International Tables for Crystallography (2006). Vol. C, Section 2.2.3.1, p. 31.

2.2.3. Rotation/oscillation geometry

The main modern book dealing with the rotation method is that of Arndt & Wonacott (1977).

2.2.3.1. *General*

The purpose of the monochromatic rotation method is to stimulate a reflection fully over its rocking width *via* an angular rotation. Different relp's are rotated successively into the reflecting position. The method, therefore, involves rotation of the sample about a single axis, and is used in conjunction with an area detector of some sort, *e.g.* film, electronic area detector or image plate. The use of a repeated rotation or oscillation, for a given exposure, is simply to average out any time-dependent changes in incident intensity or sample decay. The overall crystal rotation required to record the total accessible region of reciprocal space for a single crystal setting, and a detector picking up all the diffraction spots, is $180^\circ + 2\theta_{\max}$. If the crystal has additional symmetry, then a complete asymmetric unit of reciprocal space can be recorded within a smaller angle. There is a blind region close to the rotation axis; this is detailed in Subsection 2.2.3.5.

2.2.3.2. *Diffraction coordinates*

Figs. 2.2.3.1(*a*) to (*d*) are taken from *IT* II (1959, p. 176). They neatly summarize the geometrical principles of reflection, of a monochromatic beam, in the reciprocal lattice for the general case of an incident beam inclined at an angle (μ) to the equatorial plane. The diagrams are based on an Ewald sphere of unit radius.

With the nomenclature of Table 2.2.3.1:
Fig 2.2.3.1(*a*) gives

$$\sin\nu = \sin\mu + \zeta. \qquad (2.2.3.1)$$

Fig. 2.2.3.1(*b*) gives, by the cosine rule,

$$\cos\Upsilon = \frac{\cos^2\nu + \cos^2\mu - \xi^2}{2\cos\nu\cos\mu} \qquad (2.2.3.2)$$

and

$$\cos\tau = \frac{\cos^2\mu + \xi^2 - \cos^2\nu}{2\xi\cos\mu}, \qquad (2.2.3.3)$$

and Figs. 2.2.3.1(*a*) and (*b*) give

$$\xi^2 + \zeta^2 = d^{*2} = 4\sin^2\theta. \qquad (2.2.3.4)$$

The following special cases commonly occur:
(*a*) $\mu = 0$, normal-beam rotation method, then

$$\sin\nu = \zeta \qquad (2.2.3.5)$$

and

$$\cos\Upsilon = \frac{2 - \xi^2 - \zeta^2}{2\sqrt{1-\zeta^2}}; \qquad (2.2.3.6)$$

(*b*) $\mu = -\nu$, equi-inclination (relevant to Weissenberg upper-layer photography), then

$$\zeta = -2\sin\mu = 2\sin\nu \qquad (2.2.3.7)$$

$$\cos\Upsilon = 1 - \frac{\xi^2}{2\cos^2\nu}; \qquad (2.2.3.8)$$

(*c*) $\mu = +\nu$, anti-equi-inclination

$$\zeta = 0 \qquad (2.2.3.9)$$

$$\cos\Upsilon = 1 - \frac{\zeta^2}{2\cos^2\nu}; \qquad (2.2.3.10)$$

(*d*) $\nu = 0$, flat cone

$$\zeta = -\sin\mu \qquad (2.2.3.11)$$

$$\cos\Upsilon = \frac{2 - \xi^2 - \zeta^2}{2\sqrt{1-\zeta^2}}. \qquad (2.2.3.12)$$

In this section, we will concentrate on case (*a*), the normal-beam rotation method ($\mu = 0$). First, the case of a plane film or detector is considered.

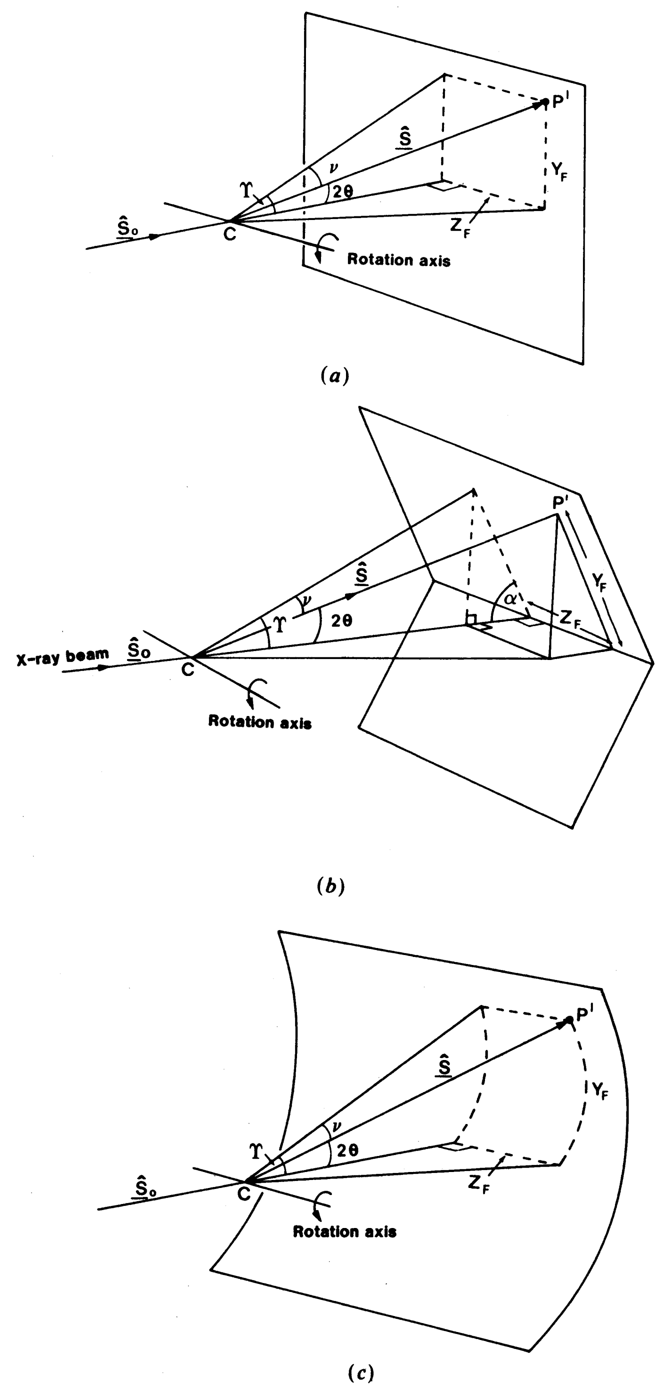

Fig. 2.2.3.2. Geometrical principles of recording the pattern on (*a*) a plane detector, (*b*) a *V*-shaped detector, (*c*) a cylindrical detector.

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references