International Tables for Crystallography (2018). Vol. H, Section 2.2.2.2.2, pp. 53–54.

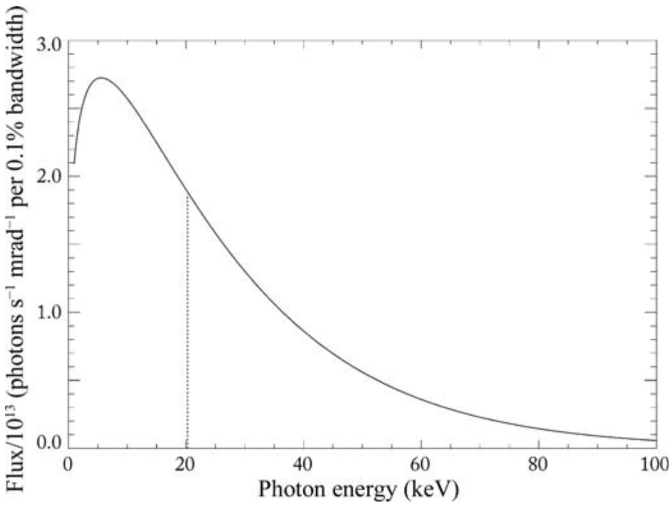

Figure 2.2.4
Spectrum of a bending magnet ($B = 0.85$ T) at the ESRF with an electron energy of 6 GeV (γ = 11 742), shown as flux per horizontal mrad for a 0.1% energy bandwidth at a storage-ring current of 200 mA. The critical energy of 20.3 keV divides the emitted power into equal halves.

$$\varepsilon \text{ [keV]} = 0.665 E_e^2 \text{ [GeV]} B.$$

The higher the critical energy, the greater the number of photons produced with short X-ray wavelengths. As an example, consider a bending magnet at the ESRF in Grenoble, France, which has a 6-GeV storage ring and bending magnets with a field of 0.85 T. The bending radius is 23.5 m and the critical photon energy is 20.3 keV (equivalent to a wavelength of 0.61 Å). The spectrum of such a device is shown in Fig. 2.2.4.

The vertical collimation of the radiation varies with photon energy in a nonlinear manner (Kim, 2001). Nevertheless, the divergence decreases with increased photon energy, so beams with the shortest wavelengths are the most vertically collimated. Various approximations can be written to describe the variation, such as for a single electron (Margaritondo, 1988),

$$\sigma_v(\varepsilon) \simeq \frac{0.565}{\gamma}\left(\frac{\varepsilon_c}{\varepsilon}\right)^{0.425},$$

where $\sigma_v(\varepsilon)$ is the standard deviation of the vertical-divergence distribution of photons of energy ε. For a population of electrons circulating in a storage ring, the distribution of the trajectories with respect to the plane of the orbit (of the order µrad) must also be considered, as these add to the vertical emission distribution. An approximation such as

$$\Psi_v(\varepsilon) = 2\sigma_v(\varepsilon) \simeq \frac{1.2}{\gamma}\left(\frac{\varepsilon_c}{\varepsilon}\right)^{1/2}$$

will often be adequate to estimate the vertical divergence Ψ_v in the vicinity of ε_c. Thus for the bending magnet illustrated in Fig. 2.2.4, photons at the critical energy of 20.3 keV will have a vertical divergence of ~100 µrad. A beamline would probably accept less than this, *e.g.* a 1.5-mm-high slit at 25 m from the source defining the beam onto a monochromator crystal defines an angle of ~60 µrad.

2.2.2.2. *Insertion devices*

Insertion devices can be classified into two main types, termed 'wigglers' and 'undulators', illustrated in Fig. 2.2.5. A wiggler has a relatively long magnetic period and the radiation from each oscillation is emitted like a series of powerful bending magnets, summing together to provide increased intensity. An undulator has a relatively short magnetic period and the radiation from sequential oscillations interferes coherently to give modified beam characteristics.

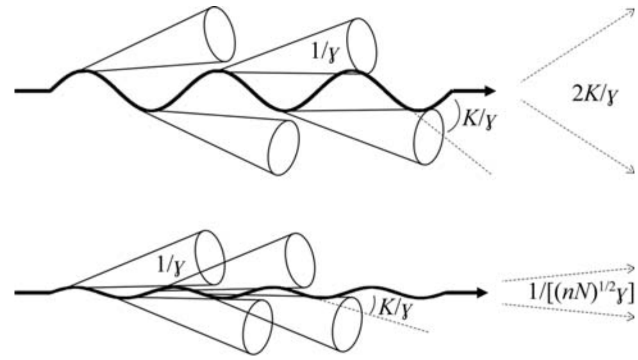

Figure 2.2.5
Schematic illustration of a wiggler (upper) and an undulator (lower).

For insertion devices the magnetic field acting on the electrons varies sinusoidally along the device,

$$B(z) = B_0 \sin(2\pi z/\lambda_u),$$

where B_0 is the peak magnetic field, z is the distance along the insertion-device axis and λ_u is the magnetic period. With a vertical field, the alternating magnetic field causes the electron path to oscillate in the horizontal plane. Note that the radiation is emitted mainly towards the outsides of the oscillations where the electrons change transverse direction, and where the magnetic field and beam-path curvature are highest. The maximum angular deflection of an electron from the axis of the insertion device is K/γ, where the deflection parameter K is given by

$$K = \frac{eB_0\lambda_u}{2\pi m_e c},$$

which simplifies to $K = 0.0934 B_0 \lambda_u$ [mm] with λ_u expressed in mm. K is a crucial parameter that determines the behaviour of the insertion device.

2.2.2.2.1. *Wigglers*

If K is large (10 or above), the insertion device is a wiggler and the electrons oscillate with an amplitude significantly greater than the emitted radiation's natural opening angle $1/\gamma$. Every oscillation along the device produces a burst of synchrotron radiation and these add together incoherently so increasing the flux in proportion to the number of magnetic periods. The radiation emerges from the wiggler in a horizontal fan with a horizontal opening angle $\sim 2K/\gamma$. The intensity of a wiggler-based beamline can be very high because each oscillation produces synchrotron radiation, and this radiation is directed close to the axis of the device. Like a bending magnet, wigglers produce a continuous spectrum but with the critical energy shifted to harder energies because the magnetic field is (usually) greater. Thus for a wiggler at a 6-GeV source, with a magnetic field of 1.2 T and a magnetic period of 125 mm, K is 14, the maximum deflection of the electrons from the straight-line path is 1.2 mrad and the critical photon energy is 28.7 keV. Magnetic fields of several tesla can be exploited using superconducting magnets to obtain even higher critical photon energies.

2.2.2.2.2. *Undulators*

If the value of K is 2 or less, the insertion device is an undulator. The deflection of the electrons is comparable to the natural opening angle of the emitted radiation $1/\gamma$. Radiation emitted from sequential oscillations interferes coherently, and the beam

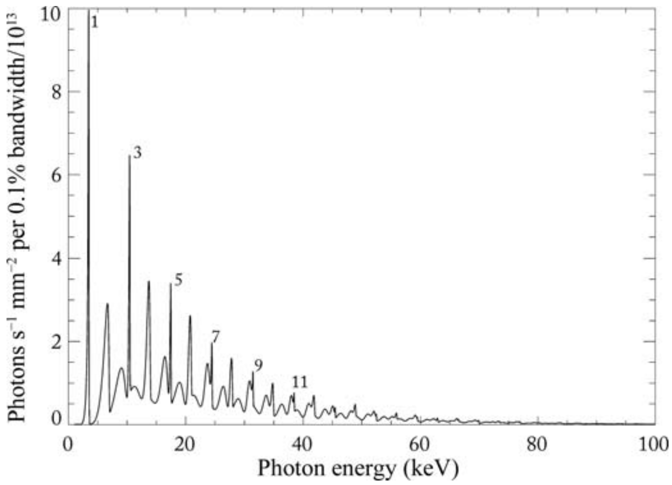

Figure 2.2.6
Photon flux *versus* energy through a 1-mm^2 aperture 30 m from the source, 0.1% bandwidth, for an ESRF u35 undulator (magnetic periodicity 35 mm, 1.6 m long, magnetic gap of 11 mm, peak magnetic field B_0 = 0.71 T, electron energy 6 GeV, K = 2.31, storage-ring current 200 mA). Odd-numbered harmonics are labelled, which are those usually employed for powder-diffraction experiments as they have maximum intensity on axis.

becomes highly collimated in the horizontal and vertical directions. Thus, the radiation from an undulator is concentrated into a central on-axis cone (fundamental and odd harmonics), surrounded by rings from higher-order even harmonics. The flux density arriving on a small sample from this central cone is therefore very high. With high on-axis intensity, it is therefore the undulators that provide the beams with the highest spectral brightness at any synchrotron-radiation source. The interference also modifies the spectrum of the device, which has a series of harmonics derived from a fundamental energy. At a horizontal angle θ to the axis of the insertion device, the wavelength of harmonic n is given by

$$\lambda_n = \frac{1 + (K^2/2) + \gamma^2\theta^2}{2n\gamma^2}\lambda_u,$$

which can be simplified on axis (θ = 0) to

$$\lambda_n\ [\text{Å}] = 1.3056\frac{1 + K^2/2}{nE_e^2\ [\text{GeV}]}\lambda_u\ [\text{mm}]$$

or

$$\varepsilon_n\ [\text{keV}] = 9.50\frac{nE_e^2\ [\text{GeV}]}{\lambda_u\ [\text{mm}](1 + K^2/2)}.$$

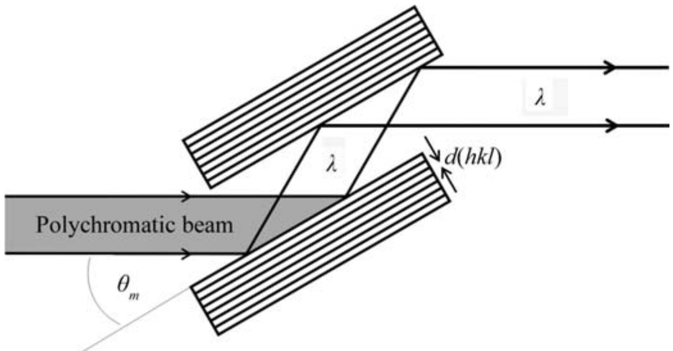

Figure 2.2.7
Double-crystal monochromator arrangement.

On axis, only odd-numbered harmonics are emitted and it is these that are usually employed in a powder-diffraction experiment. The horizontal and vertical divergence of the radiation emerging from an undulator is of the order of $1/[(nN)^{1/2}\gamma]$, where N is the number of magnetic periods making up the device. The spectrum of an undulator at a 6-GeV source with a 35-mm magnetic period is shown in Fig. 2.2.6. By carefully shimming the magnetic lattice so that it is highly regular, the higher-order harmonics persist, allowing the undulator to be a powerful source of high-energy X-rays. Any imperfections in the magnetic periodicity cause the higher-order harmonics to broaden and fade away, reducing the utility of the device at higher energies.

2.2.2.2.3. *Tuning*

For insertion devices the magnetic field can be modified by changing the vertical distance between the magnetic poles. By opening the gap, the magnetic field and K decrease following

$$B_0 \simeq B_r \exp(-\pi G/\lambda_u),$$

where B_r is proportional to the remanent magnetic field, which depends upon the nature of the magnets used in the insertion device, and G is the magnetic gap. Decreasing K for an undulator means that the energy of the fundamental harmonic increases; however, this is at the expense of the intensities of the higher harmonics. Thus the insertion device can be tuned to produce high intensity at the wavelength most suitable for a particular measurement. The smallest gap possible for a device depends on the design of the storage-ring vacuum vessel in which the electrons circulate. It is difficult to have a vessel smaller than about 10 mm high, and hence for an externally applied field a minimum magnetic gap of about 11 mm is to be expected. For smaller gaps, the magnets must be taken into the vacuum of the storage ring, a so-called ‘in-vacuum’ insertion device.

2.2.3. Optics

The intense polychromatic beam from the source needs to be conditioned before hitting the sample and diffracting. In the simplest experimental configuration, the white beam is used in an energy-dispersive experiment, and conditioning may involve no more than using slits to define the horizontal and vertical beam sizes and suppress background scattering. More usually, monochromatic radiation is employed, and the desired wavelength is chosen from the source by a monochromator. A monochromator consists of a perfect crystal, or a pair of crystals, set to select the chosen wavelength by Bragg diffraction. Additional optical elements can also be incorporated into the beamline for focusing, collimation, or for filtering out unwanted photons to reduce heat loads or remove higher-order wavelengths transmitted by the monochromator.

2.2.3.1. *Monochromator*

The monochromator is a crucial optical component in any angle-dispersive powder-diffraction beamline, and consists of one or a pair of perfect crystals (*e.g.* Beaumont & Hart, 1974), Fig. 2.2.7, set to a particular angle to the incident beam, θ_m, that transmits by diffraction wavelengths that satisfy the Bragg equation, $n\lambda = 2d(hkl)\sin\theta_m$, where $d(hkl)$ is the lattice spacing of the chosen reflection. Note that photons from higher-order reflections can also be transmitted, corresponding to wavelengths λ/n, depending on the structure factor of the nth-order reflection and its Darwin width, but these can be eliminated by use of a