Optical Aberrations from Johansson-type Incident Beam Monochromators on Bragg-Brentano Powder Diffractometers

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We present a new model of the interaction of a Johansson Incident Beam Monochromator (IBM) on a high-precision powder diffractometer with a copper anode source. This model includes two effects that result from this optical element:

- the atomic emission spectrum of the anode is trimmed due to the band-limiting effect of the monochromator, resulting in reduced interference of the spectrum with the Lorentz tails of the diffraction peaks caused by microstructure,
- the central region of the diffraction peaks are slightly broadened by the dispersion of the spectrum by the optic.

We compute these effects using full dynamical diffraction theory, including effects of finite source size and crystal focusing. This results in a straightforward analytical model, which we compare to Monte-Carlo raytracing.

These effects can be included in the Fundamental Parameters Approach (FPA) analysis of data from the machine, resulting in higher quality fits over the entire angular range to peak shapes. We will present data collected from different materials, and show that the model does improve the quality of fits, and allows valid microstructural parameter extraction for larger crystallite sizes than is possible without it. It also improves the ability to measure lattice parameters to very high precision, since the distortion of the shape of low-angle peaks due to the extra dispersion is properly computed.