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Accuracy in quantitative phase analysis: the impact of instrument geometry

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Quantitative phase analysis (QPA) by powder diffraction is a key staple of almost all diffraction laboratories around the world. There have been several Round Robins [1-3] which have probed specimen preparation, data collection, and analysis techniques, mainly in Bragg-Brentano geometry, which have shown that although the mathematics behind the technique is sound, its implementation leaves room for improvement.

With the growth in synchrotron experimentation, the use of in situ techniques, and the availability of multiple optical configurations for laboratory instruments, more measurements are being conducted in geometries that deviate from the de facto Bragg- Brentano standard. As the experimental geometry changes, so too do the peak intensities, line profiles, and how influences such as specimen displacement and absorption manifest themselves in the diffraction pattern, further complicating analysis.

One focus of our current research is generating realistic instrument models to correctly incorporate instrumental effects into our models. An understanding of the data collection geometry allows for an understanding of how peak intensities, line profiles, and other factors differ, and how to correct their effects in Rietveld modelling, potentially removing a source of error in a Rietveld refinement.

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