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# Connection of powder diffraction intensity data measured with a multiple-detector sysmtem

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## Introduction

A multiple-detector system (MDS) for powder X-ray diffraction measurement has been utilized on the powder diffraction beamline BL4B$_2$ at the Photon Factory (PF) in Tsukuba [1]. High-resolution diffraction intensity data ranging 0 – 155 deg. can be collected within about 10 hours, which has been enabled by the enhanced efficiency in data acquisition.

However, the effects of slightly different characteristics of the detectors upon the segmented intensity data may be problematic for application to detailed analysis of diffraction peak profiles. We propose a new method for correcting peak profiles measured with the MDS. The method is based on Fourier analysis of the observed intensity profiles in the overlapping regions.

## Method

### *Concept*

According to the the convolution theorem, the intensity data affected by different instrumental functions can be corrected by multiplying the Fourier transform of the data by the ratio of the instrumental functions $W_{12}(\xi)$ for the adjacent detectors. The current method is aimed to evaluate $W_{12}(\xi)$ by analyzing the experimental data in the overlapping regions.

### *Weighting scheme*

Since experimental data are affected by statistical errors, a kind of modeling or smoothing treatment is needed to extract the main features of the intrinsic deviation of the instrumental functions. In general, the characteristic features of the instrumental functions are only included in the low-$\xi$ range on the Fourier transformed scale, while the values in the high-$\xi$ range are heavily affected by the statistical errors. Therefore, appropriate weighting for data is needed to apply a least-squares modeling in order to attach greater importance to the low-$\xi$ data. The following discrete form of the weighting has been tested,

$$(W_{12})_k = \left| \sum_n \left[ (\varepsilon_1)_n^{-2} + (\varepsilon_2)_n^{-2} \right] \exp(2\pi i k n / N) \right|^2$$

where $\{(\varepsilon_1)_n\}$ and $\{(\varepsilon_2)_n\}$ are the experimental errors in the intensity data measured with the adjacent detectors and $N$ is the number of overlapping data.

## Results

### *Curve-fitting for the Fourier transformed correction function*

The powder diffraction intensity data of a capillary specimen of standard ZnO (NIST SRM674), measured with the MDS have been used to test the method. Figure 1 shows the ratio of the Fourier transformed intensity data measured with the No. 1 and No. 2 detectors, and the fitting polynomials. It is suggested that the main features of the experimentally evaluated Fourier correction are extracted by the fitting polynomials.

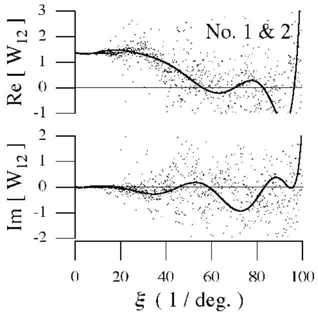

Fig. 1 Real and imaginary parts of the Fourier correction (dots: experimental, lines: fitting ).

The Fourier transformed No.2 data are multipled by the complex of the polynomials, and then inverse-Fourier transformed. The results are shown in Fig. 2. The corrected data for the No.2 detector are well coincided with the No.1 data, in the overlapping region.

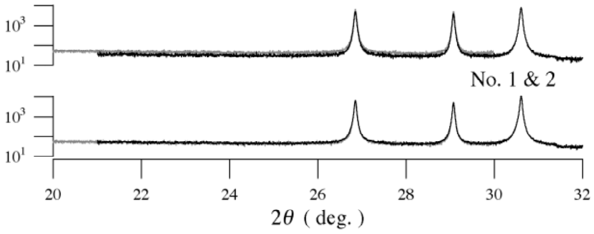

Fig. 2 Original (upper) and corrected (lower) data.

## References

[1] H. Toraya et al., *J. Synchrotron Rad.* **3**, 75 (1996).

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