[single-crystal Bragg scattering]
(Chapter 5.4.3 in *Elements*)

Single-Crystal Bragg Scattering, USANS

There are two theories for front-surface reflection, $R_D(y)$ by Darwin (1914) for very thick crystals and $R_E(y)$ by Ewald (1918) for finite-thickness crystals. Here, $y=(\theta-\theta_B)/\delta\theta_D$ is the normalized deviation from the nominal Bragg angle, $\theta_B=\sin^{-1}(\lambda/2d)$. The reflectivity functions are often idealized as top-hat functions $2\delta\theta_D$ wide with no wings and for $|y|\le 1$ $R_E(y)=R_D(y)=1.0$. However, the wings dominate the reflectivity for large *y*, where, for both functions $R(y)\propto y^{-2}$ and $R_E(y)\to 2R_D(y)$. Finite crystals reflect more neutrons because of back-face reflections, which are equal in intensity to front-face reflections.

According to dynamical diffraction theory for non-absorbing crystals, neutrons of given wavelength are reflected from a perfect single crystal within a very narrow angular range around the nominal Bragg angle. The reflection process is specular (or, mirror-like) and elastic (i.e., no wavelength change). According to the Darwin theory, which is for thick crystals, front surface only, and the Ewald theory, which is for finite-thickness crystals, front face plus multiple front- and back-face reflections, the reflected intensity is 100% for angles within the Darwin plateau $2\delta\Theta_D$. Figure 5-U1 shows the geometry.

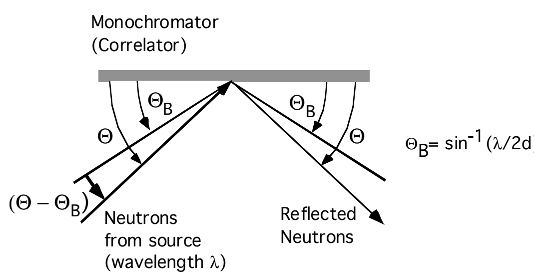

Figure 5-U1. Geometry of Bragg reflection for general angle of incidence and given wavelength. The difference angle ($\Theta - \Theta_B$) is greatly exaggerated in the figure.

For both Darwin and Ewald functions

$$R(y) = 1.0 \text{ for } |y| < 1. \tag{5-U1}$$

For |y| > 1,

$$R(y) = \begin{cases} R_D(y) = \left[|y| - \sqrt{y^2-1}\right]^2, \text{ Darwin, thick crystals, and} \\ R_E(y) = 1 - \sqrt{1-y^{-2}}, \text{ Ewald, finite crystals} \end{cases} . \tag{5-U2}$$

In the limit of large angles ($|y| >> 1$) the reflected intensity falls off as y^{-2} in both cases and $R_E(y)$ —> $2R_D(y)$. Takahashi and Hashimoto (1995) have relatively recently worked out the relationship between the Darwin and Ewald functions:

$$R_E(y) = 2R_D(y)/(1+R_D(y)). \qquad (5\text{-U3})$$

The width of the Darwin plateau is

$$2\delta\theta_D = \frac{2\lambda^2}{\pi V_{cell}\sin(2\theta_B)}\exp(-W)|F_{hkl}|, \qquad (5\text{-U4})$$

where λ is the wavelength, V_{cell} is the volume of the crystallographic unit cell, exp(-W), which appears here as W, not $2W$, is the Debye-Waller factor, θ_B is the Bragg angle, and $|F_{hkl}|$ is the magnitude of the structure factor for the hkl reflection. The Debye-Waller exponent is

$$W = B\left[\frac{\sin(\theta_B)}{\lambda^2}\right]^2, \qquad (5\text{-U5})$$

in which $B = 8\pi^2 u^2$, and u^2 is the temperature-dependent mean-squared displacement of an atom in the direction perpendicular to the scattering plane. Figure 5-U2 shows the Darwin and Ewald reflectivity functions. Table 5-U1 gives structure factors for hkl reflections of diamond cubic crystals, and for comparison those of BCC and FCC crystals, expressed in units of the coherent scattering length per atom.

References

Darwin, C. G. (1914). The theory of x-ray reflection. Part II, *Philos. Mag,* **27**, 675.

Ewald, P. P. (1917). Zur begründung der Kristalloptik; Teil III: die Kristalloptik der Röntgenstrahlung, *Annalen der Physik,* **359**, 519.

Takahashi, T., and M. Hashimoto (1995). Neutron rocking cures for nonabsorbing crystals, *Phys. Lett.,* **A 200**, 72.