Use of Pattern Correction Algorithm to Remove the Effect of Axial Divergence in Atomic Pair Distribution Function (PDF) Analysis

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The PDF technique utilizes a Fourier transformation of the X-ray powder diffraction (XRPD) data and gives information about the inter-atomic distances of the material. The accuracy of this assessment of inter-atomic distances depends strongly on the energy of the utilized radiation source and the possibility to correct for aberrations from the instrumental set-up that is used. Recent advances in laboratory X-ray diffractometer technology like e.g. new generation detectors optimized for hard radiation (like Mo and Ag radiation) allow to minimize artifacts or fluctuations in the PDF arising from statistical noise, resulting in more reliable data. Nevertheless, effects of instrumental aberrations and particularly axial divergence may still influence the accuracy of the final result. A possible way around is the use of a well collimated beam and 2D data collection or the use of small Soller collimators in combination with line focus optics. Both approaches significantly reduce the measurement intensity and increase the measurement time.

Here we present an alternative route by "cleaning" the data from axial aberration before the PDF is calculated. The used patented aberrations correction method [1, 2] is capable of correcting for systematic instrumental aberrations while considering multiple overlapping peaks as a single continuum. It is based on an integral transformation algorithm and converts the measured pattern into the corrected one without influencing resolution. The algorithm may be applied to any pattern without prior analysis; the resultant peaks appear to be symmetrical and located in the ideal (Bragg) positions regardless of the instrumental setup.

We will demonstrate the application of the correction algorithm with several examples and demonstrate the possible speed gain in PDF measurements and/or possible improvement in data quality.

[1] Kogan V.A., Kupriyanov M.F., J.Appl.Cryst, 1992, 25,16-2
[2] Kogan V.A. US7516031B2 "Apparatus and method for correcting for aberrations"