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Particle statistics in powder diffraction method

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The statistical variation in observed powder diffraction intensity is often dominated by the limited number of crystallites that satisfy the diffraction condition. This effect has been termed with particle statistics in powder diffraction method [1]. We have reported experimental validation of the theory for particle statistics about symmetric reflection mode measurements, and proposed a new method to evaluate the crystallite size and its distribution by statistical analysis based on a generalized theoretical framework [2]. We have also demostrated improvement of structure refinement by application of the maximum likelihood estimation to statistical model explicitly taking the errors caused by the particle statistics into account [3]. As the formula suitable for the particle statistics about a continuously spinning flat specimen is still unclear, three kinds of diffraction intensity measurements, (1) in-plane (Φ)-scan, rocking angle (Ω)-scans for (2) stationary and (3) spinning flat specimens, have been conducted for standard powder samples of Si (NIST SRM640c) and lanthanum hexaboride (NIST SRM660a) at a synchrotron powder diffraction beamline BL-4B2 at the Photon Factory, KEK in Tsukuba. The statistical variance observed inΦ-scan and Ω-scan measurements for stationary specimens have shown cosecant dependence of the effective number of diffracting crystallites, just as predicted by the traditional theory. The statistical variance in Ω-scan measurements for spinning specimens has also shown a cosecant behaivior rather than the squared cosecant dependence suggested by de Wolff [1].

[1] *P. M. de Wolff, Appl. Sci. Res. 1958, 7, 102-112.,* ***[2]*** *T. Ida, J. Appl. Cryst. 2011, 44, 911-920.,* ***[3]*** *T. Ida, F. Izumi, J. Appl. Cryst. 2011, 44, 921-927.*

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