 ICCES, vol.10, no.1, pp.7-7

Crystallite Size Distribution Determination By X-Ray Diffraction

D. Balzar[1]

Summary

X-ray diffraction is a useful technique for the estimation of size distributions of smaller crystallites. With the constant improvement of experimental techniques, especially with the advent of new-generation synchrotron and neutron sources with superior resolution, these size distributions can be precisely determined. Furthermore, modern methods for the analysis of X-ray diffraction patterns, such as Rietveld refinement, increasingly go beyond the determination of structural parameters and include refinable parameters for a physical crystallite size distribution.

Several common size distributions (such as lognormal and gamma) will be considered. Particularly, a lognormal distribution of both ellipsoidal and cylindrical crystals with elliptical cross-sections can be used to successfully model anisotropic size broadening. In an example (ZnO powder), the apparent crystallite most closely resembling the shape obtained by the spherical-harmonics model was obtained by using a bimodal lognormal distribution of ellipsoidal crystallites with two different shapes, corresponding to two size-distribution modes. This shape of the apparent crystallite is in agreement with those reported earlier from X-ray diffraction line broadening analysis and TEM for this sample.

[1]Department of Physics and Astronomy, University of Denver, Denver, CO 80208, USA