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Algorithms for Two-dimensional XRD Data Evaluation

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The diffracted x-rays from a polycrystalline (powder) sample form a series diffraction cones in space since large numbers of crystals oriented randomly in the space are covered by the incident x-ray beam. Each diffraction cone corresponds to the diffraction from the same family of crystalline planes in all the participating grains. When a two-dimensional (2D) detector is used for x-ray powder diffraction, the diffraction cones are intercepted by the 2D detector and the x-ray intensity distribution on the sensing area is converted to an image-like diffraction pattern. The 2D pattern contains the scattering intensity distribution as a function of two orthogonal angles. One is the Bragg angle 2θ and the other is the azimuthal angle about the incident x-ray beam, denoted by γ. A 2D diffraction pattern can be analyzed directly or by data reduction to the intensity distribution along γ or 2θ. The γ-integration can reduce the 2D pattern into a diffraction profile analogs to the conventional diffraction pattern which is the diffraction intensity distribution as a function of 2θ angles. This kind of diffraction pattern can be evaluated by most exiting software and algorithms for conventional applications, such as, phase identification, structure refinement and 2θ-profile analysis. However, the materials structure information associated to the intensity distribution along γ direction is lost through γ-integration. The intensity distribution and 2θ variations along γ contain more information, such as the orientation distribution, strain states, crystallite size and shape distribution. In order to understand and analyze 2D diffraction data, new approaches and algorithms are necessary. The diffraction vector approach has been approved to be the genuine theory in 2D data analysis. The unit diffraction vector used for 2D analysis is a function of both 2θ and γ. The unit diffraction vector for all the pixels in the 2D pattern measured in the laboratory coordinates can be transformed to the sample coordinates. The vector components can then be used to derive fundamental equations for many applications, including stress, texture, crystal orientation and crystal size evaluation by γ-profile analysis. The unit diffraction vector is also used in polarization and absorption correction.

[1] B. B. He, *Two-dimensional X-ray Diffraction, John Wiley & Sons, Hoboken, New Jersey 2009.*

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