International Tables for Crystallography (2018). Vol. H, Section 2.3.3.4, pp. 77–80.

the pulses at long-pulse spallation neutron sources (Peters *et al.*, 2006).

As an initial case study, we consider the ISIS neutron facility, located in Oxfordshire, England, at the Rutherford Appleton Laboratory. This is a well established neutron spallation source supporting a strong programme of research using neutron beams. Of particular note are the excellent facilities for powder diffraction. First neutrons were delivered in 1984, but there have been upgrades since then, including the commissioning of a second target station in 2009. Fig. 2.3.10 is a schematic showing the layout of this facility. Some details about its operation are available on the ISIS web site, at https://www.isis.stfc.ac.uk/Pages/How-ISIS-works.aspx. Briefly, an ion source and radio-frequency quadrupole accelerator (not shown) inject bunches of negative hydrogen ions, H^-, into the linear accelerator where they are accelerated to 70 MeV. These are passed through aluminium foil, which strips them of their electrons, so they become protons, H^+, which are then accelerated to 800 MeV in the proton synchrotron. The protons, then travelling in two 100 ns bunches 230 ns apart, are kicked out of their synchrotron orbits and directed toward the targets. The whole process is repeated at a frequency of 50 Hz; the kickers are arranged to send one pulse in five to Target Station 2 (so that the pulse frequency there is just 10 Hz), and the remainder to Target Station 1. Both targets are made of tantalum-coated tungsten, as a stack of water-cooled plates in Target Station 1 and as a heavy-water surface-cooled cylinder in Target Station 2. As explained earlier, the fast neutrons produced in the spallation process must be moderated, and for this purpose moderators are located adjacent to the targets: two water moderators at 300 K, one liquid-methane moderator at 100 K and one liquid-hydrogen moderator at 20 K at Target Station 1; and one decoupled solid-methane moderator at 26 K and one coupled liquid-hydrogen/methane moderator at 26 K at Target Station 2. The widths of the pulses of the moderated neutrons are typically 30–50 µs, but 300 µs for the coupled moderator at Target Station 2. The target/moderator assemblies are surrounded, apart from beam exit ports, by beryllium reflectors. The schematic of Fig. 2.3.10 indicates the placement of the various neutron-beam instruments around the target stations.

The Swiss neutron spallation source, SINQ, located at the Paul Scherrer Institute in Villigen, is the only spallation source operating in continuous mode. SINQ reached full power in 1997. Since there is no time structure to be preserved, more generous quantities of moderator can be used; in fact the target, which becomes the source of neutrons, is located centrally in a moderator tank. The situation here is not very different from that in a medium-flux research reactor. The target comprises lead rods in Zircaloy tubes, the moderator is heavy water and there is a light-water reflector outside the moderator tank. Protons accelerated first by a Cockroft–Walton accelerator, then to 72 MeV by an injector cyclotron, and finally to 590 MeV in a proton ring cyclotron are directed onto the target from below (Fig. 2.3.11). The proton current is initially 2.4 mA, but this is reduced in muon production, so that only about 1.65 mA reaches the spallation target. The power is thus close to 1.0 MW. A horizontal insert in the moderator tank houses a liquid-deuterium cold source at 25 K.

As a final example we describe the 5 MW long-pulse European Spallation Source, now under construction in Lund, Sweden (see Fig. 2.3.12). A more detailed description is available at the ESS web site, https://europeanspallationsource.se/technology. The proton-acceleration system, although comprising a number of different components, will be linear. The protons from the ion source will be accelerated through a radio-frequency quadrupole and drift tube LINAC up to 90 MeV, then through a series of superconducting cavities up to the final energy of 2 GeV. This system will deliver proton pulses of 2.86 ms duration at a 14 Hz repetition rate; the average current will be 6.26 mA and hence the total power 5 MW. The target material will be helium-cooled tungsten encased in stainless steel, in the form of a 2.5 m-diameter rotating wheel. Such an arrangement assists in dissipation of the heat deposited in the target. Coupled liquid-hydrogen moderators will be located above and below the rotating wheel, and this assembly will be partially surrounded by a water pre-moderator and beryllium reflector. Neutron choppers will be used to shape the neutron pulses as required, and neutron optical systems will deliver neutrons to the experiments. First beam on target is expected in 2019.

Characteristics of these and other neutron spallation sources are recorded in Table 2.3.4. The information included there has been taken from the respective facility web sites.

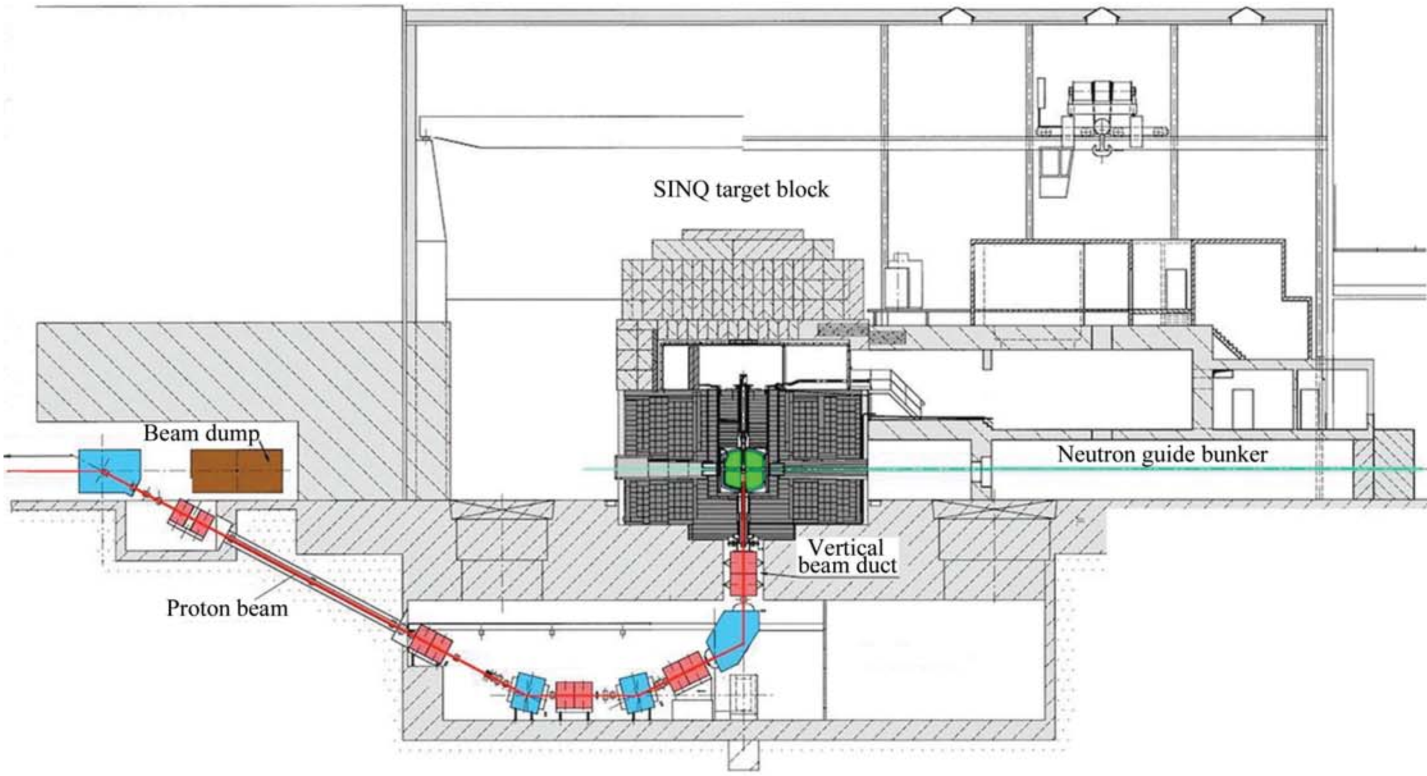
2.3.3.4. *Neutron beam tubes and guides*

Ideally, neutron diffractometers should be designed following a holistic approach, designing the source of moderated neutrons, through the delivery system, to the instrument itself. This is not often possible in practice; for example the source must often be taken as a given, and in some cases the delivery of the neutrons as well. The holistic approach is commonly a very large Monte Carlo simulation, not suitable for purposes of description; in this chapter, therefore, we provide separate descriptions of these different components.

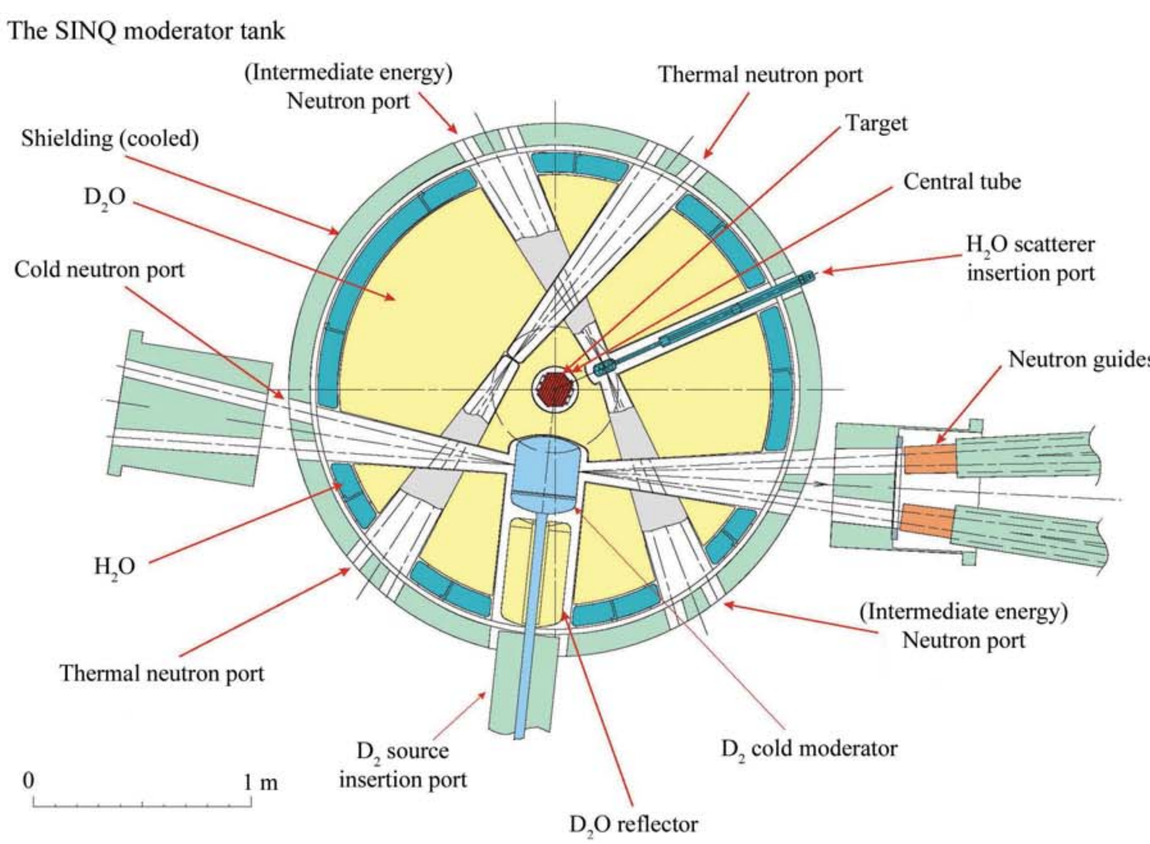
The simplest delivery system is a neutron beam tube or collimator. A collimator could comprise just two pinholes of diameters a_1 and a_2 cut into neutron-absorbing material, and placed at a distance L apart; this limits the divergence of the beam to (full angle) $2\alpha = (a_1 + a_2)/L$. It is of course possible to use apertures of different cross section, for example rectangular slits, if the divergence must be smaller in one direction than another.

Neutron guides are now widely used at both reactor and spallation neutron sources. These are able to transport neutrons over distances ranging to 100 m or more. They are evacuated tubes, normally of rectangular cross section, and transmission depends on the reflection of glancing-angle neutrons from the walls of the guide. The guides are constructed from glass plates with a reflective coating deposited on the internal surfaces.

Initially, total external reflection (Section 2.3.2.3) provided the basis for reflection; the coating was nickel, or preferably ^{58}Ni. Given that nickel has a face-centred cubic structure (4 atoms per unit cell) with lattice parameter 3.524 Å, and taking the scattering lengths from Table 2.3.2, we find from equation (2.3.6) that the critical glancing angles per unit wavelength for total external reflection are 0.10° Å^{-1} and 0.12° Å^{-1} for nickel and ^{58}Ni, respectively. Taking wavelengths of 0.4, 1.2 and 5 Å as representative of hot, thermal and cold neutrons, respectively (*cf.* Fig. 2.3.5), these angles for a nickel mirror are just 0.04, 0.12 and 0.5°. Consequently, these guides are most useful for transmitting cold neutrons and are moderately useful for thermal neutrons, but are not used for hot neutrons. The small glancing angles are demanding, not only on the precision of manufacture, but also because it is highly desirable to use a curved guide tube so there is no direct line of sight to the source (as in Fig. 2.3.13); this is a way of preventing fast neutrons and γ-radiation from impacting on the experiment. The guide tube still transmits a range of wave-



(*a*)



(*b*)

Figure 2.3.11
Layout at the SINQ neutron source. (*a*) Elevation: the target is located in the moderator tank, the high-energy protons being delivered from below. (*b*) Plan: showing the location of guide tubes relative to this central target. (Courtesy: Dr Bertrand Blau, Paul Scherrer Insitut.)

lengths, although only the longest wavelengths can travel by the zig-zag path indicated in Fig. 2.3.13. If the guide width is a, and its radius of curvature ρ (see Fig. 2.3.13), then the minimum length to avoid direct transmission is $(8a\rho)^{1/2}$. Critical to the transmission of a guide tube is the angle θ^*, which is the minimum glancing angle of incidence onto the outer surface that permits subsequent reflection from the inner surface, and is given by $\theta^* = (2a/\rho)^{1/2}$. The shortest wavelength, then, that can be transmitted involving reflection from the inner surface is given by [*cf.* equation (2.3.6)]

Table 2.3.4
Details of selected spallation neutron sources

Source	Type	Location	Proton energy	Current	Average power	Target(s)	Repetition rate (Hz)	Moderator(s)
CSNS†	Short pulse	Institute of High Energy Physics, Guangdong, China	1.6 GeV	62.5 μA	100 kW	Tungsten	25	Water, 2 × liquid hydrogen
ESS†	Long pulse	European Spallation Source, Lund, Sweden	2 GeV	2.5 mA	5 MW	Tungsten wheel (helium cooled)	14	2 × Liquid hydrogen (pancake geometry)
ISIS	Short pulse	Rutherford Appleton Laboratory, Oxfordshire, UK	800 MeV	200 μA	160 kW	2 × Tungsten	50	2 × Water, liquid methane, liquid hydrogen
							10	Hydrogen/methane, solid methane at 26 K
JSNS‡	Short pulse	J-Parc Centre, Tokai-mura, Japan	3 GeV	333 μA	1 MW	Liquid mercury	25	Supercritical hydrogen
LANSCE	Long pulse	Los Alamos National Laboratory, Los Alamos, USA	800 MeV	125 μA	100 kW	Tungsten	20	Water, 2 × liquid hydrogen
SINQ	Continuous	Paul Scherrer Institute, Villigen, Switzerland	590 MeV	1.64 mA§	0.97 MW	Lead	—	Heavy water; cold source: liquid deuterium at 20 K
SNS	Short pulse	Oak Ridge National Laboratory, Oak Ridge, USA	1 GeV	1.4 mA	1.4 MW	Liquid mercury	60	2 × Water, 2 × liquid hydrogen

† Under construction. ‡ Currently operating at <0.5 MW. § Current reaching spallation target after attenuation in muon source.

Figure 2.3.12
Schematic diagram of the ESS facility. The proton beam enters at the right, strikes the target and liberates neutrons for instruments in the three neutron experiment halls. (Image courtesy of the ESS.)

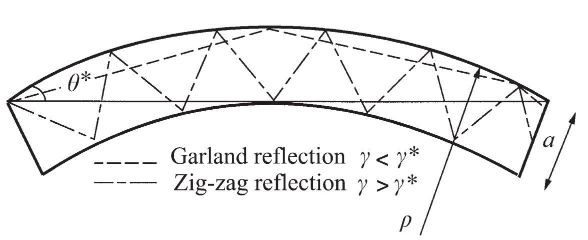


Figure 2.3.13
Plan of a curved neutron guide, indicating different possible neutron paths, labelled 'garland' and 'zig-zag'. Only the longer-wavelength neutrons can travel the zig-zag path because the glancing angles on this path (which must be less than the critical angle) are greater. In this schematic, the glancing angles, the width and the curvature have all been exaggerated. [From Section 4.4.2 of Volume C (Anderson & Schärpf, 2006).]

$$\lambda^* = \theta^* \left(\frac{\pi}{N b_{\rm coh}} \right)^{1/2}. \qquad (2.3.12)$$

This is known as the 'characteristic' wavelength of the guide [see Section 4.4.2 of Volume C by Anderson & Schärpf (2006)]; the majority of transmitted neutrons will have longer wavelengths than this.

The desire to use guides for shorter (*e.g.* thermal-neutron) wavelengths, and for retaining more neutrons at a given wavelength, has motivated the development of mirrors capable of reflecting neutrons incident at greater glancing angle. The earliest such mirrors were in fact monochromating mirrors obtained by laying down alternate layers of metals with contrasting coherent-scattering-length densities (Fig. 2.3.14). For a bilayer thickness d and angle of incidence θ these would select wavelengths according to Bragg's law [equation (1.1.3)],

$$\lambda = 2d \sin(\theta).$$

In an early implementation (Schoenborn *et al.*, 1974), the metals were Ge and Mn (which have coherent scattering lengths opposite in sign) and the bilayer thickness was of the order of 100 Å; this is a larger d-spacing giving access to longer wave-

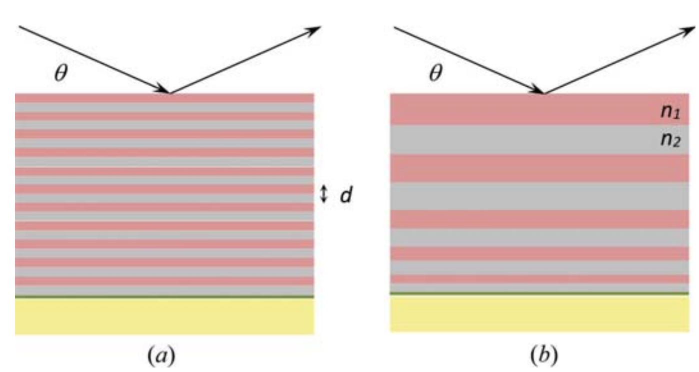


Figure 2.3.14
Schematic diagrams of (*a*) a multilayer monochromator and (*b*) a neutron supermirror.

lengths than would be accessible with the usual crystal monochromator (Section 2.3.4.1.2). The idea of supermirrors, comprising bilayers of graduated thickness, and in effect increasing the critical angle, was suggested by Turchin (1967) and Mezei (1976). For a perhaps simplistic explanation, we note first that since the bilayer dimension d is large compared with the neutron wavelength, we can approximate the above equation for reflection as

$$\theta \simeq \lambda \frac{1}{2d},$$

in which form it is reminiscent of equation (2.3.6). If we take $d_{\min}$ to be the thickness of the thinnest bilayer, then we can propose that the critical angle for reflection by the supermirror should be

$$\theta_c^{\rm SM} \simeq \lambda \frac{1}{2d_{\min}}. \qquad (2.3.13)$$

In order to ensure that all neutrons incident at angles less than this critical angle should be reflected, we need to incorporate a more-or-less continuous range of thicker bilayers into the supermirror (Fig. 2.3.14*b*). A more rigorous treatment (Hayter & Mook, 1989; Masalovich, 2013) takes account of the transmission and reflection at each interface, and lays down a prescription as to how the thicknesses should be varied. The most common pairing for the bilayer is now Ni with Ti; the coherent scattering cross sections are of opposite sign (see Table 2.3.2). The performance of a supermirror is normally quoted as the ratio m of the critical angle for the supermirror, $\theta_c^{\rm SM}$, to that for natural nickel, $\theta_c^{\rm Ni}$; a high value for reflectivity is also important. Supermirrors to m of 2 or 3 are in quite common use, while now Ni/Ti supermirrors with m up to 7 are offered for purchase (Swiss Neutronics AG; see also Maruyama *et al.*, 2007).

Consideration is currently being given to the variation of the cross section of the guide along its length. There is some loss on reflection by supermirrors, so these studies aim to reduce the number of reflections involved in transmission along the guide. One suggestion (also attributable to Mezei, 1997) is to use a 'ballistic guide', in which neutrons from the source travel through a taper of widening cross section into a length of larger guide, then through a taper of narrowing cross section to restore the original cross section at the exit. This is said to reduce the number of reflections suffered by the neutron by a factor of $(w_0/w)^2$, where w_0 is the width at entrance and exit and w the larger width along the main part of the guide (Häse *et al.*, 2002). Such a guide has been installed and is operating successfully on the vertical cold source at the Institut Laue–Langevin (Abele *et al.*, 2006). An extension of this idea is based on the well known property of ellipses that a ray emanating from one focus is reflected (just one bounce) to pass through the other; so if the guide cross section could be varied to give a very long ellipse, a source of neutrons placed at one focus, and the target point at the other, then perhaps the neutrons could be transmitted along the guide with just a single reflection (Schanzer *et al.*, 2004; Rodriguez *et al.*, 2011). Accordingly a number of neutron facilities have installed elliptical guides, and indeed a number of neutron powder diffractometers now are located on elliptical guides; these include diffractometer POWTEX at FRM-II, the high-resolution diffractometers HRPD and WISH at ISIS, and Super-HRPD at JSNS. Computer simulation by Cussen *et al.* (2013), however, questions whether, given the practicalities of finite source sizes and the approximation of elliptical variation by a number of linear segments, the theoretical improvement is fully realized.

2.3.4. Diffractometers

Put simply, the diffracted neutron beams associated with the different d-spacings in the sample under study satisfy Bragg's law,

$$\lambda = 2d\sin(\theta). \qquad (2.3.14)$$

As always, λ is the wavelength of the incident neutrons, and these neutrons are scattered through an angle 2θ.

There are basically two ways of exploiting this relationship. The first is to use a single wavelength for the investigation, in which case diffracted neutrons are observed at different angles 2θ corresponding to different d-spacings in the sample. A neutron powder diffractometer designed to carry out an investigation by this means we choose to call a 'constant wavelength' (CW) diffractometer. The other means is to fix the angle 2θ, illuminate the specimen with a range of wavelengths, and note the different wavelengths that are diffracted. In this case, we determine the wavelengths of the diffracted neutrons *via* their speed $\lambda = h/(mv)$ [equation (2.3.1)], and that in turn is measured by their flight time t over a path of length L, $v = L/t$; this leads to

$$\lambda = \frac{ht}{mL}. \qquad (2.3.15)$$

A diffractometer designed to carry out such an analysis of wavelengths we call a 'time-of-flight (TOF) diffractometer'.

The distinction between these two modes of operation can also be indicated *via* the Ewald construction in reciprocal space (Section 1.1.2.4). In this, the ideal powder is represented by concentric spheres in reciprocal space. In the constant-wavelength situation, the primary beam is fixed in direction and the Ewald sphere has a fixed radius; diffracted (reflected) beams are observed at any angle at which the surface of the Ewald sphere intersects one of the concentric spheres mentioned just above. In the wavelength-analysis (time-of-flight) situation, the directions of the primary and diffracted beams are fixed, but the radius of the Ewald sphere ($1/\lambda$) is variable through a range; diffracted beams are observed whenever the wavelength is such that the tip of the vector representing the reflected beam lies on one of the concentric spheres.

2.3.4.1. *Constant-wavelength neutron diffractometers*

The salient features of a constant-wavelength diffractometer are perhaps most easily explained by reference to a particular example; for this purpose we consider the High Resolution Powder diffractometer for Thermal neutrons (HRPT) installed at the SINQ continuous spallation source (Fischer *et al.*, 2000). Neutrons from the source travel through a guide tube to the crystal monochromator, which directs neutrons of a selected wavelength toward the sample. The diffracted neutrons are registered in a detector or detectors that cover a range of angles of scattering from the sample. Collimation is used to better define the directions of the neutron beams; in this instance a primary collimator is included in the guide tube and additional collimation is included between the sample and the position-sensitive detector. The various components will be described in more detail below.

2.3.4.1.1. *Collimation*

There need to be restrictions on the angular divergences of the neutron beams. The divergence of the beam impinging upon the crystal monochromator must be limited to better define the wavelength of the neutrons directed to the sample, whereas the divergences of the beams incident upon and diffracted from