International Tables for Crystallography (2006). Vol. C, Section 7.1.6.1.7, pp. 625–626.

processing circuits. The counting losses are affected by the time modulation, if any, of the source, as, for example, with storage rings (Arndt, 1978).

Counting losses can affect the behaviour of detectors in two different ways. In most analogue detectors and in counters with parallel read-out, each pixel behaves as an independent detector and the counting loss at any point depends only on the *local* counting rate. In other devices, such as multiwire proportional chambers with delay-line read-out (see Subsection 7.1.6.2), the whole detector becomes dead after an event anywhere in the detector and what matters is the *global* counting rate.

Fortunately, the fractional counting loss is the same for all parts of the pattern so that the *relative* intensities in a stationary pattern are not affected.

7.1.6.1.3. *Dynamic range*

The lowest practically measurable intensity is determined by the inherent background or noise of the detector. Some form of discrimination against noise pulses is usually possible with a detector that counts individual photons, but not, of course, with integrating detectors.

The maximum intensity at which a *counter* can operate is determined by the dead-time. In the case of an *integrating or analogue detector* with a variable gain, there is a trade-off between maximum intensity and DQE. Such a device can often be regarded as having an output signal with an amplitude $S = NV/M$ that is a noise-free representation of N, the number of photons detected in the integrating period of the device, where V, the maximum signal amplitude, is produced by M photons in this period. M can be varied by altering the gain of the detector. The noise can be regarded as a fixed fraction $1/r$ of the maximum amplitude V that is added to the signal. Then the DQE will be

$$\begin{aligned}\varepsilon &= S^2/\sigma^2 N\\ &= (1 + M^2/r^2 N)^{-1}.\end{aligned} \qquad (7.1.6.2)$$

This equation shows the importance of having as small a value of $1/r$ as possible; it also demonstrates that, for a given value of r, M can be increased only at the expense of a reduced DQE. This is valid for X-ray film (Arndt, Gilmore & Wonacott, 1977), for television detectors (Arndt, 1984), for the integrating gas detectors discussed in Subsection 7.1.6.2, and for many semiconductor X-ray detectors.

7.1.6.1.4. *Spatial resolution*

The spatial resolution of a PSD is determined by the number and size of resolution or picture elements (pixels) along the length or parallel to the edge of the detector. In most diffraction experiments, the size of the pattern can be scaled by altering the distance of the detector from the sample and what is important is the angular resolution of the detector when placed at a distance where it can ‘see’ the entire pattern. We shall see below that linear PSD’s can be made with up to 2000 pixels and that area detectors are mostly limited to fewer than 512 × 512 pixels. The sizes of pixels range from about 10 μm for semiconductor PSD’s to about 1 mm for most gas-filled detectors.

The *useful* number of pixels of a detector is determined by its point-spread function (PSF). This is the relative response as a function of distance from the centre of a point image on the detector. PSF’s are not necessarily radially symmetrical and may have to be specified in at least two directions at right angles, for example along and perpendicular to the lines of a television raster scan. The width of the PSF at the 50% level determines the amount of detail visible in a directly viewed image. The accuracy of intensity measurements may depend more critically upon the width of the PSF at a lower level, since a weak spot may be immeasurable when sitting on the ‘tail’ of a very intense one. For various physical reasons, the PSF’s of *all* PSD’s, including X-ray film, have appreciable tails.

The spatial resolution of a detector is affected by parallax: when an X-ray beam is absorbed in a thick planar detector at an angle φ to the normal, the width of the resultant image is smeared out exponentially and its centroid is shifted by an amount $\sin\varphi/\mu$. For 8 keV X-rays incident at 45° on a xenon-filled counter, for example, this shift is about 4 mm for a filling pressure of 1 atm and 0.4 mm for a filling pressure of 10 atm. These figures illustrate the desirability of high-pressure xenon (Fig. 7.1.6.2) for gas-ionization detectors intended for wide-angle diffraction patterns.

7.1.6.1.5. *Uniformity of response*

All PSD’s show long-range and pixel-to-pixel variations of response to larger or smaller extents. These can be corrected, in general by means of a look-up table, during data processing, but the measurements necessary for the calibration are often time-consuming. The output signals of many analogue detectors contain fixed-pattern noise that is synchronous with the read-out clock. This noise is usually removed during data processing, which in any case requires the subtraction of the background pattern.

7.1.6.1.6. *Spatial distortion*

In most detectors, there is some spatial distortion of the image. Again, the necessary calibration procedure may be time-consuming. Distortions cause point-to-point variations in pixel size, which produce response variations additional to those from other causes.

Corrections for spatial distortion and for non-uniformity of response have been discussed by Thomas (1989, 1990) and by Stanton, Phillips, Li & Kalata (1992*b*).

7.1.6.1.7. *Energy discrimination*

The amplitude of the signal due to a single photon is usually a function of the photon energy. The variance in this amplitude, or the full width at half-maximum (FWHM) of the pulse-height spectrum, for a monoenergetic input, depends on the statistics of the detection process. A sharp pulse-height-distribution (PHD) curve may permit simultaneous multi-wavelength measurements with a suitable counter, or at least afford a reduction of the background by pulse-height discrimination. In an analogue

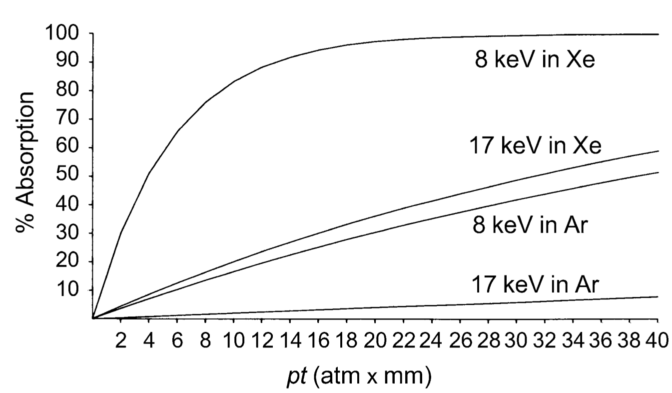

Fig. 7.1.6.2. Absorption of 8 keV and 17 keV photons in argon and xenon as a function of pressure in atm × column length in mm.

detector, the variance in the primary amplitude affects the DQE (Arndt & Gilmore, 1979).

7.1.6.1.8. *Suitability for dynamic measurements*

Many investigations, such as low-angle or fibre diffraction studies on biological materials carried out with synchrotron radiation (Boulin, Dainton, Dorrington, Elsner, Gabriel, Bordas & Koch, 1982; Huxley & Faruqi, 1983), involve the time variation of a diffraction pattern. For very short time slots, only counters can be employed; the incoming pulses must then be gated and stored in an appropriate memory (Faruqi & Bond, 1982).

Stores used for these experiments are described as histogramming memories; the contents of a given storage location are incremented by one whenever the corresponding address, which represents the position and the time of arrival of a photon, appears on the address bus (Hendricks, Seeger, Scheer & Suehiro, 1982; Hughes & Sumner, 1981).

7.1.6.1.9. *Stability*

Stability of the performance of a detector is of paramount importance. Most position-sensitive detectors are used in connection with microcomputers, which make calibration and corrections for spatial distortion, non-uniformity of response, and lack of linearity relatively easy, provided that these distortions remain constant. The long-term stability of many detectors, notably of semiconductor devices, is affected by radiation damage produced by prolonged exposure to intense irradiation.

7.1.6.1.10. *Size and weight*

The size and weight of the detector determine the ease with which the detector can be moved relative to the sample and thus the extent to which the diffractometer can be adapted to varying resolution and collimation conditions. Some detectors cannot be moved easily (Xuong, Freer, Hamlin, Nielsen & Vernon, 1978), or need very heavily engineered rotational and translational displacement devices (Phizackerley, Cork & Merritt, 1986). Others, such as spherical drift chamber multiwire proportional chambers, are designed for use at a fixed distance from the sample and may only be swung about the latter but not translated (Kahn, Fourme, Bosshard, Caudron, Santiard & Charpak, 1982).

In single-crystal diffraction patterns, the Bragg reflections may be visualized as diverging from the X-ray source while the background – fluorescence X-rays, scatter by amorphous material on the specimen crystal and its mount – diverges from the sample. Consequently, the highest reflection-to-background ratio is achieved by using a large detector at a large distance from the specimen. Of all the detectors discussed here, the image plate can most readily and economically be used to cover a large area; its present popularity is chiefly due to this property (Sakabe, 1991).

There is fairly general agreement on the specification of an ideal X-ray area detector. It should be at least 250 mm in diameter, contain at least 1000×1000 pixels, have a large dynamic range and a high detective quantum efficiency for photon energies up to 20 keV and be capable of being read-out rapidly.

Many suggestions have been made for improving the performance of existing detectors. It has become apparent, however, that the development of ideal, or even better, X-ray detectors is extremely expensive and, therefore, that their development and installation can be undertaken only in central national or international laboratories such as storage-ring synchrotron-radiation laboratories.

7.1.6.2. *Gas-filled counters*

In all gas-filled counters, whether one-, two-, or three-dimensional, the initial event is the absorption of the incoming X-ray photon in a gas molecule with the emission of a photo-, or alternatively an Auger, electron. The detection efficiency depends on the fraction of the photons absorbed in the gas and this fraction is shown in Fig. 7.1.6.2 as a function of the product of gas pressure and column length for 8 and 17 keV photons on argon and xenon. The ionization energy of noble gases is about 30 eV so that one 8 keV photon gives rise to about 270 electron–ion pairs. With adequately high collecting fields, the electrons acquire sufficient energy to produce further ionization by collision with neutral filling gas molecules; this process is often referred to as 'avalanche production' or 'gas multiplication'. The factor A by which the number of primary ion pairs is multiplied can be as great as ten to one hundred thousand. Up to a certain value of A, the total amount of ionization remains proportional to the energy of the original X-ray photon. The electrical signal generated at the anode of the counter is due very largely to the movement of the positive ions from the immediate vicinity of that electrode; at the same time, a corresponding pulse is induced on the cathode. The signal can be shaped to produce a pulse with a duration of the order of a microsecond.

In single or multiwire proportional counters, the secondary ionization (avalanche production) takes place in the highest field region, that is, within a distance of a few wire diameters of the anode wire or wires. The electrons are collected on the anode and the positive ions move towards the cathode, with very little spread of the ionization in a direction perpendicular to the field gradient, that is, parallel to the wire direction. It is thus possible to construct position-sensitive devices based on such chambers.

Proportional-counter behaviour is discussed in detail in many standard texts and review articles (Wilkinson, 1950; Price, 1964; Dyson, 1973; Rice-Evans, 1974).

The gas amplification does not have to take place in the same region of the detector as the original absorption. In so-called drift chambers, the primary ionizing event takes place in a low-field region where no avalanching takes place. The electrons drift through a grid or grids into a region where the field is sufficiently high for gas multiplication to occur. The drift field can be made cylindrical in a linear counter (Pernot, Kahn, Fourme, Leboucher, Million, Santiard & Charpak, 1982), or spherical in an area detector (Charpark, 1982; Kahn, Fourme, Bosshard, Caudron, Santiard & Charpak, 1982), centred on the point from which the X-rays diverge, that is on the specimen; the electrons then drift in a radial direction without parallax being introduced (Fig. 7.1.6.3).

In many experiments, use is made of the energy discrimination of the detector. The ratio of the full width at half-maximum to the position of the maximum of the pulse-height distribution is given by

$$w = 2.36[(F + f)/N], \qquad (7.1.6.3)$$

where N is the number of primary ion pairs produced, F is the Fano factor (Fano, 1946, 1947), which takes into account the partially stoichastic character of the gas multiplication process, and f is the avalanche factor. For proportional counters filled with typical gas mixtures (argon + methane), $F = 0.17$ and $f = 0.65$, so that for 8 keV photons $w \sim 13\%$, but, in the

references