

On the use of pseudo-Voigt function in the variance method of size-strain analysis

PRABAL DASGUPTA¹, Endale Abeba Gudeta²

¹N/A ²Jimma University

pdg23091952@gmail.com

Although pseudo-Voigt(p-V) function is widely used to describe an experimentally observed powder XRD line, mainly due to ease with which its mathematical calculations could be tackled, Dasgupta[1,2] has shown that under certain conditions fitting of an observed profile with a p-V function, may lead to erroneous results, in case of Warren-Averbach[3] analysis. Pseudo-Voigt functions may be fitted with experimentally observed X-ray powder diffraction profiles and subsequently be subjected to variance method of size-strain analysis to extract particle size and root mean square strain of a crystallite. This work mathematically shows that for spherical crystallite and also for h00 reflections of a cubic crystallite and hho reflections of an octahedron shaped crystals (for which taper parameter $L=0$), Cauchy content η must be less than 0.328, otherwise no meaningful results in terms of particle size and root-mean-square (r.m.s) strain could be extracted from such profiles. We have made use of variance equation for pseudo-voigt profile deduced by Sanchez-Bajo and Cumbreira[4] and expression for intercept of a sample related variance, W_0 given by Klug & Alexander[5]. Taper parameter values were taken from Wilson's paper[6].

References:

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