

Effect of systematic errors on lattice parameter refinement

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The Bragg-Brentano para-focusing geometry is widely used for powder diffraction measurements because of its high intensity and resolution and relatively simple hardware requirements. However, the diffraction peak positions often have systematic errors associated with the focusing nature of the geometry and those errors result in the errors of the lattice parameter analysis results. Those systematic errors can be corrected by using an internal standard reference material, but this correction technique is not necessarily cost effective because the standard materials are not reusable and the sample preparation often takes a long time.

The parallel beam geometry can eliminate all of the sample related systematic errors including the sample surface displacement, absorption, and surface flatness. The only cause of the major systematic errors is the axial x-ray beam divergence which can be corrected using an external standard reference material.

The effect of the systematic errors on the lattice parameter refinement analysis was studied using both the Bragg-Brentano para-focusing and parallel beam geometries with and without the correction using a standard reference material.