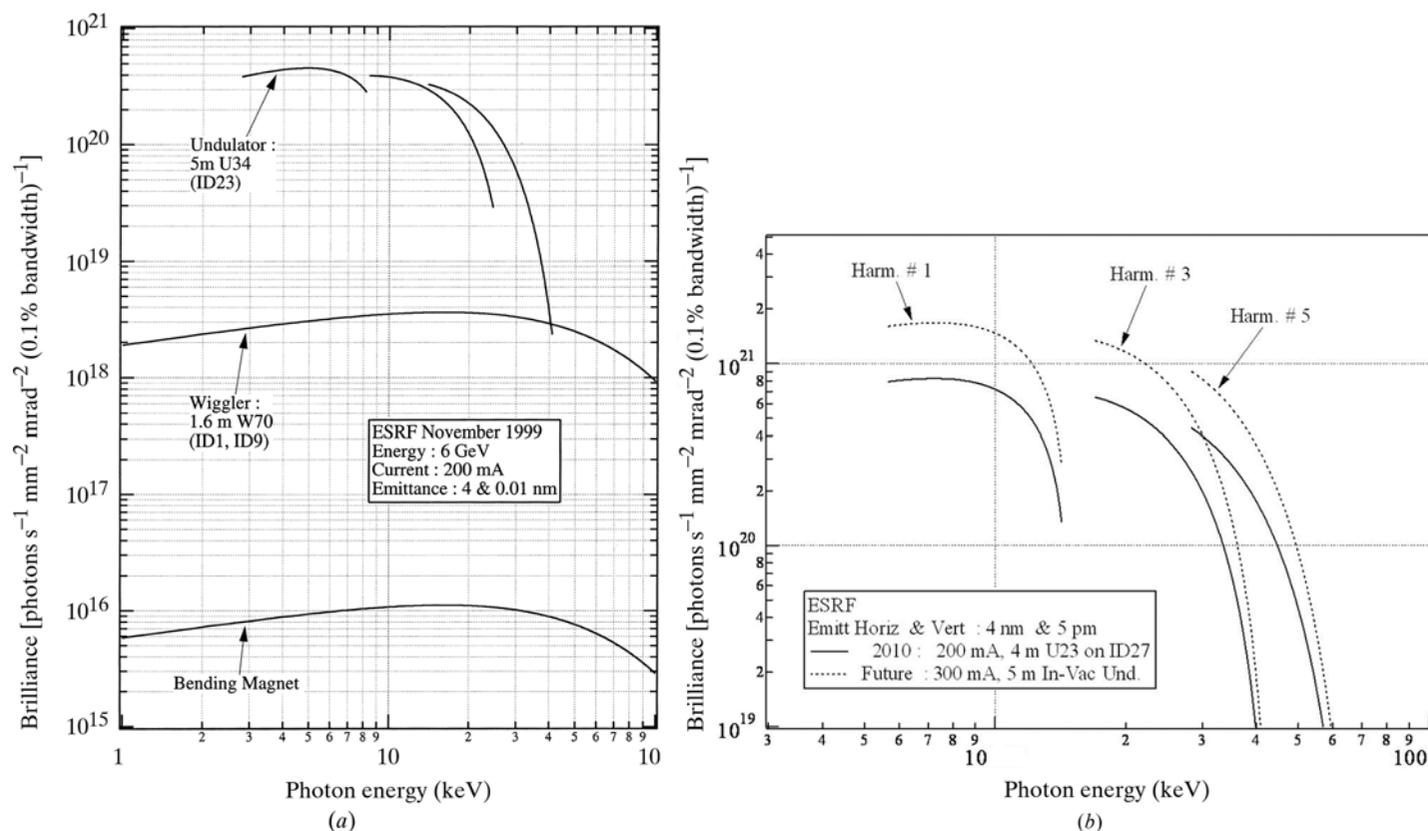


8. SYNCHROTRON CRYSTALLOGRAPHY

**Figure 8.1.2.2**

SR spectra. (a) Spectral brightness (also referred to as brilliance) of different SR source types (undulator, multipole wiggler and bending magnet) as exemplified by such types of sources at the ESRF. For the undulator, the tuning range (*i.e.* as the magnet gap is changed) is indicated. (b) Brilliance produced by the in-vacuum undulator of cell 27 of the ESRF dedicated to high-pressure studies. The plain curve corresponds to the condition in use as of September 2010. Further increase in brilliance (dotted curve) is expected in the years to come by increasing the ring current, increasing the length of the undulator and further decreasing the vertical emittance. Kindly provided by Dr Pascal Elleaume, ESRF, Grenoble, France.

units, are so ensconced in the field ‘that a drive to change this would only lead to more confusion rather than more clarity in the descriptions of synchrotron-radiation sources’. At the ESRF the term brilliance is firmly ensconced in house and with its large user community, and so is the label for the y axes used in Fig 8.1.2.2.

Another useful term is the machine emittance, ε . This is an invariant for a given machine lattice and electron/positron machine energy. It is the product of the divergence angle, σ' , and the source size, σ :

$$\varepsilon = \sigma\sigma'. \quad (8.1.2.2)$$

The horizontal and vertical emittances need to be considered separately.

The total radiated power, Q (kW), is expressed in terms of the machine energy, E (GeV), the radius of curvature of the orbiting electron/positron beam, ρ (m), and the circulating current, I (A), as

$$Q = 88.47E^4I/\rho. \quad (8.1.2.3)$$

The opening half-angle of the synchrotron radiation is $1/\gamma$ and is determined by the electron rest energy, mc^2 , and the machine energy, E :

$$\gamma^{-1} = mc^2/E. \quad (8.1.2.4)$$

The basic spectral distribution is characterized by the universal curve of synchrotron radiation, which is the number of photons per s per A per GeV per horizontal opening in mrad per 1% $\delta\lambda/\lambda$ integrated over the vertical opening angle, plotted versus λ/λ_c . Here the critical wavelength, λ_c (Å), is given by

$$\lambda_c = 5.59\rho/E^3, \quad (8.1.2.5)$$

again with ρ in m and E in GeV. Examples of SR spectral curves are shown in Fig. 8.1.2.2(a). The peak photon flux occurs close to λ_c , the useful flux extends to about $\lambda_c/10$, and exactly half of the total power radiated is above the critical wavelength and half is below this value.

In the plane of the orbit, the beam is essentially 100% plane polarized. This is what one would expect if the electron orbit was visualized edge-on. Away from the plane of the orbit there is a significant (several per cent) perpendicular component of polarization. Schiltz & Bricogne (2009) advocated definitions to use in the analysis of polarization-dependent phenomena that are instrument-independent and completely general. They have implemented these methods in the macromolecular phasing program *SHARP* for exploiting the polarization anisotropy of anomalous scattering in protein crystals.

8.1.3. Insertion devices (IDs)

These are multipole magnet devices placed (inserted) in straight sections of the synchrotron or storage ring. They can be designed to enhance specific characteristics of the SR, namely

- (1) to extend the spectral range to shorter wavelengths (wavelength shifter);
- (2) to increase the available intensity (multipole wiggler);
- (3) to increase the spectral brightness *via* interference and also yield a quasi-monochromatic beam (undulator) (Fig. 8.1.2.2b shows the distinctly different emission from an undulator);

8.1. SYNCHROTRON RADIATION

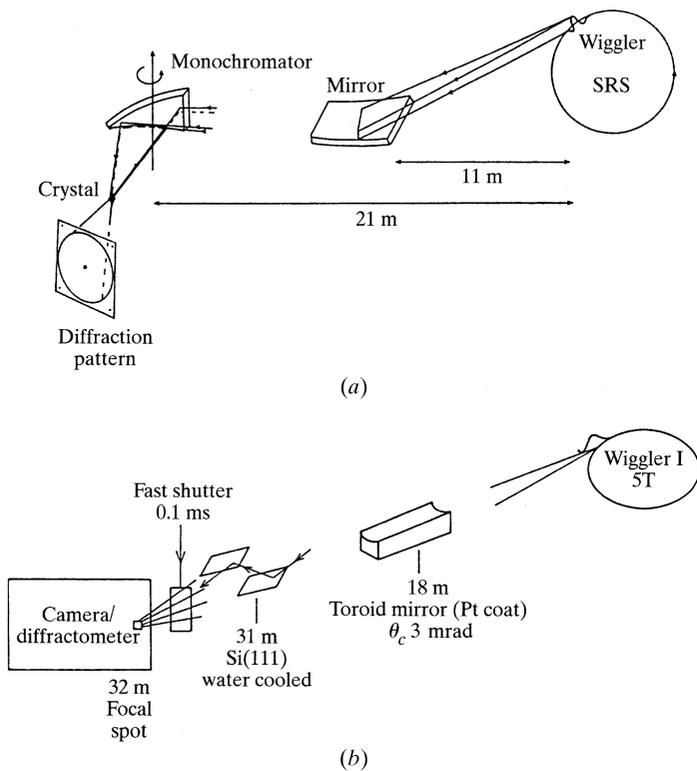


Figure 8.1.4.1 Common beamline optics modes. (a) Horizontally focusing cylindrical monochromator and vertical focusing mirror [shown here for station 9.6 as existed at the SRS (adapted from Helliwell *et al.*, 1986)]. (b) Rapidly tunable double-crystal monochromator and point-focusing toroid mirror [shown here as existed for station 9.5 at the SRS (adapted from Brammer *et al.*, 1988)].

(4) to provide a different polarization (*e.g.* to rotate the plane of polarization, to produce circularly polarized light *etc.*).

The classification of a periodic magnet ID as a wiggler or undulator is based on whether the angular deflection, δ , of the electron beam is small enough to allow radiation emitted from one pole to interfere directly with that from the next pole. In a wiggler, $\delta \gg \gamma^{-1}$, so the interference is negligible and the spectral emission (Fig. 8.1.2.2a) is very similar in shape to, but scaled up from, the universal curve (*i.e.* bending magnet spectral shape). In an undulator $\delta \leq \gamma^{-1}$ and the interference effects are highly significant (Fig. 8.1.2.2b). If the period of the ID is λ_u (cm), then the wavelengths λ_i (i integer) emitted are given by

$$\lambda_i = \frac{\lambda_u}{i2\gamma^2} \left(1 + \frac{K^2}{2} + \gamma^2\theta^2 \right), \quad (8.1.3.1)$$

where $K = \gamma\delta$.

The spectral width of each peak is

$$\Delta_i \simeq 1/iN, \quad (8.1.3.2)$$

where N is the number of poles. The angular deflection, δ , is changed by opening or closing the gap between the pole pieces.

8.1.4. Beam characteristics delivered at the crystal sample

The sample acceptance, α [equation (8.1.4.1)], is a quantity to which the synchrotron machine emittance [equation (8.1.2.2)] should be matched, *i.e.*,

$$\alpha = x\eta, \quad (8.1.4.1)$$

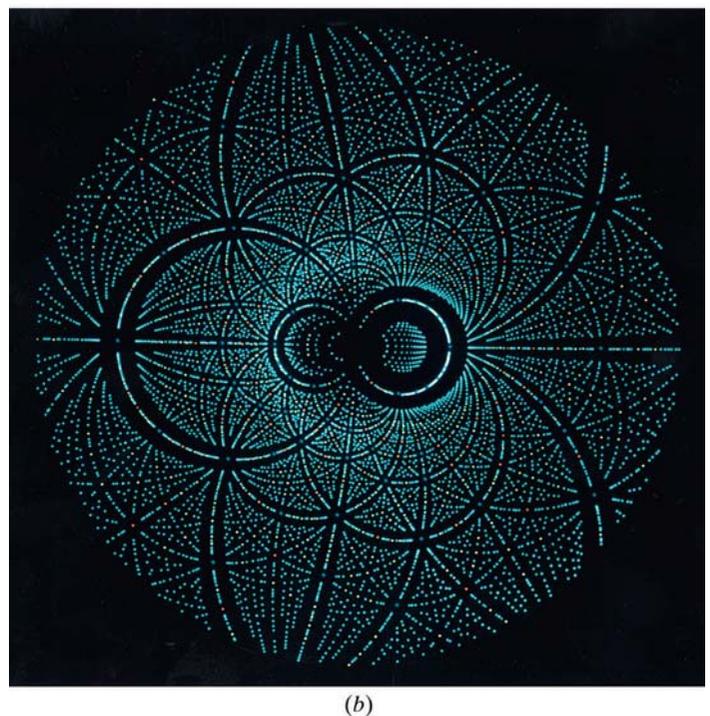
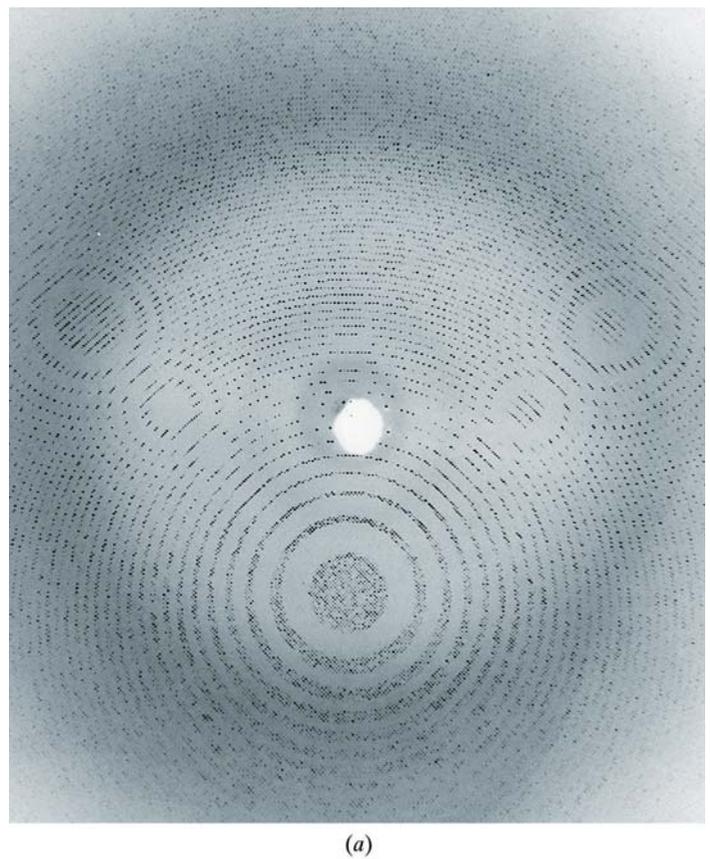


Figure 8.1.4.2 Single-crystal SR diffraction patterns. (a) Rhinovirus monochromatic oscillation photograph recorded at CHESS (Arnold *et al.* 1987; see also Rossmann & Erickson, 1983). (b) Prediction of a protein crystal Laue diffraction pattern (for an illuminating bandpass, without monochromator, $\sim 0.4 < \lambda < 2.6$ Å). The colour coding is according to the multiplicity of each spot: turquoise for singlet reflections, yellow for doublets, orange for triplets and blue for quartet or higher-multiplicity Laue spots (Cruickshank *et al.*, 1991).

where x is the sample size and η the mosaic spread. For example, if $x = 0.1$ mm and $\eta = 1$ mrad (0.057°), then $\alpha = 10^{-7}$ m rad or 100 nm rad.