International Tables for Crystallography (2018). Vol. H, Section 2.1.7.2.1, pp. 46–47.

count rate and the rate of signals generated and registered by the detector. In any detector it takes some time to process the conversion of an individual photon to a voltage pulse, which is related to the detector *dead time*: photons arriving while the detector is still processing the previous photon conversion may be lost. The detector dead time is related to the physical characteristics of the detector, *e.g.* the drift time in a gas-ionization detector, or the read-out time of the counting electronics, *e.g.* the shaping time of the amplifier. The effect of dead time becomes a substantial issue at high photon count rates, when the dead time becomes a significant part of the average time separation between two arriving photons, leading to increasing intensity losses at higher count rates. Detectors can be categorized as being non-paralysable or paralysable with respect to dead time. A nonparalysable detector is dead for a fixed time after each count, but not influenced by photons arriving during the dead time. Counting losses increase with increasing count rates, but the true count rate of a nonparalysable detector can be corrected unless the maximum observed count rate is equal to the inverse of the dead time. In a paralysable detector, a second photon arriving within the dead time can not be counted but will extend the dead time up to a point where the detector will be incapable of collecting any counts at all (saturation point). Modern detectors can stand the count rates obtained in powder diffraction experiments using fixed-target X-ray sources. At very high count rates, *e.g.* those obtained in thin-film experiments such as reflectometry, it may be necessary to attenuate the beam. Sophisticated instruments are equipped with an electronic feedback system and automatic absorbers (see Section 2.1.6.3.1.2) to ensure that detector saturation is avoided.

The *dynamic range* of a detector may be defined as the range between the smallest detectable photon count rates (determined by inherent detector noise such as readout and dark noise) to the largest acceptable photon count rates (determined by the dead time).

Energy resolution is the ability of a detector to resolve two photons that have different energies. Energy resolution is typically characterized by the size of the detector energy window, ΔE, in electron volts, as determined by the full width at half maximum (FWHM) of the detector-efficiency curve as a function of energy, with the detector and counting electronics set to a specific wavelength. Another frequently used expression for energy resolution is the ratio of the detector energy window size to the energy of the monochromatic X-ray beam, E, expressed as $\Delta E/E$.

The *proportionality* of the detector determines how the size of the generated voltage pulse is related to the energy of the absorbed X-ray photons, and electronic methods (pulse-height selection) can be used to discriminate between different energies. An accurate proportionality thus allows the use of *energy discrimination* as a form of monochromatization, where the energy is filtered by the detector rather than by an optical element such as a metal filter, crystal or mirror; see Section 2.1.6.3. Signals corresponding to photons with too high or too low energies are discarded.

The size and weight of detectors may impose several practical constraints, see also Section 2.1.4.2. For large detectors the accessible angular range may be limited owing to collision issues. For heavy detectors a horizontal goniometer may be preferred over a vertical goniometer (unless horizontal specimen positioning is imperative) in order to minimize the goniometer load.

X-ray detectors may be broadly classified as *counting detectors* or *integrating detectors*. Counting (digital) detectors are able to detect and count individual photons. The number of pulses counted per unit time is proportional to the incident X-ray flux. Integrating (or analogue) detectors accumulate photon-induced signals for a given period of time, prior to the integrated signal being read out and converted into an (analogue) electrical signal. The signal size is proportional to the flux density of the incident X-rays.

Counting and integrating detectors each have their clear advantages and disadvantages. Counting detectors normally have a greater dynamic range than integrating detectors, while integrating detectors normally have better spatial resolution (Section 2.1.7.3). Energy resolution is only possible for counting detectors. Readout and dark noise are usually higher for integrating detectors. Integrating detectors are not limited by the photon count rate as there is no dead time; nevertheless, the measurement time has to be kept sufficiently small to avoid saturation.

2.1.7.2. *Detector types*

Counting and integrating detectors can be further distinguished by their working principle, and are represented by scintillation, gas-ionization and semiconductor detectors. The most commonly used detector types and their properties are listed in Tables 2.1.1 and 2.1.6, respectively.

At the end of the 1990s the types of detectors in use were scintillation, gas-ionization, Si(Li) and image-plate detectors, with the scintillation counter being the most common by far. Usage of photographic film had already greatly diminished by that time. With the introduction of a series of new one- and two-dimensional detector technologies since the late 1990s, the X-ray detection landscape changed completely. New semiconductor-based detectors (silicon micro-strip, silicon pixel) as well as gas-ionization-based detectors (micro-gap) reached a market share of >90% in newly sold X-ray powder diffractometers within only a few years. As a consequence, classical metal-wire-based proportional counters and scintillation counters will probably become obsolete before 2020. The same is expected for CCD-based detectors, which will be replaced by the very recently introduced complementary metal–oxide–semiconductor (CMOS) active pixel sensor technology.

In the following the working principles of currently available detector types will be briefly described. Matters that are specific to zero- (0D), one- (1D) and two-dimensional (2D) detection are discussed in Section 2.1.7.3. While image plates are still in use, their market share in newly sold systems has become insignificant. Photographic film techniques are totally obsolete. For these reasons, these two detector types will not be taken into further consideration.

2.1.7.2.1. *Scintillation counters*

Scintillation counters are constructed from a scintillator crystal optically coupled to a photomultiplier tube. The crystal is typically made of sodium iodide (NaI) doped with about 1% thallium, frequently denoted as NaI(Tl). When irradiated by X-ray radiation, blue light (~415 nm) is emitted and converted to electrons in a photomultiplier and amplified; the resulting pulses are registered as photon counts.

The height of the outgoing pulses is proportional to the energy of the incoming X-ray photons. This permits the use of pulse-height selection but only allows for poor energy resolution. The relatively high count rate and a moderate noise level result in a moderate dynamic range. These characteristics are the reason for the formerly wide-ranging acceptance of the scintillation counter

Table 2.1.6
Important detector properties at 8 keV as reported by various vendors

Only typical values are given to allow approximate comparisons. Detector properties strongly depend on individual detector designs and are subject to high development rates.

		Gas ionization (Xe/CO_2 gas filling)		
	Scintillation	Wire based (0D)	Wire based (1D/2D)	Micro-gap (1D/2D)
DQE	~95%	~95%	~80%	~80%
Dynamic range	$>6 \times 10^6$	$>10^6$	$>10^4$ (1D) $>10^6$ (2D)	$>8 \times 10^7$ (1D) $>10^9$ (2D)
Maximum global count rate	$>2 \times 10^6$ c.p.s.	$>7.5 \times 10^5$	$>10^5$ (1D) $>4 \times 10^4$ c.p.s. (2D)	$>8 \times 10^5$ (1D) $>1.6 \times 10^6$ c.p.s. (2D)
Maximum local count rate	n/a	n/a	$>10^4$ (1D) $>10^4$ c.p.s. mm^{-2} (2D)	$>9 \times 10^5$ c.p.s. mm^{-2} (1D, 2D)
Noise	~0.3 c.p.s.	~1 c.p.s.	~1 c.p.s. (1D) $<5 \times 10^{-4}$ c.p.s. mm^{-2} (2D)	<0.01 c.p.s. (1D) $<5 \times 10^{-4}$ c.p.s. mm^{-2} (2D)
Energy resolution	~3500 eV (~45%)	~1600 eV (~20%)	~1600 eV (~20%)	~1600 eV (~20%)
Detection mode	Photon counting	Photon counting	Photon counting	Photon counting

	Semiconductor				
	Si(Li)	Strip	Pixel	CCD	CMOS
DQE	>98%	>98%	>98%	~20–60%	~75%
Dynamic range	$>10^6$	$>7 \times 10^6$ per strip	$>10^9$	$>5 \times 10^4$	$>1.6 \times 10^4$
Maximum global count rate	$>10^5$ c.p.s.	$>10^8$ c.p.s	$>10^7$ c.p.s. mm^{-2}	n/a	n/a
Maximum local count rate	n/a	$>7 \times 10^5$ c.p.s. per strip	$>10^4$ per pixel	n/a	n/a
Noise	~0.1 c.p.s.	~0.1 c.p.s. per strip	$\sim 2.5 \times 10^{-3}$ c.p.s. mm^{-2}	<0.1 c.p.s. per pixel	<0.05 c.p.s. per pixel
Energy resolution	~200 eV (~4%)	~1600 eV (~20%)†	>1000 eV (~12.5%)	n/a‡	n/a
Detection mode	Photon counting	Photon counting	Photon counting	Integrating§	Integrating

† ~380 eV/~5%; Wiacek *et al.* (2015). ‡ >300 eV/>6% in photon-counting mode, see text. § Photon-counting mode possible, see text.

as the detector of choice. An important disadvantage these days is the limitation to 0D detection.

2.1.7.2.2. *Gas-ionization detectors*

The gas-ionization detectors in current use are proportional counters and can be of the 0D, 1D or 2D detection type. Common to all proportional counters is a gas-filled chamber permeated by a non-uniform electric field between positive and negative electrodes, held at a constant potential difference relative to each other. Typically the noble gases Ar or Xe are used as gas fill, mixed with a small amount of quenching gas such as CH_4 or CO_2 to limit discharges. When an X-ray photon travels through the gas-filled volume, it may be absorbed by a noble-gas atom, resulting in the ejection of an electron (photoelectric and Compton recoil). This electron, accelerated by the electric field towards the anode, will cause an avalanche by subsequent ionization along its path (gas amplification), generating an electric pulse which can be registered. The height of the generated pulse is proportional to the energy of the incoming X-ray photon and permits the use of pulse-height selection to achieve moderate energy resolution.

2.1.7.2.2.1. Wire-based proportional counters

In a point proportional detector (0D detection), the pulses generated are measured at one end of a wire (or a knife edge). Position-sensitive (1D and 2D detection) proportional detectors have the added capability of detecting the location of an X-ray photon absorption event. In a 1D proportional detector, pulses are detected at both ends of the wire. Thus the time difference between the measurements of a given pulse can be used to determine the location of the discharge. 2D proportional counters consist of three arrays of wires (multiwire proportional counter, MWPC; Sauli, 1977; Charpak *et al.*, 1968), where one array forming the anode plane is placed between two cathode arrays with their wires oriented parallel and orthogonal to the anode-plane wires, respectively.

Low count rates and low-to-moderate detector noise result in low-to-moderate dynamic ranges. Wire-based proportional counters are not competitive with micro-gap and semiconductor detectors, as can be seen in Table 2.1.6, and are therefore being driven out of the market.

2.1.7.2.2.2. Micro-gap detectors

The maximum count rates in 'classical' metal-wire-based proportional counters are severely limited by the long ion-drift times in the chamber (which typically have a cathode to anode spacing of ~10 mm). This issue has been successfully addressed by so-called micro-gap technology using parallel-plate avalanche chambers with a readout electrode separated from a resistive anode. The key feature is the resistive anode, which allows a very small amplification gap (1–2 mm cathode to anode spacing) at an increased average electric field intensity, while preventing discharges (Durst *et al.*, 2003; Khazins *et al.*, 2004). As a result, micro-gap detectors can achieve count rates several orders of magnitude higher than classical proportional counters at higher position sensitivity. Micro-gap detectors of the 1D and 2D detection type are available. Moderate count rates and very small

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