

Analysis of Powder Diffraction Data Measured with Synchrotron X-ray and 2D Detector

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A powder diffraction measurement system constructed on a beam-line BL5S2 at Aichi Synchrotron Radiation Center in Seto, Japan, has been modified for extensive use of two-dimensional (2D) X-ray detectors. Four flat 2D detectors (Dectris, PILATUS-100K) are mounted on the movable stages on supporting rods radially attached to the 2 Θ -wheel of the goniometer (Huber, 401-440) with the interval of 25°. Any camera length from 340 mm to 1000 mm can be applied, when the detectors are located on the meridian positions.

The 2D powder diffraction intensity data are reduced to conventional 1D format of powder diffraction data by the method proposed by Sulyanov *et al.* [1]. As the method is based on averaging of the pixel intensities with geometrical corrections, it is quite easy to incorporate evaluation of standard uncertainties about the reduced intensity data.

The uncertainties estimated for the diffraction data from fine quartz powder filled in 0.5 mm-capillary has shown double-peak profile, which is naturally assigned to the propagation of errors in the diffraction angle 2θ , as has been suggested for laboratory powder diffraction data by one of the authors [2]. The lattice constants of the quartz sample have been estimated at $a = 4.9131(4)$ Å and $c = 5.4043(2)$ Å by a Rietveld code, RIETAN-FP [3], ($R_{wp} = 0.84$ %) from the intensity and uncertainty data including 9 reflection peaks. No significant peak shift or asymmetry of peak profile has been detected.

The reduced diffraction data of 0.1 mm-capillary LaB₆ (NIST SRM660b) sample have also shown almost symmetric peak profile, but slight asymmetry has been detected, which can be simulated by a Beta-distribution profile function.

[1] Sulyanov S. N., Popov A. N. and Kheiker D. M. *J. Appl. Cryst.*, 1994, 27, 934. [2] Ida T. *Solid State Phenomena*, 2013, 203/204, 3. [3] Izumi F. and Momma K. *Solid State Phenomena* 2007, 130, 15.

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