

## GEOMETRY, POLARIZATION AND ABSORPTION CORRECTIONS FOR TWO-DIMENSIONAL XRD

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Two-dimensional x-ray diffraction systems have been widely used in the pharmaceutical industry for drug discovery and process analysis. A two-dimensional diffraction pattern contains information for phase identification, polymorphous structures, crystallinity, particle size and distribution, phase transformation, melting point, and preferred orientation. Any one or group of these parameters can be used as criteria for high-throughput screening. Two-dimensional x-ray diffraction has enhanced phase identification in many respects. Because of its ability to collect diffracted x-rays in a large angular range in both  $2\theta$  and  $\gamma$  directions, it can collect diffraction data with high speed and better sampling statistics. Due to point beam illumination on the sample, a relatively small sample size is required for phase identification. The large area detector allows for a large  $2\theta$  range to be analyzed without scanning of the detector. This makes it possible to perform high-throughput screening or in-situ phase investigation on samples measured during phase transformation. The diffraction information in the  $\gamma$  direction allows accurate phase identification of samples with large grains and a preferred orientation.

With the increased usage of area detectors, many users have also noticed some discrepancies between the diffraction patterns collected with a Bragg-Brentano system and a system with linear or area detector. In the Bragg-Brentano geometry, the  $2\theta$  resolution is controlled by the selection of the divergence slit and receiving slit in the diffractometer plane, and the axial divergence is controlled by soller slits, while in a diffractometer with a linear or area detector, the  $2\theta$  resolution is mainly determined by the spatial resolution of the detector and the sample-to-detector distance. The relative peak intensity in a diffraction pattern from a sample with texture measured with linear or area detector can be significantly different from the results measured with the Bragg-Brentano geometry. It is imperative to study the nature of these discrepancies so that the diffraction patterns collected with linear and area detectors can be used for phase ID with proper understanding and correction if necessary. This presentation compares the conventional Bragg-Brentano diffractometer with diffractometers using linear or area detectors in terms of geometry conventions, x-ray optics, data collection and processing strategies. The correction algorithms for geometry, polarization, absorption and preferred orientation are given to interpret and eliminate the discrepancies between two-dimensional diffraction and conventional Bragg-Brentano geometry. Fortunately, in most applications, the  $\gamma$ -integrated profile can be used for phase identification without these corrections.