Symmetrisation of Powder Diffraction Peak Profiles by a Fourier Method

Takashi Ida, Ceramics Research Laboratory, Nagoya Institute of Technology. Tajimi, Japan. E-mail: ida.takashi@nitech.ac.jp

Powder diffraction intensity data with asymmetric peak profiles measured with a conventional Bragg-Brentano diffractometer and a high-resolution synchrotron diffractometer are treated with a fast Fourier transformation method [1, 2] to obtain intensity data with symmetric peak profiles. The method is based on deconvolution of analytical expressions of the optical aberrations of the diffractometers [3-6]. The symmetrised peak profiles enable simplified analytical procedures for individual peak profile fitting, whole pattern decomposition and Rietveld refinement.

The symmetrised diffraction data of fine SiC powder (JFCC, RP-2) measured with a conventional powder diffractometer has revealed a "super-Lorentzian" character of intrinsic diffraction peak profiles, which is reasonably explained by a theory for diffraction from small spherical crystallites with broad log-normal size distribution [7]. The results of a least-squares refinement applied to integrated intensity values of 42 reflections extracted from symmetrised high-resolution diffraction data of standard ZnO powder (NIST, SRM674) measured at Photon Factory in Tsukuba has been coincidence factor of R = 0.45% with reasonable structure parameters.

[1] Ida T., Toraya H., J. Appl. Cryst., 2002, 35, 58. [2] Ida T., Toraya H., J. Appl. Cryst., 2003, 36, 890. [3] Ida T., Rev. Sci. Instrum., 1998, 69, 3837. [4] Ida T., Kimura K., J. Appl. Cryst., 1999, 32, 634. [5] Ida T., Kimura K., J. Appl. Cryst., 1999, 32, 982. [6] Ida T., Hibino H., Toraya H., J. Appl. Cryst., 2001, 34, 144. [7] Ida T., Shimazaki, S., Hibino H., Toraya H., J. Appl. Cryst., 2003, 36, 1107.

Keywords: powder diffraction, profile analysis, Fourier methods