direction and the other giving the vertical position. A detector of this kind is used on the WOMBAT diffractometer at the OPAL reactor. MSGC detectors can also be adapted to provide two-dimensional positional information after printing a set of cathodes orthogonal to the primary set on the back surface of the glass.

A few general comments about detecting systems are in order. The time for a detector to recover after registering a neutron count is known as the dead time, and this may be significant when count rates are high, in which case corrections are needed [Chapter 7.3 of Volume C (Convert & Chieux, 2006)]. For banks of detectors, and also for position-sensitive detectors, calibration for position and sensitivity becomes a critical issue. In the case of a smaller bank of detectors, it may be possible to scan the detector bank so the same diffraction pattern is recorded in the different detectors, in which case the relative positions and efficiencies of the different detectors can be determined quite well (see Section 4.1 of Kisi & Howard, 2008). For more extensive banks or large position-sensitive detectors, detector sensitivity calibration is performed by examining the very nearly isotropic incoherent scattering from vanadium. In this case checking for angular accuracy can be more difficult. The time taken to register a neutron count cannot be said to be a fundamental issue in CW powder diffraction, since in some applications it is scarcely relevant, although in other applications, such in the study of very fast reaction kinetics (Riley *et al.*, 2002), the constraints on time are very demanding.

2.3.4.1.4. *Resolution and intensity*

The resolution and intensity of a CW powder diffractometer are strongly influenced by the divergences α_1, α_2 and α_3 of the primary, monochromatic and diffracted beams, respectively, along with the mosaic spread β of the crystal monochromator. The situation was analysed by Caglioti *et al.* (1958) on the basis that the triangular transmission factor of each collimator, total width 2α, could be approximated by a Gaussian with full-width at half-maximum (FWHM) α, that the mosaic distribution of the monochromator could also be described by a Gaussian with FWHM β, but that there was no sample contribution to the peak widths. On this basis the diffraction peaks were found to be Gaussian, with the FWHM of the diffraction peak occurring at scattering angle 2θ given by (Hewat, 1975)

$$\mathrm{FWHM}^2 = U\tan^2\theta + V\tan\theta + W, \tag{2.3.18}$$

where

$$U = \frac{4(\alpha_1^2\alpha_2^2 + \alpha_1^2\beta^2 + \alpha_2^2\beta^2)}{\tan^2\theta_M(\alpha_1^2 + \alpha_2^2 + 4\beta^2)}, \tag{2.3.18a}$$

$$V = \frac{-4\alpha_2^2(\alpha_1^2 + 2\beta^2)}{\tan\theta_M(\alpha_1^2 + \alpha_2^2 + 4\beta^2)}, \tag{2.3.18b}$$

$$W = \frac{\alpha_1^2\alpha_2^2 + \alpha_1^2\alpha_3^2 + \alpha_2^2\alpha_3^2 + 4\beta^2(\alpha_2^2 + \alpha_3^2)}{\alpha_1^2 + \alpha_2^2 + 4\beta^2} \tag{2.3.18c}$$

and θ_M is the Bragg angle ($2\theta_M$ is the take-off angle) at the monochromator. Under these conditions the total (integrated) intensity in the diffraction peak is given by

$$L \propto \frac{\alpha_1\alpha_2\alpha_3\beta}{(\alpha_1^2 + \alpha_2^2 + 4\beta^2)^{1/2}}. \tag{2.3.19}$$

These equations have important implications and accordingly have received a good deal of attention. They return at once the well known resolution advantage in setting up the diffractometer in the parallel configuration (that seen in Fig. 2.3.15, in this configuration θ_M taken to be positive). Caglioti *et al.* (1958) deduced that for the simple case of $\alpha_1 = \alpha_2 = \alpha_3 = \beta = \alpha$ equations (2.3.18) and (2.3.19) reduce to

$$\mathrm{FWHM} = \alpha\left(\frac{11 - 12a + 12a^2}{6}\right)^{1/2} \text{ and } L \propto \alpha^3/(6)^{1/2},$$

where $a = \tan\theta/\tan\theta_M$; they went on to record results for a number of other combinations. In his design for a high-resolution diffractometer, Hewat (1975) considered the case $\alpha_2 = 2\beta > \alpha_1 \simeq \alpha_3$. Under these conditions, the peak widths are close to their minimum around the parallel focusing condition $\theta = \theta_M$, their widths there are given by

$$\mathrm{FWHM}^2 = (\alpha_1^2 + \alpha_3^2) - \frac{\alpha_1^4}{\alpha_1^2 + \alpha_2^2 + 4\beta^2} \simeq \alpha_1^2 + \alpha_3^2,$$

and the total intensity is approximately

$$L \propto \alpha_1\alpha_3\beta/(2)^{1/2}.$$

Hewat's conclusions, put briefly, were that good resolution could be obtained by keeping divergences α_1 and α_3 small, while intensity could be somewhat recovered by adopting relatively large values for the monochromator mosaic spread β and divergence α_2 of the monochromatic beam. Hewat also argued for a high monochromator take-off angle $2\theta_M$, not only to reduce peak widths [through the term $\cot\theta_M$ appearing in equation (2.3.17) and reappearing in equations (2.3.18)], but also to match the region of best resolution to that of the most closely spaced peaks in the diffraction pattern. Hewat's design was implemented in the D1A diffractometer at the Institut Laue–Langevin (Hewat & Bailey, 1976), subsequently in the D2B diffractometer at the same establishment, and elsewhere. In a version installed at the (now retired) HIFAR reactor in Sydney, Howard *et al.* (1983), using an Al_2O_3 (corundum) ceramic sample, reported a peak-width variation in close agreement with that calculated from equation (2.3.18). Although more sophisticated analyses are available in the literature (Cussen, 2000), this result would suggest that equations (2.3.18) still provide a good starting point.

The usual trade-off between intensity and resolution applies, and since neutron sources are rather less intense than X-ray sources, this is an important consideration. Intensity is sacrificed by using high monochromator take-off angles to limit the wavelength spread [equation (2.3.17)], and by using tight collimation [equation (2.3.19)]. Evidently intensities could be increased by relaxing these constraints. These days it is more common to build diffractometers of good-to-high resolution, and then to seek other means to improve data-collection rates. Focusing monochromators, such as described in Section 2.3.4.1.2, serve to increase the neutron intensity at the sample position without seriously degrading the resolution. In addition, the use of multi-detector banks and the development and deployment of position-sensitive detectors, as described in Section 2.3.4.1.3, has been very much driven by the desire to increase the speed of data collection. As mentioned earlier, the design and analysis of neutron powder diffractometers should be treated in a holistic fashion, and although some advanced analytical methods have been applied (Cussen, 2016 and references therein), Monte Carlo analyses using programs such as *McStas* (Willendrup *et al.*, 2014) and *VITESS* (Zendler *et al.*, 2014) to track large numbers of neutrons from the source right through to the neutron detectors are now widely employed.