Geometry and Algorithms to Expand 2θ Coverage of 2D Detector

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A 2D diffraction pattern is an image representing the diffraction intensity distribution over the detected area. For data evaluations of various materials characterization, such as phase identification, stress, texture, and crystal size, this distribution is further converted to the intensity distribution over both 2θ and γ angles. For many applications, especially phase analysis and structure refinement, it is crucial for the 2D pattern to have a large 2θ range sufficient to cover as many diffraction rings as necessary. The 2θ range covered by a 2D detector is mostly determined by the size of the detector active area and the detector distance from the sample. It is possible to increase the 2θ range by reducing the sample-to-detector distance, but it may be counterproductive due to the deteriorated angular resolution associated with a short detector distance.

There are two methods to expand 2θ coverage of the collected 2D pattern. One is to collect several 2D frames at various swing angles and then merge the multiple frames to create a 2D pattern with large 2θ coverage. The other method is to scan the 2D detector over the desired 2θ range during the data collection. For a flat 2D detector, the distance of the detector pixels to the sample varies depending on the pixel position within the 2D detector. Due to the detection plane of the detector at different swing angles are not within the same plane, the images collected at various detector positions cannot be simply merged or superposed to form an accurate two-dimensional diffraction image. A smearing effect will be observed if the final 2D pattern is incorrectly constructed. In order to obtain the accurate 2D diffraction pattern within the desired 2θ range, the best strategy is to project each of the images into a cylinder detection surface so the merged or scanned diffraction pattern can be stored and displayed accurately. This presentation introduces the geometry and algorithms to project the images and to construct a 2D diffraction pattern with the expanded 2θ coverage. The position and counts of all pixels in the final 2D diffraction pattern will be as accurate as if it were collected by a detector with a cylindrical detection surface and pixels of the same size and nature. The data evaluation can then be done with the geometry and algorithms for cylindrical 2D detectors.

Reference:

Bob He, *Two-dimensional X-ray Diffraction*, John Wiley & Sons, 2009.