International Tables for Crystallography (2018). Vol. H, Section 2.5.3.2.3, pp. 127–128.

where $F(x, y)$ is the flux (in photons s^{-1}) intercepted by the pixel and B is the brightness of the source (in photons s^{-1} $mrad^{-2}$) or scattering from the sample. The ratio of the flux in pixel $P(x, y)$ to that in the centre pixel $P(0, 0)$ is then given as

$$\frac{F(x, y)}{F(0, 0)} = \frac{D^3}{R^3} = \frac{D^3}{(D^2 + x^2 + y^2)^{3/2}} = \cos^3\phi, \qquad (2.5.20)$$

where ϕ is the angle between the X-rays to the pixel $P(x, y)$ and the line from S to the detector in perpendicular direction. It can be seen that the greater the sample-to-detector distance, the smaller the difference between the centre pixel and the edge pixel in terms of the flux from the homogeneous source. This is the main reason why a data frame collected at a short sample-to-detector distance has a higher contrast between the edge and centre than one collected at a long sample-to-detector distance.

2.5.3.2.2. *Spatial resolution of area detectors*

In a 2D diffraction frame, each pixel contains the X-ray intensity collected by the detector corresponding to the pixel element. The pixel size of a 2D detector can be determined by or related to the actual feature sizes of the detector structure, or artificially determined by the readout electronics or data-acquisition software. Many detector techniques allow multiple settings for variable pixel size, for instance a frame of 2048 × 2048 pixels or 512 × 512 pixels. Then the pixel size in 512 mode is 16 (4 × 4) times that of a pixel in 2048 mode. The pixel size of a 2D detector determines the space between two adjacent pixels and also the minimum angular steps in the diffraction data, therefore the pixel size is also referred to as pixel resolution.

The pixel size does not necessarily represent the true spatial resolution or the angular resolution of the detector. The resolving power of a 2D detector is also limited by its point-spread function (PSF) (Bourgeois *et al.*, 1994). The PSF is the two-dimensional response of a 2D detector to a parallel point beam smaller than one pixel. When the sharp parallel point beam strikes the detector, not only does the pixel directly hit by the beam record counts, but the surrounding pixels may also record some counts. The phenomenon is observed as if the point beam has spread over a certain region adjacent to the pixel. In other words, the PSF gives a mapping of the probability density that an X-ray photon is recorded by a pixel in the vicinity of the point where the X-ray beam hits the detector. Therefore, the PSF is also referred to as the spatial redistribution function. Fig. 2.5.12(*a*) shows the PSF produced from a parallel point beam. A plane at half the maximum intensity defines a cross-sectional region within the PSF. The FWHM can be measured at any direction crossing the centroid of the cross section. Generally, the PSF is isotropic, so the FWHMs measured in any direction should be the same.

Measuring the PSF directly by using a small parallel point beam is difficult because the small PSF spot covers a few pixels and it is hard to establish the distribution profile. Instead, the line-spread function (LSF) can be measured with a sharp line beam from a narrow slit (Ponchut, 2006). Fig. 2.5.12(*b*) is the intensity profile of the image from a sharp line beam. The LSF can be obtained by integrating the image from the line beam along the direction of the line. The FWHM of the integrated profile can be used to describe the LSF. Theoretically, LSF and PSF profiles are not equivalent, but in practice they are not distinguished and may be referenced by the detector specification interchangeably. For accurate LSF measurement, the line beam is intentionally positioned with a tilt angle from the orthogonal direction of the pixel array so that the LSF can have smaller steps in the integrated profile (Fujita *et al.*, 1992).

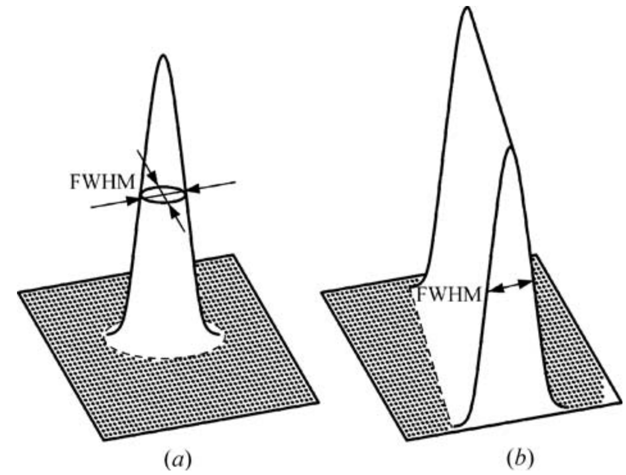

Figure 2.5.12
(*a*) Point-spread function (PSF) from a parallel point beam; (*b*) line-spread function (LSF) from a sharp line beam.

The RMS (root-mean-square) of the distribution of counts is another parameter often used to describe the PSF. The normal distribution, also called the Gaussian distribution, is the most common shape of a PSF. The RMS of a Gaussian distribution is its standard deviation, σ. Therefore, the FWHM and RMS have the following relation, assuming that the PSF has a Gaussian distribution:

$$\text{FWHM} = 2[-2\ln(1/2)]^{1/2}\text{RMS} = 2.3548 \times \text{RMS}. \qquad (2.5.21)$$

The values of the FWHM and RMS are significantly different, so it is important to be precise about which parameter is used when the value is given for a PSF.

For most area detectors, the pixel size is smaller than the FWHM of the PSF. The pixel size should be small enough that at least a 50% drop in counts from the centre of the PSF can be observed by the pixel adjacent to the centre pixel. In practice, an FWHM of 3 to 6 times the pixel size is a reasonable choice if use of a smaller pixel does not have other detrimental effects. A further reduction in pixel size does not necessarily improve the resolution. Some 2D detectors, such as pixel-array detectors, can achieve a single-pixel PSF. In this case, the spatial resolution is determined by the pixel size.

2.5.3.2.3. *Detective quantum efficiency and energy range*

The detective quantum efficiency (DQE), also referred to as the detector quantum efficiency or quantum counting efficiency, is measured by the percentage of incident photons that are converted by the detector into electrons that constitute a measurable signal. For an ideal detector, in which every X-ray photon is converted to a detectable signal without additional noise added, the DQE is 100%. The DQE of a real detector is less than 100% because not every incident X-ray photon is detected, and because there is always some detector noise. The DQE is a parameter defined as the square of the ratio of the output and input signal-to-noise ratios (SNRs) (Stanton *et al.*, 1992):

$$\text{DQE} = \left(\frac{(S/N)_{\text{out}}}{(S/N)_{\text{in}}}\right)^2. \qquad (2.5.22)$$

The DQE of a detector is affected by many variables, for example the X-ray photon energy and the counting rate. The dependence of the DQE on the X-ray photon energy defines the energy range of a detector. The DQE drops significantly if a detector is used out of its energy range. For instance, the energy range of MWPC and microgap detectors is about 3 to 15 keV. The DQE with Cu $K\alpha$ radiation (8.06 keV) is about 80%, but drops gradually when approaching the lower or higher energy limits. The energy range of imaging plates is much wider (4–48 keV). The energy range of a CCD, depending on the phosphor, covers from 5 keV up to the hard X-ray region.

2.5.3.2.4. *Detection limit and dynamic range*

The detection limit is the lowest number of counts that can be distinguished from the absence of true counts within a specified confidence level. The detection limit is estimated from the mean of the noise, the standard deviation of the noise and some confidence factor. In order to have the incoming X-ray photons counted with a reasonable statistical certainty, the counts produced by the X-ray photons should be above the detector background-noise counts.

The dynamic range is defined as the range extending from the detection limit to the maximum count measured in the same length of counting time. The linear dynamic range is the dynamic range within which the maximum counts are collected within the specified linearity. For X-ray detectors, the dynamic range most often refers to linear dynamic range, since only a diffraction pattern collected within the linear dynamic range can be correctly interpreted and analysed. When the detection limit in count rate approaches the noise rate at extended counting time, the dynamic range can be approximated by the ratio of the maximum count rate to the noise rate.

Dynamic range is very often confused with the maximum count rate, but must be distinguished. With a low noise rate, a detector can achieve a dynamic range much higher than its count rate. For example, if a detector has a maximum linear count rate of 10^5 s^{-1} with a noise rate of 10^{-3} s^{-1}, the dynamic range can approach 10^8 for an extended measurement time. The dynamic range for a 2D detector has the same definition as for a point detector, except that with a 2D detector the whole dynamic range extending from the detection limit to the maximum count can be observed from different pixels simultaneously. In order to record the entire two-dimensional diffraction pattern, it is necessary for the dynamic range of the detector to be at least the dynamic range of the diffraction pattern, which is typically in the range 10^2 to 10^6 for most applications. If the range of reflection intensities exceeds the dynamic range of the detector, then the detector will either saturate or have low-intensity patterns truncated. Therefore, it is desirable that the detector has as large a dynamic range as possible.

2.5.3.2.5. *Types of 2D detectors*

2D detectors can be classified into two broad categories: photon-counting detectors and integrating detectors (Lewis, 1994). Photon-counting area detectors can detect a single X-ray photon entering the active area. In a photon-counting detector, each X-ray photon is absorbed and converted to an electrical pulse. The number of pulses counted per unit time is proportional to the incident X-ray flux. Photon-counting detectors typically have high counting efficiency, approaching 100% at low count rate. The most commonly used photon-counting 2D detectors include MWPCs, Si-pixel arrays and microgap detectors. Integrating area detectors, also referred to as analogue X-ray imagers, record the X-ray intensity by measuring the analogue electrical signals converted from the incoming X-ray flux. The signal size of each pixel is proportional to the fluence of incident X-rays. The most commonly used integrating 2D detectors include image plates (IPs) and charge-coupled devices (CCDs).

The selection of an appropriate 2D detector depends on the X-ray diffraction application, the sample condition and the X-ray beam intensity. In addition to geometry features, such as the active area and pixel format, the most important performance characteristics of a detector are its sensitivity, dynamic range, spatial resolution and background noise. The detector type, either photon-counting or integrating, also leads to important differences in performance. Photon-counting 2D detectors typically have high counting efficiency at low count rate, while integrating 2D detectors are not so efficient at low count rate because of the relatively high noise background. An MWPC has a high DQE of about 0.8 when exposed to incoming local fluence from single photons up to about 10^3 photons s^{-1} mm^{-2}. The diffracted X-ray intensities from a polycrystalline or powder sample with a typical laboratory X-ray source fall into this fluence range. This is especially true with microdiffraction, where high sensitivity and low noise are crucial to reveal the weak diffraction pattern. Owing to the counting losses at a high count rate, the DQE of an MWPC decreases with increasing count rate and quickly saturates above 10^3 photons s^{-1} mm^{-2}. Therefore, an MWPC is not suitable for collecting strong diffraction patterns or for use with high intensity sources, such as synchrotron X-ray sources. An IP can be used in a large fluence range from 10 photons s^{-1} mm^{-2} and up with a DQE of 0.2 or lower. An IP is suitable for strong diffraction from single crystals with high-intensity X-ray sources, such as a rotating-anode generator or synchrotron X-ray source. With weak diffraction signals, the image plate cannot resolve the diffraction data near the noise floor. A CCD detector can also be used over a large X-ray fluence range from 10 photons s^{-1} mm^{-2} to very high fluence with a much higher DQE of 0.7 or higher. It is suitable for collecting diffraction of medium to strong intensity from single-crystal or polycrystalline samples. Owing to the relatively high sensitivity and high local count rate, CCDs can be used in systems with either sealed-tube X-ray sources, rotating-anode generators or synchrotron X-ray sources. With a low DQE at low fluence and the presence of dark-current noise, a CCD is not a good choice for applications with weak diffraction signals. A microgap detector has the best combination of high DQE, low noise and high count rate. It has a DQE of about 0.8 at an X-ray fluence from single photons up to about 10^5 photons s^{-1} mm^2. It is suitable for microdiffraction when high sensitivity and low noise are crucial to reveal weak diffraction patterns. It can also handle high X-ray fluence from strong diffraction patterns or be used with high-intensity sources, such as rotating-anode generators or synchrotron X-ray sources.

2.5.3.3. *Data corrections and integration*

2D diffraction patterns contain abundant information. In order to interpret and analyse 2D patterns accurately it is necessary to apply some data-treatment processes (Sulyanov *et al.*, 1994; Scheidegger *et al.*, 2000; Cervellino *et al.*, 2006; Boesecke, 2007; Rowe, 2009). Most data-treatment processes can be categorized as having one of the following four purposes: to eliminate or reduce errors caused by detector defects; to remove undesirable effects of instrument and sample geometry; to transfer a 2D frame into a format such that the data can be presented or further analysed by conventional means and software; and cosmetic treatment, such as smoothing a frame for reports and publications.

references