Poster Presentation

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Deconvolution-convolution treatment of powder diffraction data collected in Bragg-Brentano geometry

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A deconvolution-convolution method to correct shift and asymmetric deformation of observed diffraction peak profile, caused by instrumental aberrations of Bragg-Brentano geometry [1], has been improved. The method is based on scale-transform of abscissa, interpolation of data, and fast Fourier transform. The main improvement about this method has been achieved by cumulant analysis of theoretical axial-divergence aberration function, and finding of mathematical formulas that can precisely reproduce the angular dependence of the first and third order cumulants of the axial-divergence aberration function by double convolution on appropriate scales.
The effects of the even order cumulants of the aberration function are kept unchanged just by multiplication of absolute value of the Fourier transform on division by the Fourier transform of component instrumental model function. It means that the powder diffraction data treated by the method will provide the peak profile with the same integrated intensity, width and kurtosis (sharpness) etc as the peak profile in the source data, because all the characteristics of the symmetric part of a function are determined by the even order cumulants of the function.
The deconvolution-convolution treatment also enables incorporation of a realistic spectroscopic profile model, such as combination of Cu Kα quartet and Cu Kβ quintet models [2] and white X-ray caused by bremsstrahlung and absorption of Ni foil. The deconvolution with a realistic spectroscopic profile model and convolution with hypothetical singlet Cu Kα1 profile without contribution of white X-ray have been applied to the diffraction data of standard LaB6 (NIST SRM660a) and Si (NIST SRM640c) samples. The structures originated from Cu Kα2 and Cu Kβ emissions and Ni K-absorption edge have effectively been reduced in the processed data, but it has been found that there still remain some unidentified small peaks.
The intensities of the small peaks have also been reduced by the treatment on assumption that those peaks are caused by emissions from tungsten and nickel in the X-ray tube.
Magnified plots of observed and deconvolved-convolved powder diffraction data of Si are shown in Figure 1.

[1] Ida, T. & Toraya, H. (2002). J. Appl. Cryst., 35, 58-68.
[2] Deutsch, M. et al. (2004). J. Res. Natl. Inst. Stand. Technol., 109, 75-98.

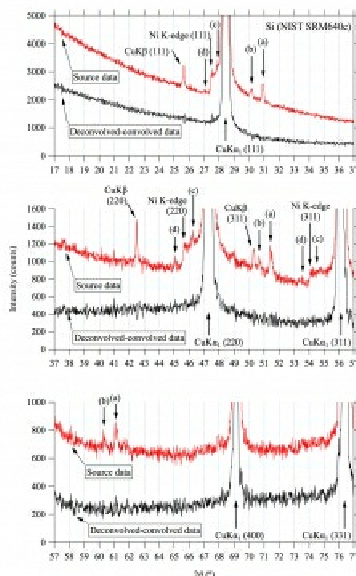

Figure 1 Magnified plots of the observed and deconvolved-convolved powder diffraction data of Si. Unidentified peaks are marked by (a)–(d).

Keywords: deconvolution, Bragg-Brentano geometry, axial-diverence aberration