

"Studies on Instruments and Analytical Methods Aiming at Evaluation of Crystallite Size from Powder Diffraction Data"

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It is well known that the size of small crystallites can be evaluated by line-broadening analysis of powder diffraction intensity data. The statistical distribution of crystallite size may also be evaluated by detailed analysis of the size-broadened profile. However, experimental evaluation of the size-broadened profile is difficult for materials having average crystallite sizes larger than 100 nm, mainly because of instrumental broadening or smearing effect of the observed diffraction peak profile, which is expressed by the convolution with the instrumental function. Instrumental broadening for a diffractometer is modeled by the multiple convolution of the spectroscopic distribution of the X-ray source and optical aberrations of the diffractometer. The speaker has originally found approximate formulas for the axial-divergence aberration function of laboratory X-ray and synchrotron powder diffractometers, and also a practical numerical method to calculate the convolution. In attempting to apply Fourier-based deconvolution methods to remove the instrumental function from experimental diffraction data, it has been found that a fast Fourier transform algorithm can be applied to treat wide-angle powder diffraction data; when appropriate abscissa scaling is used. Propagation of statistical errors through the deconvolution is also discussed. A deconvoluted diffraction peak profiles from SiC fine particles with broad size distribution shows a sharp peaktop and long tails, both of which are well reproduced by a theoretical diffraction peak profile from lognormal distributed crystallite size broadened profile.