ESTIMATION OF ERRORS IN THE MEASUREMENT OF UNIT-CELL PARAMETERS: STATISTICAL UNCERTAINTIES OF PEAK POSITIONS OF POWDER DIFFRACTION LINES DETERMINED BY INDIVIDUAL PROFILE FITTING

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A formula for estimating a statistical uncertainty of peak position, determined by individual profile fitting, has been derived. A magnitude of the statistical uncertainty is given by (sum of peak profile intensities)$^{-1/2}$ × full-width at half-maximum × form factor × correlation factor × quality factor × the goodness-of-fit index. The form factor depends on a shape of diffraction profile, and it becomes smaller by 40% when the profile shape changes from Lorentzian to Gaussian. The correlation factor represents the parameter correlation between the peak position and the parameter for profile asymmetry, and it becomes unity when the profile shape is symmetric or the parameter for profile asymmetry is fixed during the least-squares fitting. The quality factor depends on a peak-to-background ratio. The formula was experimentally verified by using diffraction data sets of CeO_2 and Si powders. The statistical uncertainty is essentially based on the counting statistics and profile width. Therefore, the peak position of a strong and sharp peak in the low angle region can be determined more precisely than that of a weak and broadened peak in the high angle region. The formula gives a guideline for optimizing experimental parameters for required precision.