### Development of Trichromator at SPring-8 RIKEN Beamline I

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### 1. Introduction

With tunability over a wide energy range of the synchrotron radiation, the multi-wavelength anomalous diffraction (MAD) method, which gives crystallographic phase information from anomalous scatterers [1], has been developed [2]. Utilizing a third-generation SR facility and with the maximized advantage of the MAD method, RIKEN beamline I (BL45XU) at SPring-8 is designed to contribute to ward studies on structural biology by the Institute of Physical and Chemical Research (RIKEN) [3, 4].

To insure the accuracy in MAD experiments, it is essential to minimize systematic errors. In these experiments, at least three sets of diffraction data have to be collected at three different wavelengths. The wavelengths have to be tuned as quickly as possible with good reproducibility. To achieve such an experimental environment, the 'trichromatic concept' has been introduced to SPring-8 by the development of a tandem vertical undulator and the trichromator equipped with high-quality diamond crystals.

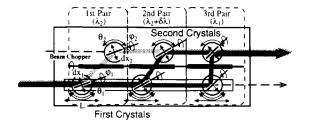


Fig. 1 Schematic draw of the trichromator

### 2. Trichromator design

Dichromatic synchrotron radiation is branched out by a beam-splitter, i.e. a transparent diamond monochromator. The beam-splitter plays the role of a first monochromator for the small-angle X-ray scattering (SAXS) branch beamline. The beam of the transparent part through the beam-splitter is guided to the trichromator for the protein crystallography station. The trichromator uses synthetic

diamonds [5] delivered by Sumitomo Electric Industries Co. Ltd., and the crystal sizes range from  $5\times4$  mm² to  $7\times5$  mm². The reflection planes of the diamonds are (4 0 0) with Bragg geometries and the fundamental energy cover range is from 7 keV to 16 keV. The mechanisms of the trichromator are illustrated in Fig. 1. Construction of the trichromator was completed by Sigma Koki Co. Ltd., Japan.



Fig. 2 The first image of three undulator spots

## 3. The first observation of trichromatic undulator beams

The initial test of the trichromator was performed by using diamond crystals with a thickness of 1 mm under 1.0 mA operation of the storage ring. The trichromator successfully monochromatized three wavelengths at the same time, and three beams were observed on a phosphor screen.

The image of the three spots is shown in Fig. 2. In the figure, the spots are displaced from each other to give a different energy. The three spots were independently controlled by each of the monochromator pairs of the trichromator. Then, the energies of the individual pairs were set at 9.7 keV, 9.9 keV, and 10.2 keV, respectively. Each diamond crystal with a thickness of 1 mm transmitted almost 70% of the incident beam in the energy region. The energies of the three beams were detected by measuring the scattering X-rays by air. The spectrum of the beams was measured by using a Si-SSD detector

(Fig. 3).

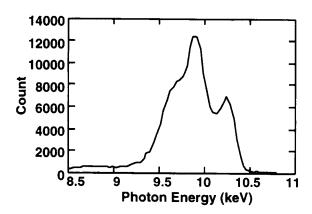


Fig. 3: Spectrum of trichromatized undulator beams

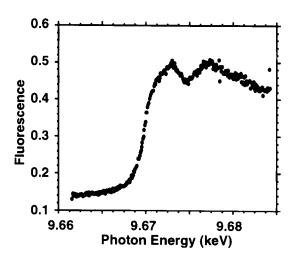


Fig. 4: X-ray fluorescent spectrum of a zincprotease

# 4. Measurement of X-ray fluorescence spectra

X-ray fluorescent spectra are needed to optimize the anomalous effects of MAD data sets. Energy scan control is carried out on the trichromator and fluorescent photons are counted using an NaI scintillation counter. A *Grifola frondosa* metalloprotease crystal is supplied to measure the spectra (Fig. 4).

### 5. Examination of diffraction data collection

For the examination of the beamline, some protein crystals were used to collect diffraction data. First of all, diffraction images of a tetragonal crystal of hen egg white lysozyme were taken with a coaxial three-color beam (Fig. 5). Diffraction data sets for the crystals of the lysozyme and isopropyl malate dehydrogenase from *Thermus thermophilus* were collected using a Rigaku R-AXIS IV image plate detector with monochrome X-ray.

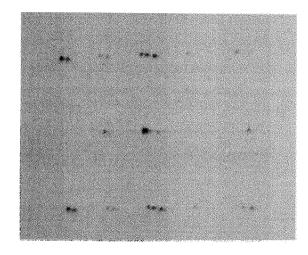


Fig. 5: Diffraction spots of a lysozyme crystal with trichromated X-ray

### 6. Summary

For the PX station at RIKEN beamline I, the 'trichromatic concept' optimized for MAD data collection was newly designed and put into effect. Initial construction plans have been completed, and we are now proceeding on to the commissioning phase with synchrotron radiation. As the first step in this phase, the trichromator 'trichro-'matized an undulator beam and diffraction data sets were collected for some protein crystals, successfully.

### 7. Acknowledgment

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#### References

- J. Karle, Int. J. Quant. Chem. 7, 356-367 (1980).
- [2] W.A. Hendrickson et al., Proteins 4, 77-88 (1988).
- [3] M. Yamamoto et. al., Rev. Sci. Instrum. 66, 1833 (1995).
- [4] T. Ueki et al., SPring-8 Ann. Rep. 1996, 105-108 (1996).
- [5] T. Uruga et al., Rev. Sci. Instrum. 66, 2254-2256 (1995).