International Tables for Crystallography (2006). Vol. C, Figure 2.2.7.4, p. 40.

In the case of the single-crystal monochromator, the actual curvature employed is very important in the diffraction geometry. For a point source and a flat monochromator crystal, there is a gradual change in the photon wavelength selected from the white beam as the length of the monochromator is traversed [Fig. 2.2.7.2(*a*)]. For a point source and a curved monochromator crystal, one specific curvature can compensate for this variation in incidence angle [Fig. 2.2.7.2(*b*)]. The reflected spectral bandwidth is then at a minimum; this setting is known as the 'Guinier position'. If the curvature of the monochromator crystal is increased further, a range of photon wavelengths, $(\delta\lambda/\lambda)_{\rm corr}$, is selected along its length so that the rays converging towards the focus have a correlation of photon wavelength and direction [Fig. 2.2.7.2(*c*)]. The effect of a finite source is to cause a change in incidence angle at the monochromator crystal, so that at the focus there is a photon-wavelength gradient across the width of the focus (for all curvatures) [Fig. 2.2.7.2(*d*)]. The use of a slit in the focal plane is akin to placing a slit at the tangent point to limit the source size.

The double-crystal monochromator with two parallel or nearly parallel perfect crystals of germanium or silicon is a common configuration. The advantage of this is that the outgoing monochromatic beam is parallel to the incoming beam, although it is slightly displaced vertically by an amount $2d\cos\theta$, where d is the perpendicular distance between the crystals and θ the monochromator Bragg angle. The monochromator can be rapidly tuned, since the diffractometer or camera need not be re-aligned significantly in a scan across an absorption edge. Between absorption edges, some vertical adjustment of the diffractometer is required. Since the rocking width of the fundamental is broader than the harmonic reflections, the strict parallelism of the pair of crystal planes can be relaxed, *i.e.* detuned so that the harmonic can be rejected with little loss of the fundamental intensity. The spectral spread in the reflected monochromatic beam is determined by the source divergence accepted by the monochromator, the angular size of the source, and the monochromator rocking width (see Fig. 2.2.7.3).

The double-crystal monochromator is often used with a toroid focusing mirror; the functions of monochromatization are then separated from the focusing (Hastings, Kincaid & Eisenberger, 1978).

The rocking width of a reflection depends on the horizontal and vertical beam divergences/convergences (after due account for collimation is taken) γ_H and γ_V, the spectral spreads $(\delta\lambda/\lambda)_{\rm conv}$ and $(\delta\lambda/\lambda)_{\rm corr}$, and the mosaic spread η. We assume that $\eta \gg \omega$, where ω is the angular broadening of a relp due to a finite sample. In the case of synchrotron radiation, γ_H and γ_V are usually widely asymmetric. On a conventional source, usually $\gamma_H \simeq \gamma_V$.

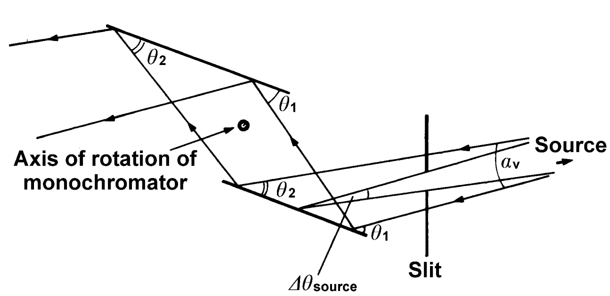

Fig. 2.2.7.3. Double-crystal monochromator illuminated by synchrotron radiation. The contributions of the source divergence α_V and angular source size $\Delta\theta_{\rm source}$ to the range of energies reflected by the monochromator are shown.

Two types of spectral spread occur with synchrotron and neutron sources. The term $(\delta\lambda/\lambda)_{\rm conv}$ is the spread that is passed down each incident ray in a divergent or convergent incident beam; the subscript refers to conventional source type. This is because it is similar to the $K\alpha_1$, $K\alpha_2$ line widths and separation. At the synchrotron, this component also exists and arises from the monochromator rocking width and finite-source-size effects. The term $(\delta\lambda/\lambda)_{\rm corr}$ is special to the synchrotron or neutron case. The subscript 'corr' refers to the fact that the ray direction can be correlated with the photon or neutron wavelength. Usually, an instrument is set to have $(\delta\lambda/\lambda)_{\rm corr} = 0$. In the most general case, for a $(\delta\lambda/\lambda)_{\rm corr}$ arising from the horizontal ray direction correlation with photon energy, and the case of a horizontal rotation axis, then the rocking width φ_R of an individual reflection is given by

$$\varphi_R = \left\{ L^2 \left[\left(\frac{\delta\lambda}{\lambda} \right)_{\rm corr} d^{*2} + \zeta\gamma_H \right]^2 + \gamma_V^2 \right\}^{1/2} + 2\varepsilon_s L, \qquad (2.2.7.11)$$

where

$$\varepsilon_s = \frac{d^*\cos\theta}{2} \left[\eta + \left(\frac{\delta\lambda}{\lambda} \right)_{\rm conv} \tan\theta \right] \qquad (2.2.7.12)$$

and L is the Lorentz factor $1/(\sin^2 2\theta - \zeta^2)^{1/2}$.

The Guinier setting of the instrument gives $(\delta\lambda/\lambda)_{\rm corr} = 0$. The equation for φ_R then reduces to

$$\varphi_R = L[(\zeta^2\gamma_H^2 + \gamma_V^2/L^2)^{1/2} + 2\varepsilon_s] \qquad (2.2.7.13)$$

(from Greenhough & Helliwell, 1982). For example, for $\zeta = 0$, $\gamma_V = 0.2$ mrad (0.01°), $\theta = 15^\circ$, $(\delta\lambda/\lambda)_{\rm conv} = 1 \times 10^{-3}$ and $\eta = 0.8$ mrad (0.05°), then $\varphi_R = 0.08^\circ$. But φ_R increases as ζ increases [see Greenhough & Helliwell (1982, Table 5)].

In the rotation/oscillation method as applied to protein and virus crystals, a small angular range is used per exposure

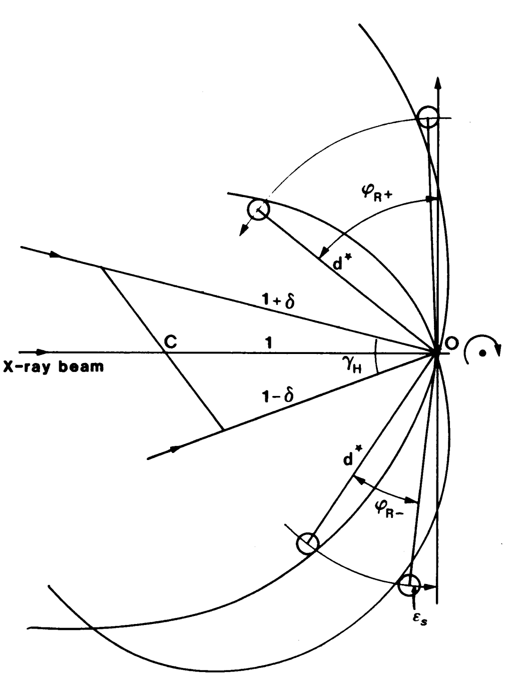

Fig. 2.2.7.4. The rocking width of an individual reflection for the case of Fig. 2.2.7.2(*c*) and a vertical rotation axis. φ_R is determined by the passage of a spherical volume of radius ε_s (determined by sample mosaicity and a conventional-source-type spectral spread) through a nest of Ewald spheres of radii set by $\delta = \frac{1}{2}[\delta\lambda/\lambda]_{\rm corr}$ and the horizontal convergence angle γ_H. From Greenhough & Helliwell (1982).

references