New Model-free Method of Aberrations Correction for X-ray Powder Diffractometry

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The influence of instrumental aberrations is different for different experimental XRD set-ups. Proper correction for aberrations is required for accurate analysis, comparison, and storage of patterns in databases. Most of the current methods for aberration correction are based on simulation, which requires the introduction a model of peaks in the pattern. The introduction and refinement of peaks model is not always possible based on the available information.

We will describe the new method capable to correct instrumental aberrations while considering the diffraction pattern as a single "unknown" continuum. No input information about the sample microstructure or peak positions is required, and generally, there are no variable parameters to be refined.

An algorithm named "cleaning procedure" [1] incorporating the mathematical model of instrumental aberrations [2], converts an experimental pattern to one corrected for instrumental aberrations. The peaks in the corrected pattern appear to be symmetrical and positioned in the ideal (Bragg) positions regardless of the instrumental setup. The corrected pattern may be processed later by any analytical package or stored in the database.

The advantage of this approach is that the aberration correction stage is split from the analytical stage and may be performed with minimum sample information. The application of the method to patterns of different structures including bio-polymers will be presented for reflection, transmission, focusing and parallel beam geometries.

[1] patent pending. [2] Kogan V.A., Kupriyanov M.F., J.Appl.Cryst, 1992, 25,16-25.

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