where z and $T(z)$ are the path lengths for the incident and diffracted beams, respectively. τ is the radius, along the line of the incident beam, of the ellipse described by the cross section of the crystal in the plane of diffraction, shown in Fig. 6.3.3.2. The equation for the ellipse is

$$\tau = R(1 - \sin^2\theta \sin^2\chi)^{-1/2}. \qquad (6.3.3.15)$$

The outgoing elliptical radius v satisfies

$$Av^4 + Bv^2 + C = 0, \qquad (6.3.3.16)$$

where

$$\begin{aligned} A &= [1 - \sin^2\theta \sin^2\chi]^2 \\ B &= -2R^2[1 - \sin^2\theta \sin^2\chi] \\ &\quad - 2(\tau - z)^2[\cos^2\theta - \sin^2\theta \cos^2\chi]\sin^2 2\theta \sin^2\chi \\ C &= R^4 + 2R^2(\tau - z)^2 \sin^2 2\theta \sin^2\chi \cos 2\theta \\ &\quad + (\tau - z)^4 \sin^4 2\theta \sin^4\chi. \end{aligned}$$

In the case where the cylinder axis is inclined at an angle Γ to the φ axis, these equations become

$$\begin{aligned} A &= [1 - \sin^2(\theta + \beta)\sin^2\chi_1]^2 \\ B &= -2R^2[1 - \sin^2(\theta + \beta)\sin^2\chi_1] \\ &\quad - 2(\tau - z)^2[\cos^2(\theta + \beta) \\ &\quad - \sin^2(\theta + \beta)\cos^2\chi_1]\sin^2 2\theta \sin^2\chi_1 \\ C &= R^4 + 2R^2(\tau - z)^2 \sin^2 2\theta \sin^2\chi_1 \cos 2(\theta + \beta) \\ &\quad + (\tau - z)^4 \sin^4 2\theta \sin^4\chi_1, \end{aligned}$$

where

$$\tan\beta = \sin\Gamma \sin\varphi / [\sin\Gamma \cos\chi \cos\varphi + \sin\chi \cos\Gamma].$$

The roots of the quadratic equation (6.3.3.16) for v^2 are real and positive for reflection from within the crystal. The convergent path length T is given by the positive root of the triangle formula

$$T^2 - 2T(\tau - z)\cos 2\theta + (\tau - z)^2 - v^2 = 0. \qquad (6.3.3.17)$$

It should be noted that the volume of the specimen irradiated changes with the angular settings of the diffractometer. Normalization to constant volume requires that the absorption correction be multiplied by the volume-correction factor $[1 - \sin^2(\theta - \beta)\sin^2\chi_1]^{-1/2}$.

The method readily extends to the case of a cylindrical window or sheath, such as used for mounting an unstable crystal of conventional size. The correction in this case is

$$\begin{aligned} &\exp[-\mu(\tau_2 - \tau_1 + v_2 - v_1)] \\ &\quad = \exp\Big(-\mu(R_2 - R_1)\{[1 - \sin^2(\theta - \beta)\sin^2\chi_1]^{-1/2} \\ &\qquad + [1 - \sin^2(\theta + \beta)\sin^2\chi_1]^{-1/2}\}\Big), \end{aligned} \qquad (6.3.3.18)$$

where the subscripts 1 and 2 apply to the inner and outer radii, respectively.

The integral in equation (6.3.3.14) may be evaluated by Gaussian quadrature, *i.e.* by approximation as a weighted sum of the values of the function at the N zeros X_i of the Legendre polynomial of degree N in the interval $[-1, +1]$. The weights w_i for the points are tabulated by Abramowitz & Stegun (1964). Further details are given in Subsection 6.3.3.4. The emergent path lengths $T(z_1)$ and $T(z_2)$ for the case of the sheath are calculated as functions of the Gaussian variable X_i using the linear transformation

$$z_i = \tau_1 X_i + \tau_2, \quad i = 1, 2, \ldots, N. \qquad (6.3.3.19)$$

This transformation converts the Gaussian variable X into the beam coordinate z for each i of the N summation points.

6.3.3.3. *Analytical method for crystals with regular faces*

For a crystal with regular faces, (6.3.3.1) may be integrated exactly, giving the correction in analytical form. In its simplest form, the analytical method applies to specimens with no re-entrant angles. It is efficient for crystals with a small number of faces. Its accuracy does not depend on the size of the absorption coefficient. The principles can be illustrated by reference to the two-dimensional case of a triangular crystal shown in Fig. 6.3.3.3.

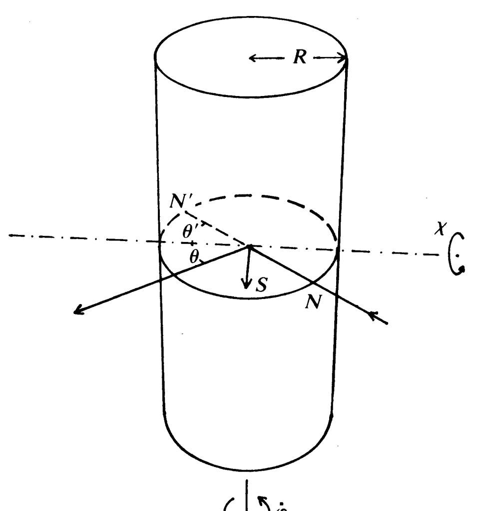

Fig. 6.3.3.1. Geometry of the Eulerian cradle with the axis of a cylindrical specimen coincident with the φ axis.

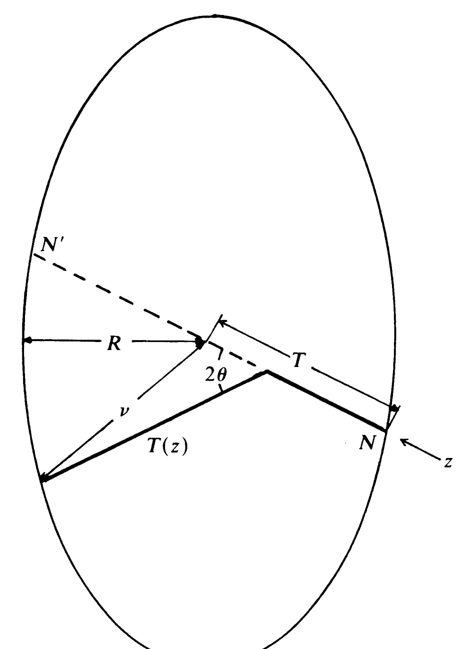

Fig. 6.3.3.2. Cross section of the plane of diffraction for a cylindrical specimen coincident with the φ axis.