

Improvement of Deconvolution-Convolution Method for Powder Diffractometry

Takashi Ida¹, Daiki Hattan¹ and Katsuhiro Nomura²

¹ACRC, Nagoya Institute of Technology, Asahigaoka, Tajimi, Gifu 507-0071, Japan

²Inorganic Functional Materials Research Institute, National Institute of Advanced Industrial Science and Technology, Anagahora, Shimoshidami, Moriyama, Nagoya, Aichi 463-8560, Japan

The whole-pattern deconvolution-convolution method [1] has been improved to remove the shift and deformation caused by axial-divergence aberration in Bragg-Brentano geometry. The improvement has been achieved by cumulant analysis of the theoretical axial-divergence aberration function [2]. Powder diffraction data collected with Cu K α X-ray and Ni K β filter have been analyzed. The method is easily extended to remove small unwanted peaks from the observed data caused by contamination of Cu-target X-ray tube. Figure 1 shows the peak profile of observed and deconvolved-convolved powder diffraction data of LaB₆, where the expected peak positions are marked by arrows. Small peaks detected in the observed data are effectively removed in the deconvolved-convolved data.

References:

[1] Ida, T. and Toraya, H. (2012). *J. Appl. Crystallogr.* 35, 58–68.

[2] Ida, T., Ono S., Hattan, D., Yoshida, T., Takatsu Y. and Nomura, K. (submitted) *Powder Diffraction*.

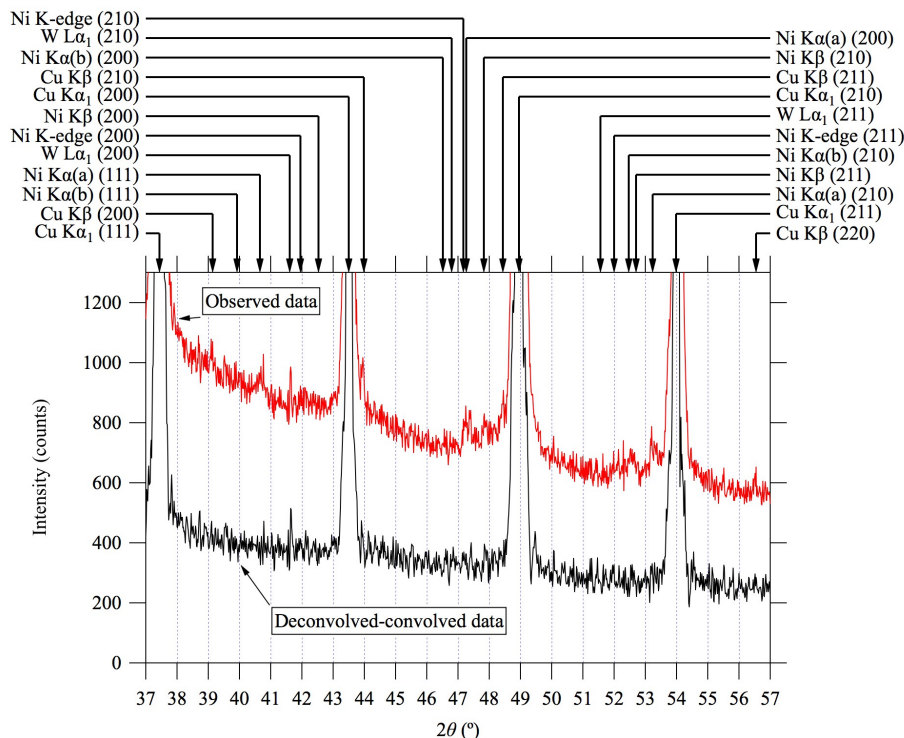


Figure 1 Observed and deconvolved-convolved powder diffraction profile of LaB₆.