

## 2. INSTRUMENTATION AND SAMPLE PREPARATION

speed  $v$  is

$$E_e = \frac{m_e c^2}{(1 - v^2/c^2)^{1/2}} = \gamma m_e c^2,$$

where  $m_e$  is the rest mass of the electron,  $9.10938356(11) \times 10^{-31}$  kg. The term  $1/(1 - v^2/c^2)^{1/2}$  is referred to as  $\gamma$  and is the factor by which the mass of the electron increases from its rest mass because of its relativistic speed. Expressed in eV (the conversion factor from kg to eV is  $c^2/e$ ), the electron rest mass is  $5.109989461(31) \times 10^5$  eV, so that

$$\gamma \simeq 1957 E_e [\text{GeV}]$$

when  $E_e$  is given in the customary units of GeV. Thus for a 3-GeV machine, a common energy for a synchrotron-radiation source,  $\gamma$  has the value of 5871. The mass of an electron with energy 3 GeV is therefore 3.22 atomic mass units, so around 7% more massive than a stationary atom of  $^3\text{H}$  or  $^3\text{He}$ .

Electrons do not circulate individually in the storage ring but in a series of bunches that are in phase with the accelerating radio frequency. Radiation is therefore emitted in pulses as each bunch passes through a bending magnet or insertion device. Thus the number and distribution of the electron bunches around the orbit determine the time structure of the emitted radiation. For most powder-diffraction applications using synchrotron radiation, the pulsed nature of the source can be neglected and the radiation can be regarded as continuous, although attention should also be paid to the performance of detectors that are more susceptible to pulse pile-up problems when the radiation arrives at very high average rates or in concentrated bursts (Cousins, 1994; Laundry & Collins, 2003; Honkimäki & Suortti, 2007), which can happen with certain bunch-filling modes. Certain specialized experiments requiring very fast time resolution can exploit the time structure of the source. In such experiments the longitudinal dimension of the bunches controls the pulse duration, which is usually a few tens of picoseconds.

In discussing the performance of different beamlines, the spectral brightness (Mills *et al.*, 2005) is often quoted for the source and is defined as

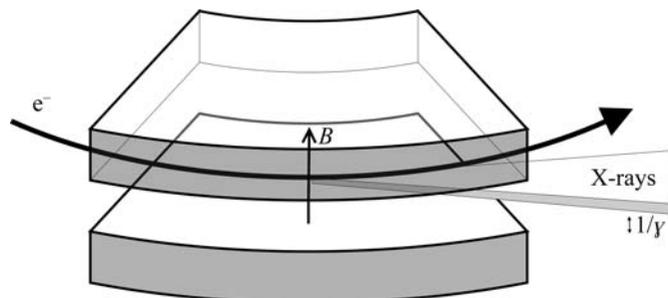
spectral brightness =

$$\text{photons per second per } 0.1\% \text{ bandwidth per mrad}^2 \text{ per mm}^2,$$

where ‘0.1% bandwidth’ represents  $\delta\lambda/\lambda = 0.001$ , the  $\text{mrad}^2$  term expresses the solid-angle of the emission of the X-rays from the source and the  $\text{mm}^2$  term relates to the cross-sectional area of the source. Thus a source of high spectral brightness emits many photons per second of the specified energy, into a narrow solid angle, with a small source size. The source size, which may well differ in the horizontal and vertical directions, is an important consideration as source size and beam divergence ultimately limit the performance of the beamline optical system in terms of collimation, energy resolution and focal spot size.

### 2.2.2.1. Bending magnets

A bending magnet provides a vertical magnetic field to deflect the electrons laterally in the horizontal plane from a straight-line trajectory, and thereby causes the emission of synchrotron radiation (see Fig. 2.2.2). The lateral Lorentz force,  $F$ , acting on an electron travelling at velocity  $v$  in a magnetic field  $B$  is mutually perpendicular to both the magnetic field and the direction of travel of the electron, and is given by



**Figure 2.2.2**

Emission of a fan of radiation by the electron beam as it curves in a bending magnet from one straight section of the ring to the next.

$$F = evB.$$

In a bending magnet the magnetic field is applied over an extended distance leading to a curved path of radius  $\rho$ . The centripetal acceleration is  $F/\gamma m_e$ , which for circular motion is equal to  $v^2/\rho$ . Since  $v \simeq c$ ,

$$\rho = \frac{\gamma m_e c}{eB},$$

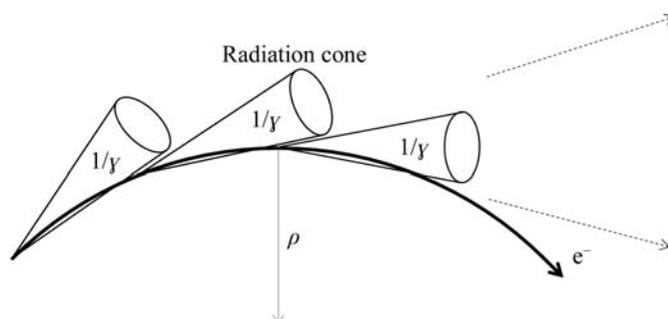
so the radius of curvature decreases with magnetic field strength and increases with machine energy *via* increased  $\gamma$ . With the electron energy expressed in GeV, this can be approximated to  $\rho \simeq 3.34 E_e [\text{GeV}]/B$  (where  $10^9/c \simeq 3.34$ ).

Synchrotron radiation is emitted in a forward cone tangential to the direction of the electrons' motion (Fig. 2.2.3) with a nominal Gaussian distribution and an opening angle of the order of  $1/\gamma$ . Thus the radiation is highly collimated in the vertical plane. In the horizontal plane, synchrotron radiation is emitted in a broad fan, tangential to the curved trajectory of the electrons as they sweep through the bending magnet. Only a fraction of the radiation emitted by a bending magnet enters the associated beamline *via* a cooled aperture defining a horizontal acceptance angle of a few mrad. The radiation is polarized in the plane of the synchrotron orbit. Sometimes, more than one beamline can be built on a bending magnet with a suitable angular separation between them.

Photons are emitted over a broad spectral range. The critical photon energy,  $\varepsilon_c$ , divides the emitted power into equal halves and is given by

$$\varepsilon_c = \frac{3\hbar c \gamma^3}{2\rho} = \frac{3\hbar \gamma^2 e B}{2m_e} = \frac{3\hbar e E_e^2 B}{2m_e^3 c^4} = 4.151 E_e^2 B,$$

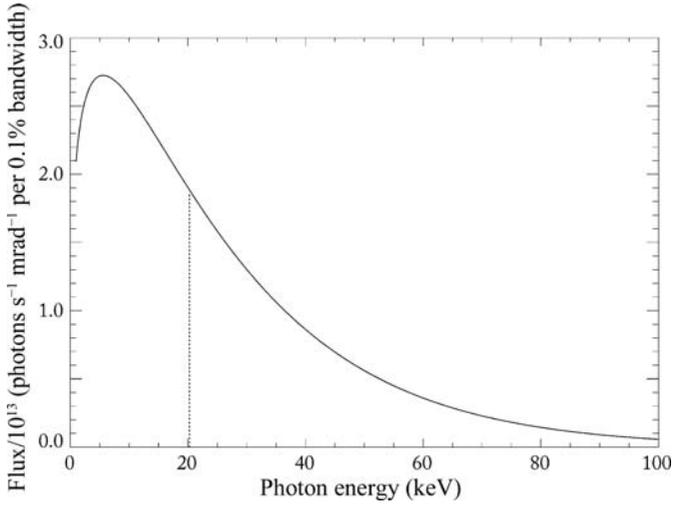
or, with photon and electron energies in keV and GeV, respectively,



**Figure 2.2.3**

Synchrotron radiation is emitted in a cone of opening angle of the order of  $1/\gamma$  tangential to the electrons as they follow a curved trajectory through the bending magnet.

## 2.2. SYNCHROTRON RADIATION



**Figure 2.2.4**

Spectrum of a bending magnet ( $B = 0.85$  T) at the ESRF with an electron energy of 6 GeV ( $\gamma = 11\,742$ ), 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),

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

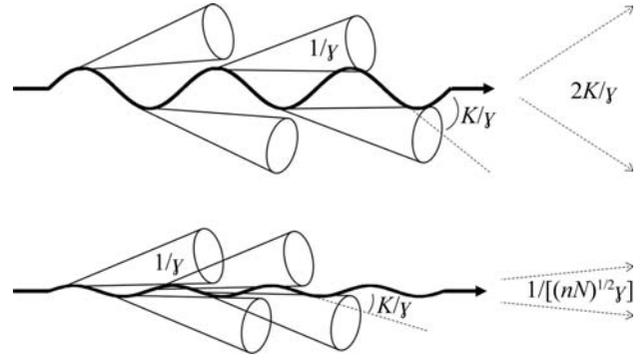
where  $\sigma_v(\varepsilon)$  is the standard deviation of the vertical-divergence distribution of photons of energy  $\varepsilon$ . For a population of electrons circulating in a storage ring, the distribution of the trajectories with respect to the plane of the orbit (of the order  $\mu\text{rad}$ ) 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  $\Psi_v$  in the vicinity of  $\varepsilon_c$ . 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  $\sim 100 \mu\text{rad}$ . 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  $\sim 60 \mu\text{rad}$ .

### 2.2.2.2. Insertion devices

Insertion devices can be classified into two main types, termed ‘wiguers’ 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



**Figure 2.2.5**

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

has a relatively short magnetic period and the radiation from sequential oscillations interferes coherently to give modified beam characteristics.

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  $\lambda_u$  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  $K/\gamma$ , 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  $\lambda_u$  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