually increases. X-ray topography experiments dominated the beamtime since the start of the operation of BL28B2 as a public beamline dedicated to white X-ray topography. At present, however, the beamtime is assigned almost equally to the four research fields.

Three staff members are supporting users' experiments according to their responsibilities. Their contributions to the development of experimental instruments are intensively evaluated. A professional staff member of medical application is assigned to microangiography experiments, and skillful users who can set up the instruments carry out their own experiments by themselves. We consider that the present user-supporting system is sufficient for most of the users' experiments.

In the future, it is important to develop a system that enables the publication of results as early as possible by exchanging information between the in-house staff and the skillful users' groups.

It is required to advertise the advantage of the instruments, the research results, and the possibilities of future development, in order to invite new users and develop new research fields. For this, close collaborations with skillful users are indispensable.

A manual is provided in this beamline. However, to invite new users, the manual must be upgraded to make it more user-friendly.

2.4 Future Development and Research Direction

The beamline staff has drawn up well the future plan for the instruments at the experimental stations. However, they need to strengthen the strategic view on future research. The coexistence of the four research fields may continue in the near future, but their beamtime distribution should be prioritized from a long-term viewpoint. We suggest putting a high priority on X-ray topography and DXAFS by moving the microangiography activities to another beamline and terminating high-pressure research.

We point out the following for each field.

1) X-ray Topography

The installation of a new device for a variable beam size (including the measure for background reduction) is important in broadening the scope of research. Ambitiously, it is required to consider the possibility of constructing a long beamline to take full advantage of high-brilliance synchrotron radiation. For this, it is indispensable to increase the number of users' groups and the scope of research.

It is required to broaden the range of target materials (for example, heavy-element materials, various oxides, low-dimensional materials, and magnetic materials). It is also required to develop a spectroscattering topography technique toward the quantitative elemental analyses and position-momentum measurements. Following subjects can be considered.

(A) Evaluation of Industrial Materials

(1) Evaluation of Single Crystals:

Many industries and research laboratories require the three-dimensional mapping of domain structures and lattice imperfections in materials. A mapping technique will attract new users from the industries and laboratories. Therefore, an instrument that enables three-dimensional mapping is required to develop an effective system for user support.

(2) Application of Scattering Topography:

In addition to the on-going development for a higher resolution, a multipurpose instrument that can be used in various experiments should be developed to invite new users to perform scattering topography experiments at this beamline. For example, developments for easily adjusting the beam size and obtaining scattering topography data are necessary. Demonstrations of what can be achieved with this technique are also important.

(B) Application in Earth Science

(1) Development in Nano-Geoscience:

In recent years, the investigation of geoscientific samples, such as piston cores, using the new information extracted from the microscopic structure of the samples has been growing. We propose the development of a new technique, white X-ray CT, which has additional functions compared to conventional X-ray CT. For example, it can identify the crystal structure from an X-ray diffraction pattern, which is simultaneously obtained with a transmission CT measurement, and map out the spatial distribution of a specific element using an absorption edge. We consider that

such development be carried out since the IODP has just started.

(2) Microstructural Analyses of Environmental Index Samples and Natural Samples:

The scattering-topography technique is useful for the analyses of various natural samples. In addition, some users want to know the chemical state (identification of molecules) and the elements contained in a local volume. A combination of the scattering-topography technique and the Raman scattering measurement or AFM probing is considered as a new method of meeting the above-mentioned requirements.

2) DXAFS

The JASRI plans to develop a gas-handling system and an in-situ cell, and also to install a microstrip detector into the experimental station. This is expected to improve research on chemical processes, such as catalysis. It is required to develop an instrument that can probe the rapid, dynamical changes in atomic structures using a pulse-valve or pump-and-probe technique. It is also important to broaden the range of applications toward various physical and chemical dynamical processes, such as phase transition and catalysis.

User-friendly that can measure a large number of samples within a short time should be developed by making the most of the rapidity of DXAFS measurement. Thus, it is reasonable to give priority to the use of high-energy x-rays in DXAFS.

3) Beamline Operation

(A) Collaboration with Users' Group

We expect that the JASRI in collaboration with the users' group will further improve the beamline infrastructure for users. Such an improvement is expected to expand the scope of research and to increase the number of target samples.

(B) Increase in Number of Users' Groups

The usefulness of white X-ray topography and DXAFS should be advertised on the net and in academic meetings. Inviting new users' groups and expanding the scope of research are required.

(C) Industrial Applications

The JASRI should consider a system that willingly accepts non-proprietary proposals from industries in order to use the beamline more effectively. It is also required to develop a service and support system which is easily accessible to industries.

3. Summary

The committee suggests that the BL28B2 beamline should continue research studies that make the most of the advantages of white X-rays from a bending magnet. The committee recommends the following:

(1) The JASRI should continue to develop techniques for white X-ray topography and DXAFS. The JASRI should also actively advertise results and possibilities to potential users and invite new users and broaden the range of applications.

(2) The JASRI, in close collaboration with users' groups, should further improve the infrastructures at the experimental stations.