noted that the substantial neutron shielding surrounding the detector chamber (known as the blockhouse) is not shown.

2.3.4.2.1. *Instrument resolution and design*

In a TOF instrument, all of the incident spectrum of neutron wavelengths is utilized, appropriately trimmed by the chopper system as previously described. The different wavelengths (λ) are identified through their time-of-flight (t) according to equation (2.3.15). Substituting that equation into Bragg's law, we obtain

$$\begin{aligned} d_{hkl} &= \frac{ht}{2mL\sin\theta} \\ &= \frac{t}{505.554L\sin\theta} \end{aligned} \quad (2.3.20)$$

for t in microseconds, d in ångstroms and L in metres.

The resolution of a TOF diffractometer is defined by the uncertainty in the d-spacing (Δd) relative to its absolute value d. Apparent as the width of the diffraction peaks, the resolution is given primarily by (Buras & Holas, 1968; Worlton *et al.*, 1976)

$$\frac{\Delta d}{d} = \left[\Delta\theta^2 \cot^2\theta + \left(\frac{\Delta t}{t}\right)^2 + \left(\frac{\Delta L}{L}\right)^2\right]^{1/2}. \quad (2.3.21)$$

There are a number of important things to note concerning this equation:

(i) The terms $\Delta\theta\cot\theta$ and $\Delta L/L$ are fixed and independent of flight time once the diffractometer is constructed; in addition, as we have already noted (Section 2.3.3.3), for a spallation source with a suitably poisoned moderator the time resolution $\Delta t/t$ is practically constant. Thus the resolution of a TOF diffraction pattern is virtually constant across the entire range of d-spacing explored in a given detector bank.[17]

(ii) Uncertainties in the neutron path length, ΔL, can arise due to measurement uncertainty in determining L; however, these are usually overshadowed by the uncertainty that arises because neutrons can emerge into the neutron guide from any position within the finite-sized moderator and this uncertainty constitutes the major contribution to ΔL.

(iii) As ΔL is a constant, a linear improvement in resolution can be achieved merely by making the instrument longer, such as HRPD at ISIS and S-HRPD at J-PARC, which are almost 100 m long.

(iv) The contribution of the diffraction angle 2θ to resolution is considerable. For a fixed angular uncertainty (detector positioning and finite width) the $\cot\theta$ term varies from infinite at $2\theta = 0$ to zero at $2\theta = 180°$. Therefore, the higher the detector angle, the better the resolution.

With these matters considered, we can return to our example of a modern TOF diffractometer in Fig. 2.3.18 and in particular the arrangement of the detectors. The strategy employed is to group multiple individual detector elements into a number of discrete banks. It may be seen from equation (2.3.21) that decreasing 2θ and increasing L have opposing effects on resolution. By appropriate manipulation of the equation and by expressing the overall neutron flight path as $L = L_1 + L_2$ where L_1 is the moderator-to-sample distance and L_2 is that from the sample to the detector, it is straightforward to obtain

$$L_2 = \Delta L\left[\left(\frac{\Delta d}{d}\right)^2 - \left(\frac{\Delta\theta}{\tan\theta}\right)^2 - \left(\frac{\Delta t}{t}\right)^2\right]^{-1/2} - L_1. \quad (2.3.22)$$

Therefore by adjusting 2θ and L_2 correctly, it is possible to construct banks of detectors covering a range of 2θ, for which the resolution is identical. This allows neutrons recorded in the entire detector bank to be 'focused' into a single diffraction pattern. The resulting curved detector arrangement is obvious in the high-resolution detector bank labelled 5 and 6 in Fig. 2.3.18(*a*). For a fixed (small) value of $\Delta d/d$, eventually space limitations impose restrictions on L_2 and a new, lower-resolution detector bank (4) commences. As the benefits of a curved arrangement become insignificant, the appropriate curve is approximated by a straight arrangement in the lower-angle banks and dispensed with altogether in the very low angle bank. In Fig. 2.3.18 the backscattering (5, 6), 90° (4), two separate low-angle (2 & 3) and the very low angle (1) detector banks of POLARIS are identified. These have average 2θ angles of 146.72, 92.59, 52.21, 25.99 and 10.40°, respectively.

Raw diffraction patterns recorded in the various detector banks are compared in Fig. 2.3.19. Note that the curved background due to the incident spectrum is flattened when the patterns are normalized. A logarithmic scale is necessary to display the very wide range of d-spacings accessible across the whole instrument and this scale emphasises the near-constant resolution across each pattern. In keeping with equations (2.3.21) and (2.3.20), the effects of changing the detector angle are obviously greater resolution and access to shorter d-spacings as 2θ increases. Each detector bank can provide data for a different purpose according to its resolution and d-spacing coverage. For example, the combination of good resolution (4×10^{-3}) and a wide range of d-spacing (0.2–2.7 Å) makes data from the backscattering bank (Fig. 2.3.19*e*) ideal for the refinement of medium- to large-scale crystal structures. The 90° bank (Fig. 2.3.19*d*) is optimized for use with complex sample environments such as high-pressure cells or reaction vessels, as this geometry combined with appropriate collimation of the incident and scattered neutron beams enables diffraction patterns to be collected that only contain Bragg reflections from the sample being studied. It can be used to obtain good-resolution data (7×10^{-3}) during a variety of *in situ* studies. The low-angle and very low angle banks with their access to very large d-spacings up to 20 Å are invaluable in determining unknown crystal structures and complex magnetic structures by allowing the indexing of low-index reflections and determining reflection conditions.

In order to reduce unwanted background counts and give better localization of the diffraction pattern from the sample, *i.e.* to better exclude sample environments such as cryostats or furnaces, the instrument is fitted with a radial collimator surrounding the sample position.[18] For more common sample environments, *e.g.* furnaces, this collimation allows all detector banks to view the sample unimpeded. The detector banks are contained within the large vacuum vessel shown in Fig. 2.3.18(*b*). This reduces attenuation and background due to scattering by air. The detector coverage on such an instrument is very large, in the case of POLARIS up to 45% of the available solid angle is covered. A full description of this instrument may be found in Smith *et al.* (2018).

[17] A small effect due to a time-dependent component of $\Delta t/t$ might be observed depending on the source and instrument configuration.

[18] Although typically constructed from planar vanes which are oscillated to average their shadow across all the detectors, the POLARIS collimator vanes are stationary, and are conical to follow the Debye–Scherrer cones of the diffracted neutrons.