XRD PHASE IDENTIFICATION WITH LINEAR AND AREA DETECTORS

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X-ray diffractometer in the Bragg-Brentano geometry has been the preferred configuration for collecting phase identification data from bulk powder or polycrystalline samples. However, the reality can not be ignored that more and more users are using linear or area detectors to collect phase ID data, for many reasons, such as high speed, small sample size, or sample with large grain size and/or preferred orientation. With the increased usage of liner and area detector, 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 2θ 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 linear or area detector, the 2θ resolution is mainly determined by the spatial resolution of the detector and the sample-to-detector distance. The complete diffraction pattern can be collected by a single scan in Bragg-Brentano geometry, but several 2θ ranges may have to be collected and merged with a linear or area detector. The 2θ resolution may vary with the 2θ measurement range and sample geometry. 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 Bragg-Brentano geometry.

It is imperative to study the nature of these discrepancies so that the diffraction patterns collected with liner 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 convention, X-ray optics, data collection and processing strategies.