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7. X-RAY DETECTORS

7.1. Comparison of X-ray detectors

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7.1.1. Commonly used detectors: general considerations

This chapter summarizes detector characteristics and provides practical advice on the selection of crystallographic detectors. Important types of detectors for crystallographic applications are summarized in Section 7.1.2 and listed in Table 7.1.1.1. To be detected by any device, an X-ray must be absorbed within a detective medium through electrodynamic interactions with the atoms in the detecting layer. These interactions usually result in an energetic electron being liberated which, by secondary and tertiary interactions, produces the signal that will be measured, *e.g.* luminescence in phosphors, electron–hole pairs in semiconductors or ionized atoms in gaseous ionization detectors. As we shall see, there are many schemes for recording these signals. The various detector designs, as well as the fundamental detection processes, have particular advantages and weaknesses. In practice, detector suitability is constrained by the experimental situation (*e.g.* home laboratory X-ray generator *versus* synchrotron-radiation source; fine-slicing *versus* large-angle oscillations), by the sample (*e.g.* whether radiation damages it readily) and by availability. An assessment of detector suitability in a given situation requires an understanding of how detectors are evaluated and characterized. Some of the more important criteria are discussed below.

The *detective quantum efficiency* (DQE) is an overall measure of the efficiency and noise performance of a detector (Gruner *et al.*, 1978). The DQE is defined as

$$\mathrm{DQE} = (S_o/N_o)^2/(S_i/N_i)^2, \qquad (7.1.1.1)$$

where S is the signal, N is the noise, and the subscripts o and i refer to the output and input of the detector, respectively. The DQE measures the degradation owing to detection in the signal-to-noise ratio. For a signal source that obeys Poisson statistics, the inherent noise is equal to the square root of the number of incident photons, so that the incident signal-to-noise ratio is just $S_i/N_i = (S_i)^{1/2}$. The ideal detector introduces no additional noise in the detection process, thereby preserving the incident signal-to-noise ratio, *i.e.* DQE = 1. Real detectors always have DQE < 1 because some noise is always added in the detection process. The DQE automatically accounts for the fact that the input and output signals may be of a different nature (*e.g.* X-rays in, stored electrons out), since it is a ratio of dimensionless numbers.

A single number does not characterize the DQE of a system. Rather, the DQE is a function of the integrated dose, the X-ray spot size, the length of exposure, the rate of signal accumulation, the X-ray energy *etc.* Noise in the detector system will limit the DQE at low dose, while the inability to remove all systematic nonuniformities will limit the high-dose behaviour.

The *accuracy*, ρ, measures the output noise relative to the signal, *i.e.* $\rho = N_o/S_o$. For a Poisson X-ray source, it follows that the accuracy and the DQE are related by

$$\rho = (N_i \mathrm{DQE})^{-1/2}. \qquad (7.1.1.2)$$

This allows the determination of the number of X-rays needed to measure a signal to a given accuracy with a detector of a given DQE. The accuracy for an ideal detector is $1/(S_i)^{1/2}$, *e.g.* 100 X-rays are required to measure to 10% accuracy, and 10^4 X-rays are needed for a 1% accuracy. Nonideal detectors (DQE < 1) always require more X-rays than the ideal to measure to a given accuracy.

Spatial resolution refers to the ability of a detector to measure adjacent signals independently. The spatial resolution is characterized by the *point spread function* (PSF), which, for most detectors, is simply the spread of intensity in the output image as a result of an incident point signal. An alternative measure of resolution is the *line*

Table 7.1.1.1. *X-ray detectors for crystallography*

(*a*) Commercially available detectors

Technology	Primary X-ray converter	Format
Film	AgBr	Area
Storage phosphor	BaFBr	Area
Scintillating crystal	NaI, CsI	Point
Gas discharge	Xe	Point, linear, area
Television	Phosphor	Area
CCD	Phosphor	Area
Silicon diode	Si	Linear, area
Avalanche diode	Si	Point, area

(*b*) Detectors under development

Technology	Primary X-ray converter	Format
Pixel array	Si, GaAs, CdZnTe	Area
Amorphous silicon flat panel + phosphor	CsI, Gd_2O_2S	Area
Amorphous silicon flat panel + photoconductor	PbI_2, CdZnTe, TlBr, HgI_2	Area

spread function (Fujita *et al.*, 1992). Although a detector might have a narrow PSF at 50% of the peak level, poor performance of the PSF at the 1% level and below can severely hamper the ability to measure closely spaced spots. It is important to realize that the PSF is a two-dimensional function, which is often illustrated by a graph of the PSF cross section; therefore, the integrated intensity at a radius R pixels from the centre of the PSF is the value of the PSF cross section times the number of pixels at that radius. Often the wings of the PSF decay slowly, so that considerable integrated signal is in the image far from the spot centre. In this case, a bright spot can easily overwhelm a nearby weak spot. Another consequence is that bright spots appear considerably larger than dim ones, thereby complicating analysis.

The *stopping power* is the fraction of the incident X-rays that are stopped in the active detector recording medium. In low-noise detectors, the DQE is proportional to the stopping power. A detector with low stopping power may be suitable for experiments in which there is a strong X-ray signal from a specimen that is not readily damaged by radiation. On the other hand, even a noiseless detector with a low stopping power will have a low DQE, because most of the incident X-rays are not recorded.

Unfortunately, many definitions of *dynamic range* are used for detectors. For an integrating detector, the dynamic range per pixel is taken to be the ratio of the saturation signal per pixel to the zero-dose noise per pixel for a single frame readout. For photon counters, the dynamic range per pixel refers to the largest signal-to-noise ratio, *i.e.* the number of true counts per pixel that are accumulated on average before a false count is registered. In practice, the dynamic range is frequently limited by the readout apparatus or the reproducibility of the detector medium. For example, the large dynamic range of storage phosphors is almost always limited by the capabilities of the reading apparatus, which constrains the saturation signal and limits the zero-dose noise by the inability to erase the phosphor completely. The number of bits in the output word does not indicate the dynamic range, since the number of stored bits can only constrain the dynamic range, but, obviously, cannot increase it.

The dynamic range is sometimes given with respect to an integrated signal that spans more than one pixel. For a signal S per pixel which spans M pixels, the integrated signal is MS, and, assuming the noise adds in quadrature, the noise is $N(M)^{1/2}$, yielding a factor of $(M)^{1/2}$ larger dynamic range. For most detectors, the noise in nearby pixels does not add in quadrature, so this is an upper limit.

The characteristics of a detector may be severely compromised by practical considerations of *nonlinearity*, *reproducibility* and *calibration.* For example, the optical density of X-ray film varies nonlinearly with the incident dose. Although it is possible to calibrate the optical density *versus* dose response, in practice it is difficult to reproduce exactly the film-developing conditions required to utilize the highly nonlinear portions of the response. A detector is no better than its practical calibration. This is especially true for area detectors in which the sensitivity varies across the face of the detector. The proper calibration of an area detector is replete with subtleties and constrained by the long-term stability of the calibration. Faulty calibrations are responsible for much of the difference between the possible and actual performance of detectors (Barna *et al.*, 1999).

The response of a detector may be nonlinear with respect to position, dose, intensity and X-ray energy. Nonuniformity of response across the active area is compensated by the *flat-field* correction. Frequently, nonuniformity of response varies with the angle of incidence of the X-ray beam to the detector surface, which is a significant consideration when flat detectors are used to collect wide-angle data. Although this may be compensated by an energy-dependent *obliquity* correction, few detector vendors provide this calibration. An X-ray image may also be spatially distorted; this *geometric distortion* can be calibrated if it is stable.

Other important detector considerations include the *format* of the detector (*e.g.* the number of pixels across the height and width of the detector). The format and the PSF together determine the number of Bragg orders that can be resolved across the active area of the detector. *Robustness* of the detector is also important: as examples, gas-filled area detectors may be sensitive to vibration of the high-voltage wires; detectors containing image intensifiers are sensitive to magnetic fields; or the detector may simply be easily damaged or lose its calibration during routine handling. Some detectors are readily damaged by too large an X-ray signal. *Count-rate* considerations severely limit the use of many photon counters, especially at synchrotron-radiation sources. Detector *speed*, both during exposure and during read out, can be important. Some detector designs are highly *flexible*, permitting special readout modes, such as a selected region of interest for use during alignment, or operation as a streak camera.

Ease of use is especially important. A detector may simply be hard to use because, for example, it is exceptionally delicate, requires frequent fills of liquid nitrogen, or is physically awkward in size. A final, often compelling, consideration is whether a detector is *well integrated into an application* with the appropriate analysis software and whether the control software is well interfaced to the other X-ray hardware.

7.1.2. Evaluating and comparing detectors

The DQE comprehensively characterizes the ultimate quantitative capabilities of an X-ray detector. The DQE may be determined from an analysis of the reproducibility of recorded X-ray test images of known statistics *via* equation (7.1.1.1): given M incident X-rays per exposure, the expected incident signal-to-noise is $(M)^{1/2}$. The DQE is determined by measuring the variance in the recorded signal in repeated measurements of the test image. Repetition of this process for different values of M maps out the DQE curve. Since the DQE is dependent on the structure of the image, the integration area, the X-ray background and the long-term detector calibration, it is essential that the test images realistically simulate these features as expected in experiments. Thus, if the detector is to be used to obtain images of diffraction spots, the test images should consist of comparably sized spots superimposed on a suitable background.

A comprehensive DQE determination is nontrivial and requires specialized tools, such as test masks, uniform X-ray sources *etc.* Unfortunately, published DQE curves are frequently incorrect and misleading. Users can, however, set up and perform a simple DQE assessment, detailed below, which gives a great deal of information about the sensitivity and usefulness of a given area detector. Other sources of stable X-ray spots (of appropriate size and intensity) can also be used in similar tests.

The materials needed are sheet lead and aluminium, a sewing needle, a stable collimated X-ray source, X-ray capillaries filled with saturated salt solutions, an X-ray shutter with timing capability and a scintillator/phototube X-ray counting arrangement. Arrange a fluorescent X-ray source to provide a diffuse X-ray signal. An X-ray capillary filled with a saturated solution of iron chloride makes a suitable source for a copper anode machine. Next, make an X-ray-opaque metal mask by punching a clean pinhole with a sewing needle in a lead sheet. The size of the hole should be representative of an X-ray spot, say 0.3 mm in diameter. The mask should be firmly and reproducibly secured a few cm from the fluorescent source at a wide angle to the incident beam. Using a scintillator/phototube combination, measure the number of X-rays per second emerging through the hole at a given X-ray source loading. A sufficient number of X-rays per measurement (say 10^5) is necessary

references