

#### *Total scattering study of chaotic/statistical microstructure with traditional crystallographic tools*

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Total scattering commonly identify the analysis of a diffraction pattern by considering both Bragg and diffuse features. For most of the scientific community, the term is synonym of the Pair Distribution Function (PDF) or the Debye Scattering Equation (DSE) methods, both widely employed for structure/microstructure studies in the nanomaterials field. This is however a misconception.

Pointwise, the powder diffraction pattern is the spherical mean of the intensity of the Fourier transform of the electron density of the (powder or polycrystalline) specimen under study. Based on the knowledge of all atomic positions, the DSE obtains the pattern by considering the intensity contribution from all couples of atoms in the system, with the drawback of a computing load that scales with the sixth power of the number of atoms. The PDF takes a completely different approach, based on the relationship between the radial distribution of atoms and the Fourier transform of the diffraction pattern. In this case a virtually infinite diffraction pattern has to be measured to avoid artefacts in the Fourier transformation. Further, the DSE calculation can be directly compared with the measured data, whereas a remapping and a Fourier transform are needed for the PDF comparison in real space.

More traditional tools (e.g. Rietveld method, WPPM), are seldom considered in the total scattering community, as they have been developed/tuned for Bragg scattering only. In the case of fully periodic systems, they are the winners, as they reproduce the powder pattern fast and accurately by performing most of the transformation and averaging operations analytically. With the periodicity limitation, they perform the same task as the DSE (generating a powder pattern in measurement space), but much faster (one of the main advantages of the PDF approach).

In several practical cases it is possible to extend those traditional tools to perform fast total scattering studies directly on the measured data. When diffuse features are present, the determinism has to be abandoned for statistical/chaotic microstructure features. The latest developments of line profile analysis (LPA), relating physical (microstructure) features with the shape of the diffraction lines, aim in this direction. In simple cases (e.g. finite size domains, diluted defects), the microstructure causes just Bragg peak broadening; in more complex ones (e.g. stacking faults), diffuse scattering appears due to the statistical nature of the defects: a global model for the specimen can then be made, for which the intensity (Bragg plus diffuse) can be obtained analytically. Instrumental features and thermal diffuse scattering can also be considered.

Total scattering analysis is therefore possible without the DSE or the PDF, i.e. without explicitly considering all atomic positions, with a clear computational advantage. Working directly on the measured data with a global model for the specimen, we can directly observe the effects of model/parameters choice and work with any source, avoiding possible artefacts resulting from limited measurement of the reciprocal space, loss of directional information or the need to use multiple models for the short and long range behaviour.

Theory and supporting examples will be shown and discussed.

**Keywords:** [microstructure](#), [defects](#)