2.1.7.3. *Position sensitivity and associated scanning modes*

2.1.7.3.1. *Pixel size, spatial resolution and angular resolution*

Detectors of the line (1D) or area (2D) type have the important property of position sensitivity, which is characterized by the two parameters pixel size and spatial resolution.

The pixel size of a position-sensitive detector (PSD) can be represented either by the intrinsic size of the smallest addressable sensitive component of a detector (*e.g.* the actual size of the diodes), which can be binned to form larger pixels, or is set by the readout electronics (*e.g.* for wire-based detectors such as proportional counters). The spatial resolution is determined by the actual pixel size, the point-spread function (PSF) and parallax. The PSF represents the spread of a signal produced by a single photon over several pixels by mapping the probability density that a photon is recorded by a pixel in the vicinity of the point that the photon hit. Parallax will lead to an additional smearing if the photon travels at an angle to the detector normal. The final angular resolution of a detector system is given by the spatial detector resolution and the specimen-to-detector distance.

Point (0D) detectors do not provide position sensitivity, regardless of the actual size of the active window (representing a single pixel). Simply speaking, in analogy to PSDs, the spatial resolution of a point detector is determined by the goniometer step size representing the actual pixel size, and the size of the detector slit representing the PSF. As for PSDs, the angular resolution is given by the spatial resolution and the specimen-to-detector distance.

Detectors can be operated in fixed as well as in (2θ) scanning mode, where the step size is usually determined by the detector pixel size. Subsampling, that is scanning using an angular step size smaller than the angular pixel resolution, may be used to improve observed line profile shapes if the pixel resolution is too small. As a rule of thumb some 5–8 data points need be collected over the FWHM of a diffraction peak to allow for an appropriate description of the line-profile shape.

2.1.7.3.2. *Dimensionality*

Area detectors can be operated as line or point detectors. Electronic binning of the pixels into columns will form a line detector, while binning all pixels together will form a point detector, each associated with improvements of count rates and thus dynamic ranges. Alternatively, 1D or 0D 'regions of interest' can be defined electronically and/or by mounting suitable diffracted-beam-path X-ray optics. Area detectors – when operated as such – require point-focus operation.

Line detectors can be used as point detectors, which may be formed in several ways. One way is to only use one or more central pixels by either electronically switching off outer pixels and/or by mounting suitable X-ray optics. Another way is to turn the detector by 90° and to bin all pixels, leading to an improved count rate and thus dynamic range.

Obviously, when turning a line detector by 90°, it will function as an area detector if it is scanned over an angular range; the trace of the scan will form a cylindrical surface that is a two-dimensional diffraction image (He, 2009). This scan mode may be associated with a few advantages, in addition to lower costs. For example, the elimination of parallax and the possibility of using diffracted-beam-path optics improve the angular resolution in the 2θ direction and allow air scattering to be reduced.

2.1.7.3.3. *Size and shape*

PSDs are available in different sizes with flat (1D, 2D), curved (1D), cylindrical (2D) and spherical (2D) detection surfaces. Curved, cylindrical and spherical detectors are designed for focusing or parallel-beam geometries with a fixed specimen-to-detector distance, and cannot normally be used with the Bragg–Brentano geometry because of its 2θ-dependent focusing circle (Section 2.1.4.1). Flat detectors can be used at different specimen-to-detector distances, with either high angular resolution at a large distance or large angular coverage at a short distance. For large flat detectors, parallax errors must be addressed. Small flat detectors are perfectly suited for operation in Bragg–Brentano geometry but the angular coverage should not exceed about 10° 2θ (Section 2.1.4.1) to minimize defocusing, particularly at small 2θ angles.

References

Bartels, W. J. (1983). *Characterization of thin layers on perfect crystals with a multipurpose high resolution X-ray diffractometer*. *J. Vac. Sci. Technol. B*, **1**, 338–345.

Bilderback, D. H. (2003). *Review of capillary X-ray optics from the 2nd International Capillary Optics Meeting*. *X-ray Spectrom.* **32**, 195–207.

Bohlin, H. (1920). *Eine neue Anordnung für röntgenkristallographische Untersuchungen von Kristallpulver*. *Ann. Phys.* **366**, 421–439.

Bonse, U. & Hart, M. (1965). *Tailless X-ray single crystal reflection curves obtained by multiple reflection*. *Appl. Phys. Lett.* **7**, 238–240.

Bowen, D. K. & Tanner, B. K. (1998). *High Resolution X-ray Diffractometry and Topography*. London: Taylor & Francis.

Brentano, J. C. M. (1924). *Focussing method of crystal powder analysis by X-rays*. *Proc. Phys. Soc.* **37**, 184–193.

Charpak, G., Bouclier, R., Bressani, T., Favier, J. & Zupančič, Č. (1968). *The use of multiwire proportional counters to select and localize charged particles*. *Nucl. Instrum. Methods*, **62**, 262–268.

Clearfield, A., Reibenspiess, J. & Bhuvanesh, N. (2008). *Principles and Applications of Powder Diffraction*. New York: Wiley.

Debye, P. & Scherrer, P. (1916). *Interference of X-rays, employing amorphous substances*. *Phys. Z.* **17**, 277–283.

Durst, R. D., Diawara, Y., Khazins, D. M., Medved, S., Becker, B. L. & Thorson, T. A. (2003). *Novel, photon counting X-ray detectors*. *Powder Diffr.* **18**, 103–105.

EN 1330–11 (2007). *Non-Destructive Testing*. Part 11. *Terms used in X-ray Diffraction from Polycrystalline and Amorphous Materials*. Brussels: European Committee for Standardization (CEN).

Fankuchen, I. (1937). *A condensing monochromator for X-rays*. *Nature (London)*, **139**, 193–194.

Fewster, P. F. (2003). *X-ray Scattering from Semiconductors*. London: Imperial College Press.

Friedmann, H. (1945). *Geiger counter spectrometer for industrial research*. *Electronics*, **18**, 132–137.

Göbel, H. E. (1980). *The use and accuracy of continuously scanning position-sensitive detector data in X-ray powder diffraction*. *Adv. X-ray Anal.* **24**, 123–138.

Guinier, A. (1937). *Arrangement for obtaining intense diffraction diagrams of crystalline powders with monochromatic radiation*. *C. R. Acad. Sci. Paris*, **204**, 1115–1116.

Hanawalt, J. D., Rinn, H. W. & Frevel, L. K. (1938). *Chemical analysis by X-ray diffraction*. *Ind. Eng. Chem. Anal.* **10**, 457–512.

Hart, M. (1971). *Bragg-reflection X-ray optics*. *Rep. Prog. Phys.* **34**, 435–490.

He, B. B. (2009). *Two-Dimensional X-ray Diffraction*. New York: Wiley.

He, T., Durst, R. D., Becker, B. L., Kaercher, J. & Wachter, G. (2011). *A large area X-ray imager with online linearization and noise suppression*. *Proc. SPIE*, **8142**, 81421Q.

Hemberg, O. E., Otendal, M. & Hertz, H. M. (2003). *Liquid-metal-jet anode electron-impact X-ray source*. *Appl. Phys. Lett.* **83**, 1483–1485.

Hull, A. W. (1917). *A new method of X-ray crystal analysis*. *Phys. Rev.* **10**, 661–696.

Hull, A. W. (1919). *A new method of chemical analysis*. *J. Am. Chem. Soc.* **41**, 1168–1175.

International Tables for Crystallography (2004). Volume C, 3rd ed., edited by E. Prince. Dordrecht: Kluwer Academic Publishers.

  references