Poster Presentation

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Characterization of a diffraction profile using the fourth cumulant

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In this study, line broadening in a diffraction intensity profile of powder crystalline materials due to particle size and lattice strain has been characterized by a new function- the fourth cumulant of the diffraction profile. Diffraction intensity profile is usually characterized in terms of half intensity width (FWHM), Fourier Transforms, second and fourth restricted moments etc. The cumulants, with addtional property of additivity[1], can be used to de-convolute the contribution of several effects such as crystallite size, lattice strain, stacking fault, dislocation, etc., to the line broadening. Since the first three cumulants are the same as the corresponding moments, we investigate the fourth cumulant, which is a function of fourth and second moments. Here, line broadening has only been due to particle size and lattice strain. Previous reports [1] showed that fourth cumulant of a Gaussian was zero, where as we now show that for Cauchy, Voigt and pseudo-Voigt distributions, the fourth cumulant is non-zero. Hence, the fourth cumulant of functions describing particle size and lattice strain for the latter types of distribution has been derived, as well as those for crystalline and para-crystalline materials. For crystalline materials, it was shown that fourth cumulant for particle size and strain (jointly) is the simple sum of the 4th cumulant for particle size and that of strain individually- thus proving the additivity of the fourth cumulant. This work illustrates the advantages of considering the fourth cumulant for characterizing line broadening in terms of particle size and strain.

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