

Use of “Cleaning” Algorithm for Model-Free Correction of Instrumental Aberrations in XRPD Patterns

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XRPD patterns of pharmaceutical substances are often constituted by a significant number of peaks at low angles. As a result, XRPD patterns of pharmaceuticals are strongly influenced by instrumental aberrations, particularly by the aberration originated from the axial divergence of X-Rays. These instrumental aberration effects result in additional peak broadening, peak asymmetry and peak center gravity shifts from the "ideal" Bragg position.

Traditionally, methods for the correction of instrumental aberrations were based on modeling of individual peaks. In this poster we present a methodology for the correction of instrumental aberration effects by considering an XRPD pattern as single "unknown" continuum without the need for introduction of separate peak models. No prior knowledge about the crystallographic unit cell or peak indexes is required.

The method is based on the integral transformation algorithm disclosed in reference [1]. As input for the correction the algorithm uses Fourier coefficients of instrumental functions as described in reference [2].

The algorithm converts the measured pattern into a corrected pattern without influencing the resolution. The resulting peaks appear to be symmetrical and located in the ideal (Bragg) positions regardless of the instrumental setup. This method is beneficial for indexing, search-match, full-pattern refinement and polymorph discrimination. The main advantage of this approach is the possibility to make the peak positions of "cleaned" patterns independent from the instrumental setup without the need for immediate analysis.

We will present examples of this methodology as general pretreatment for patterns of pharmaceutical substances.

[1] Kogan V.A. US7516031B2 “Apparatus and method for correcting for aberrations”

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