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Detector Characteristics and Data Processing. J.W. Pflugrath, Rigaku/MSO, Inc., 9009 New Trails Drive, The Woodlands, TX 77381.

The single crystal X-ray diffraction experiment consists of an X-ray source, a crystal, a crystal goniometer, a crystal cryosystem and a detector to capture the diffracted X-ray photons. Electronic position-sensitive detectors, as pioneered by Dr. Nguyen-Huu Xuong and colleagues, have revolutionized the collection of diffraction data. For those of us who collected data on single-counter diffractometers and/or on photographic film, electronic area detectors were simply miraculous.

While different area detector characteristics require different methods of data processing, the fundamental ideas can be applied to all detectors with special cases encapsulated to achieve some independence in the processing algorithms. For example, each detector must be calibrated. Data collection strategy depends on the detector characteristics, especially aperture size, dynamic range, and readout time, as well as properties of the source and sample.

The images produced by area detectors required advances in data processing, too. The steps of diffraction image processing include spot finding, indexing, refinement of the crystal(s), detector and source properties, then Bragg reflection prediction, integration, and finally scaling and averaging of the reflections. These steps will be briefly discussed so that one can achieve the best results.