The coordinates Y_F and Z_F are related to film-scanner raster units *via* a scanner-rotation matrix and translation vector. This is necessary because the film is placed arbitrarily on the scanner drum. Details can be found in Rossmann (1985) or Arndt & Wonacott (1977).

2.2.3.3. *Relationship of reciprocal-lattice coordinates to crystal system parameters*

The reciprocal-lattice coordinates, $\zeta, \xi, \Upsilon, \nu$, *etc*. used earlier, refer to an axial system fixed to the crystal, $X_0Y_0Z_0$ of Fig. 2.2.3.3. Clearly, a given relp needs to be brought into the Ewald sphere by the rotation about the rotation axis. The treatment here follows Arndt & Wonacott (1977).

The rotation angle required, φ, is with respect to some reference 'zero-angle' direction and is determined by the particular crystal parameters. It is necessary to define a standard orientation of the crystal (*i.e.* datum) when $\varphi = 0^\circ$. If we define an axial system $X_0Y_0Z_0$ fixed to the crystal and a laboratory axis system XYZ with X parallel to the beam and Z coincident with the rotation axis then $\varphi = 0^\circ$ corresponds to these axial systems being coincident (Fig. 2.2.3.3).

The angle of the crystal at which a given relp diffracts is

$$\tan(\varphi/2) = \frac{2y_0 \pm (4y_0^2 + 4x_0^2 - d^{*4})^{1/2}}{(d^{*2} - 2x_0)}. \qquad (2.2.3.21)$$

The two solutions correspond to the two rotation angles at which the relp P cuts the sphere of reflection. Note that Y_F, Z_F (Subsection 2.2.3.2) are independent of φ.

The values of x_0 and y_0 are calculated from the particular crystal system parameters. The relationships between the coordinates x_0, y_0, z_0 and ξ and ζ are

$$\xi = (x_0^2 + y_0^2)^{1/2}, \qquad (2.2.3.22)$$

$$\zeta = z_0. \qquad (2.2.3.23)$$

$\mathbf{X}_0$ can be related to the crystal parameters by

$$\mathbf{X}_0 = \boldsymbol{A}\mathbf{h}. \qquad (2.2.3.24)$$

$\boldsymbol{A}$ is a crystal-orientation matrix defining the standard datum orientation of the crystal.

For example, if, by convention, $\mathbf{a}^*$ is chosen as parallel to the X-ray beam at $\varphi = 0^\circ$ and $\mathbf{c}$ is chosen as the rotation axis, then, for the general case,

$$\boldsymbol{A} = \begin{bmatrix} a^* & b^*\cos\gamma^* & c^*\cos\beta^* \\ 0 & b^*\sin\gamma^* & -c^*\sin\beta\cos\alpha \\ 0 & 0 & c^* \end{bmatrix}. \qquad (2.2.3.25)$$

If the crystal is mounted on the goniometer head differently from this then $\boldsymbol{A}$ can be modified by another matrix, $\boldsymbol{M}$, say, or the terms permuted. This exercise becomes clear if the reader takes an orthogonal case ($\alpha = \beta = \gamma = 90^\circ$). For the general case, see Higashi (1989).

The crystal will most likely be misaligned (slightly or grossly) from the ideal orientation. To correct for this, the misorientation matrices $\boldsymbol{\Phi}_x$, $\boldsymbol{\Phi}_y$, and $\boldsymbol{\Phi}_z$ are introduced, *i.e.*

$$\boldsymbol{\Phi}_x = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\Delta\varphi_x & -\sin\Delta\varphi_x \\ 0 & \sin\Delta\varphi_x & \cos\Delta\varphi_x \end{bmatrix} \qquad (2.2.3.26)$$

$$\boldsymbol{\Phi}_y = \begin{bmatrix} \cos\Delta\varphi_y & 0 & \sin\Delta\varphi_y \\ 0 & 1 & 0 \\ -\sin\Delta\varphi_y & 0 & \cos\Delta\varphi_y \end{bmatrix} \qquad (2.2.3.27)$$

$$\boldsymbol{\Phi}_z = \begin{bmatrix} \cos\Delta\varphi_z & -\sin\Delta\varphi_z & 0 \\ \sin\Delta\varphi_z & \cos\Delta\varphi_z & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad (2.2.3.28)$$

where $\Delta\varphi_x$, $\Delta\varphi_y$, and $\Delta\varphi_z$ are angles around the X_0, Y_0, and Z_0 axes, respectively.

Hence, the relationship between $\mathbf{X}_0$ and $\mathbf{h}$ is

$$\boldsymbol{X}_0 = \boldsymbol{\Phi}_z\boldsymbol{\Phi}_y\boldsymbol{\Phi}_x\boldsymbol{M}\boldsymbol{A}\mathbf{h}. \qquad (2.2.3.29)$$

2.2.3.4. *Maximum oscillation angle without spot overlap*

For a given oscillation photograph, there is maximum value of the oscillation range, $\Delta\varphi$, that avoids overlapping of spots on a film. The overlap is most likely to occur in the region of the diffraction pattern perpendicular to the rotation axis and at the maximum Bragg angle. This is where relp's pass through the Ewald sphere with the greatest velocity. For such a separation between successive relp's of a^*, then the maximum allowable rotation angle to avoid spatial overlap is given by

$$\Delta\varphi_{\max} = \left[\frac{a^*}{d^*_{\max}} - \Delta\right], \qquad (2.2.3.30)$$

where Δ is the sample reflecting range (see Section 2.2.7). $\Delta\varphi_{\max}$ is a function of φ, even in the case of identical cell parameters. This is because it is necessary to consider, for a given orientation, the relevant reciprocal-lattice vector perpendicular to $d^*_{\max}$. In the case where the cell dimensions are quite different in magnitude (excluding the axis parallel to the rotation axis), then $\Delta\varphi_{\max}$ is a marked function of the orientation.

In rotation photography, as large an angle as possible is used up to $\Delta\varphi_{\max}$. This reduces the number of images that need to be processed and the number of partially stimulated reflections per image but at the expense of signal-to-noise ratio for individual spots, which accumulate more background since $\Delta < \Delta\varphi_{\max}$. In the case of a CCD detector system, $\Delta\varphi$ is chosen usually to be

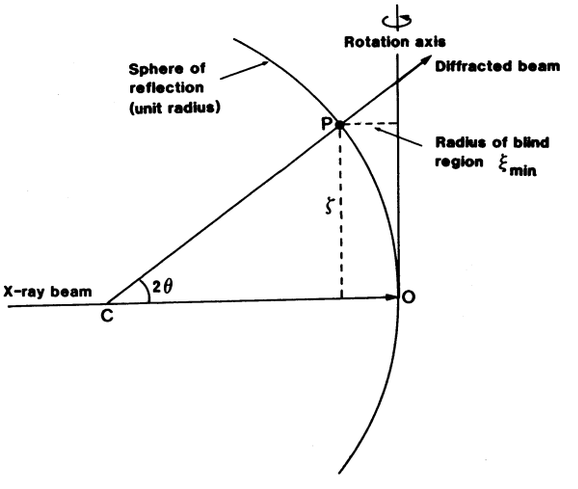

Fig. 2.2.3.4. The rotation method. The blind region associated with a single rotation axis. From Arndt & Wonacott (1977).

references