DECONTAMINATION OF POWDER DIFFRACTION DATA MEASURED WITH COPPER Kα X-RAY AND NICKEL FILTER

Takashi Ida[1], Daiki Hattan[1] and Katsuhiro Nomura[2]
[1]Advanced Ceramics Research Center, Nagoya Institute of Technology, Asahigaoka, Tajimi, Gifu 507-0071, Japan
[2]Inorganic Functional Materials Research Institute, National Institute of Advanced Industrial Science and Technology, Anagahora, Shimoshidami, Moriyama, Nagoya, Aichi 463-8560, Japan

One-dimensional X-ray detector has become widely used in laboratory powder diffraction measurement. We have analyzed the diffraction data from standard Si (NIST SRM640c) and LaB_6 (NST SRM660a) powder samples collected with a combination of a Cu Kα X-ray tube, a flat powder specimen, a Ni foil Kβ filter, a couple of Soller slits and a one-dimensional detector arranged in Bragg-Brentano geometry.

The deconvolution-convolution method [1] has been improved to remove the shift and deformation caused by axial-divergence aberration more precisely than the previous method [2]. It has been found that the contribution of white X-ray emitted from the tube should be taken into account to simulate the step structure caused by Ni K-absorption edge [3]. Cu Kα_2, Cu Kβ and Ni K-absorption edge structures and unidentified four series of small peaks (a), (b), (c), (d) marked in Figure 1 have effectively been removed by the current deconvolution-convolution method applying a realistic spectroscopic profile model of the source X-ray. Origins of peaks (a)–(d) are not fully identified, but they are likely to be caused by contamination of tungsten and nickel in the X-ray tube.

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

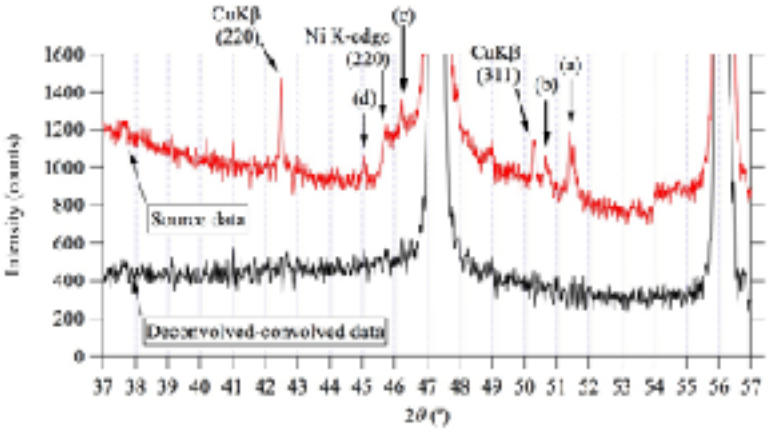

Figure 1 Magnified plots of the observed and deconvolved-convolved powder diffraction data of Si.