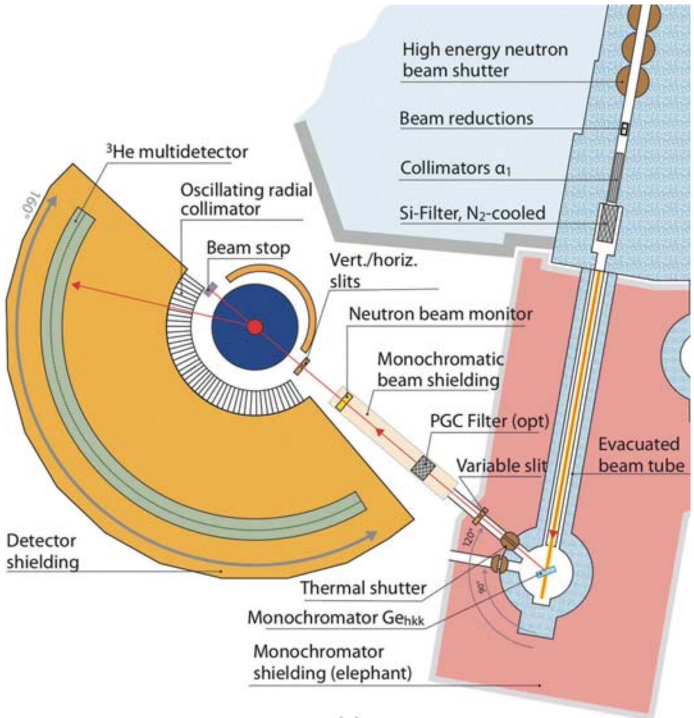

(*a*)

(*b*)

Figure 2.3.15
A constant-wavelength neutron powder diffractometer. This figure shows (*a*) a layout diagram and (*b*) the physical appearance (dominated by the monochromator and detector shieldings) for the HRPT diffractometer installed at the SINQ continuous spallation source. (Figures from https://www.psi.ch/sinq/hrpt/.)

the sample will control the precision with which the scattering angle 2θ can be determined. For a diffractometer detecting neutrons and measuring scattering angles in the horizontal plane (as shown in Fig. 2.3.15) the horizontal divergences are critical, the vertical divergences less so.[11] Indeed, the horizontal divergences are key parameters in the determination of resolution and intensity (Section 2.3.4.1.4); for this reason we denote by α_1, α_2 and α_3 the (half-angle) angular divergences of the primary beam (*i.e.* the beam onto the monochromator), the monochromatic beam (from monochromator to sample) and the diffracted beam (from sample to detector), respectively.

[11] For this reason large vertical divergences are employed to increase intensity; they do however have second-order impacts on the shapes (asymmetry) and positions of diffraction peaks (Howard, 1982; Finger *et al.*, 1994; see also Section 4.2 in Kisi & Howard, 2008).

The divergences are limited by various forms of collimation. The divergence of the primary beam will be limited in the first instance by the delivery system. For delivery through a simple beam tube of length L, with entrance and exit apertures of dimensions a_1 and a_2, respectively, the angular divergence (half-angle) is given by (as already noted in Section 2.3.3.4)

$$\alpha_1 = \frac{a_1 + a_2}{2L}. \qquad (2.3.16)$$

Neutrons emerging from a guide tube would have divergence equal to the critical angle of the guide, $\alpha_1 = \theta_c$. Soller collimators (see below) can be used if there is a need to further reduce the horizontal divergence of the primary beam. The divergence of the monochromatic beam may be limited by slits, or a beam tube. The divergence of the diffracted beam, α_3, is often defined using another Soller collimator. Sometimes this divergence is limited just by the dimensions of the sample and the detecting elements; equation (2.3.16) gives α_3 if it now references the sample and detector element dimensions and the distance between them. Even in this circumstance (as in HRPT), Soller collimators may be used in front of the detector to reduce scattering from ancillary equipment and other background contributions.

Soller collimators (Soller, 1924) are used to transmit beams of large cross section while limiting (for example) horizontal divergence. They are in effect narrow but tall rectangular collimators stacked side by side; in practice they comprise thin neutron-absorbing blades equally spaced in a mounting box. It should be evident from equation (2.3.16) that if the length of the collimator is L and the separation between the blades is a, then the (half-angle) horizontal divergence is a/L. The transmission function for a Soller collimator is ideally triangular. It is technologically challenging to make compact Soller collimators, since, for a given collimation, a shorter collimator needs a smaller blade spacing. One very successful approach, due to Carlile *et al.* (1977), has been to make the neutron-absorbing blades from Mylar, stretched on thin steel or aluminium alloy frames, and subsequently coated with gadolinium oxide paint; these blades are stacked and connected *via* the frames which become the spacers in the final product. The collimators made by Carlile *et al.* were 34 cm long, and the blade spacing was 1 mm, giving a horizontal divergence of 0.17°. Compact Soller collimators of this type (Fig. 2.3.16) are now commercially available, with blade spacings down to 0.5 mm.

Even more compact collimators can be produced by eliminating the gaps in favour of solid layers of neutron-transmitting material; for example, a collimator only 2.75 cm long made by stacking 0.16 mm thick gadolinium-coated silicon wafers gave a divergence of 0.33° (Cussen *et al.*, 2001). Microchannel plates (Wilkins *et al.*, 1989) may offer additional possibilities for collimation and focusing.

2.3.4.1.2. *Monochromators*

The wavelength in a constant-wavelength powder diffractometer is almost invariably selected by a single-crystal monochromator. If the primary beam is incident onto the monochromator in such a way as to make an angle θ_M with a chosen set of planes in the crystal, then the wavelength that will be reflected from these planes is given by Bragg's law,

$$\lambda = 2d\sin(\theta_M),$$

where d is the spacing of the chosen planes. A spread of angles of incidence represented by $\Delta\theta_M$ will result in the selection of a

references