MS72.O02

Preferred Orientation, PDF and Debye Equation

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The effect of preferred orientation is currently neglected in the Debye Equation and PDF calculations. This is to a large extend justified, especially for the PDF, as the scattering by large sample volumes is detected by an area detector. The integration of powder rings reduces the effects of preferred orientation. As more laboratory PDF measurements become available that use linear position sensitive detectors or single counter detectors, preferred orientation needs to be reconsidered. A Rietveld calculation treats preferred orientation by multiplying the Bragg intensity by a factor that depends on the angle between the reciprocal space vector and the preferred orientation axis. The powder intensity I(Q) is thus multiplied by a complex function that depends at each Q on the degree of preferred orientation, the lattice parameters, reflection multiplicity etc. The effect on the PDF is therefore the convolution by the Fourier transform of this complex function. The Debye equation is derived from a spherical average of the scattering intensity of a finite object. Thus completely random orientation of the powder grains is implicitly assumed. Both, the Debye algorithm and the PDF algorithm calculate the powder pattern, respectively the PDF from a histogram of interatomic distances, which correspond to a spherical average of all interatomic distance vectors. This histogram does not allow for a Rietveld preferred orientation correction. The effects of preferred orientation on the PDF will be presented on the basis of simulated diffraction pattern. An algorithm to describe the changes in the PDF and the inverse sine Fourier transform as a convenient tool to calculate the powder diffraction pattern will be introduced. This is a good alternative to the Debye equation and allows to take preferred orientation into account both for the PDF and the calculated powder.

Keywords: pair distribution function, preferred orientation, nanomaterials