XRD Peak Profiles in the Case of the Lognormal Crystallite Size Distribution

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Since the lognormal distribution of a crystallite size in a powder simple is the most realizable one in practice, determination of the size distribution parameters (the median and logarithmic standard deviation) from X-ray diffraction peak profile characteristics (FWHM or integral width and shape factor) is an important problem of structure analysis.

Langford *et al.* [1] have shown in principle that the size distribution can be determined directly by a profile fitting method. However, their evaluation restricted to a small variance of the distribution.

In this paper, effect of the lognormal distribution parameters on the peak profile is examined without any assumption of the parameter rage. For that the diffraction peak intensity profiles from lognormally distributed spherical crystallites is simulated and analyzed thoroughly.

Unique correlation between the distribution parameters and the XRD peak characteristics was found to exist within a wide range of the parameter values.

[1] Langford J.I., Louer D., Scardi P., *J. Appl. Cryst.*, 2000, **33**, 964. Keywords: powder, crystallite size distribution, XRD