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2.2. Synchrotron radiation and powder diffraction

A. Fitch

2.2.1. Introduction

X-rays produced at a synchrotron source are exploited in a wide range of applications in crystallography and structural science, and this includes studies by powder diffraction. Many synchrotron-radiation facilities have one or more dedicated powder-diffraction beamlines or end stations in regular user service. The high intensity, collimation and wavelength tunability of the radiation allow instruments to be designed whose performance and flexibility surpass what is possible with conventional laboratory apparatus. The majority of instruments operate with monochromatic radiation and an angle-dispersive diffractometer, but the polychromatic nature of synchrotron radiation means that an energy-dispersive setup is also possible. The general properties of synchrotron radiation include:

(*a*) High brightness, *i.e.* a highly collimated, intense X-ray beam and small source size.

(*b*) High flux of photons delivered to the sample.

(*c*) A range of wavelengths is available, possibly extending from the soft to the hard X-ray regimes, depending on the facility.

(*d*) Polarized source: synchrotron radiation is linearly polarized with the electric vector lying in the plane of the synchrotron orbit, but becomes progressively less polarized out of the plane.

(*e*) Pulsed source: the distribution of the bunches of electrons circulating in the storage ring allows the time structure to be exploited for specialized experiments.

Further information about the nature of synchrotron radiation can be found in texts by, for example, Margaritondo (1988), Als-Nielsen & McMorrow (2001) and Kim (2001).

Synchrotrons are usually user facilities, where scientists from external laboratories visit to perform experiments that have been approved by a peer-review or other procedure, and are supported by the scientific and technical staff for the beamlines. Most facilities have regular rounds in which users submit proposals for beam time, with special arrangements for access to carry out proprietary research. Arrangements can also usually be made for urgent access to the facility (when justified), and some beamlines run a routine mail-in service, allowing samples to be measured under defined conditions without the user needing to attend.

For any powder X-ray diffraction experiment, the wavelength of the radiation to be used is of high importance. The wavelength, λ, is a measure of the photon energy, ε, and the terms ‘photon energy’ and ‘wavelength’ tend to be used interchangeably at synchrotron beamlines. They can readily be converted by

$$\varepsilon = h\nu = hc/\lambda,$$

where h is the Planck constant, ν is the frequency of the radiation and c is the speed of light. If expressed in convenient units with λ in Å and ε in keV then

$$\varepsilon\ [\text{keV}] = hc/e\lambda \times 10^7\ [\text{Å}] \simeq 12.3984/\lambda\ [\text{Å}] \simeq 12.4/\lambda\ [\text{Å}],$$

where e is the elementary charge.

2.2.2. Production of synchrotron radiation

Synchrotron radiation is emitted by charged particles travelling at relativistic speeds when they are accelerated to move in a curved trajectory. In a modern synchrotron facility dedicated to the production of X-ray beams for scientific experiments, electrons are circulated in a closed horizontal orbit in a storage ring at an energy of several GeV, steered by magnetic fields from bending magnets. The overall circumference of the orbit can be several hundred metres depending on the design and specifications of an individual ring. The synchrotron ring is built up of cells (Fig. 2.2.1) comprising a straight section and a bending magnet by which the electrons are guided into the following straight section. Beamlines emerge tangentially from the bending magnets where synchrotron radiation is emitted by the electrons as they curve from one straight section into the next. Beamlines are also constructed on the straight sections where insertion devices, arrays of magnets providing an alternating magnetic field, are placed to cause the path of the electrons to oscillate and so also emit synchrotron radiation. By choosing the period of the magnetic array and by varying the strength of the magnetic field, the wavelength distribution and divergence of the X-rays emitted from an insertion device can be controlled. A straight section may accommodate more than one insertion device in series, allowing greater intensity or flexibility in the emitted radiation for the associated beamline. In the storage ring, the energy that the electrons lose by emitting synchrotron radiation is replaced by coupling the electrons to radio-frequency radiation supplied from klystrons or solid-state devices. Thus the synchrotron facility converts electrical energy, *via* radio waves and relativistic electrons, into powerful beams of electromagnetic radiation.

One key parameter of a storage ring is the energy of the circulating electrons. The energy of an electron moving with

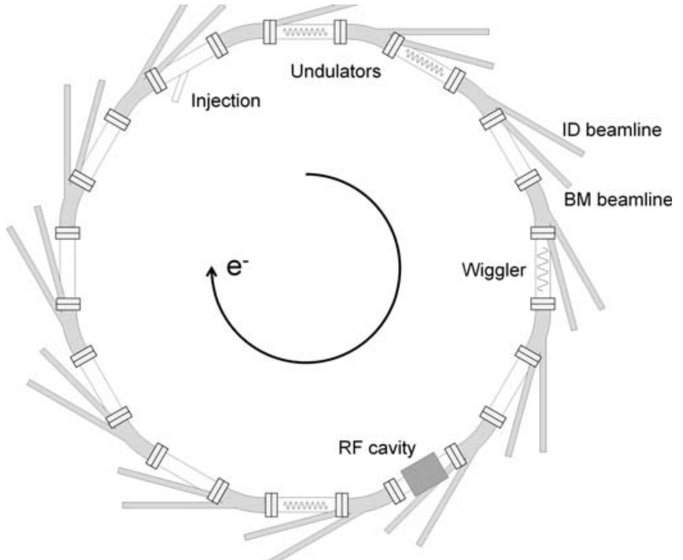

Figure 2.2.1
Schematic representation of a synchrotron storage ring with beamlines radiating tangentially from the bending magnets and in line with the straight sections. ID = insertion device, BM = bending magnet; RF = radio-frequency.