time distribution. With the elimination of all liners and poisons, a fully coupled system is obtained with a flux gain of about 6 × but with poorer wavelength resolution. The wavelength distribution at a given distance from the moderator is shown in Fig. 6.2.2.3(*a*) for the fully decoupled case and in Fig. 6.2.2.3(*b*) for the fully coupled case. For a decoupled moderator, the slowing-down power of the reflector is not as critical as it is for the coupled one. In the coupled moderator, it is beneficial to use a thermal reflector in the volume immediately surrounding the moderator because this enhances the peak thermal neutron flux. The decay constant of the neutron pulse can be tailored to match the diffractometer resolution by using a composite reflector composed of an inner thermal reflector and an outer fast reflector. The outer reflector can have a moderate thermal neutron absorption cross section, or the inner reflector can be decoupled from the outer reflector in the same manner that a moderator is decoupled from a reflector. The decay constant can then be varied by simply adjusting the size of the inner reflector (Russell *et al.*, 1996). The wavelength or energy distribution of thermal neutrons produced in the moderator is dependent on the temperature of the moderating medium, as described in Section 6.2.1.2.

For neutron protein crystallography, a moderator with an intermediate temperature between a cold and thermal moderator would be most appropriate. This can be achieved with a composite moderator composed of a thermal and a cold moderator in a symbiotic configuration, or a cold methane system.

6.2.2.3. *Beamline optics*

A chosen wavelength band (say, 1 to 6 Å) is selected by the use of rotating disks (called choppers) composed of neutron absorbing and transparent material. These choppers are synchronized to the proton pulse. The T0 chopper can open the beam a short time after the impact of the proton pulse and stop the high- and intermediate-energy radiation from reaching the sample and the detector. The T1 chopper can select the long-wavelength edge and prevent frame overlap. Since the T0 chopper is designed to stop the initial γ and high-energy neutron radiation, it is usually made of thick (30 cm) blades of Ni, while the T1 chopper is simpler in construction since it is designed to stop only thermal neutrons.

The flight-path lengths of relevant spallation neutron instruments are quite long; the Los Alamos Spallation Neutron Source has a 28 m path length for its protein crystallography station on a partially decoupled moderator. For a fully decoupled system, a flight-path length of 10 m would provide adequate energy resolution.

For protein crystallography, a beam divergence matched to the mosaicity of the crystal provides the best peak-to-background ratio. For such cases, a beam divergence of $\pm 0.1°$ can be achieved using circular collimating disks of Boral or Boron-Poly to form a cone that views most of the moderator (typically 12×12 cm) and channels the neutron beam onto the detector with a final aperture of millimetre dimensions. Another approach uses focusing mirrors, and calculations show that toroidal geometry will produce a gain in intensity of 1.5 to 2 times, depending on flight distance and beam divergence (Schoenborn, 1992*a*).

6.2.2.4. *Time-of-flight techniques*

Because of the time structure inherent at a spallation source, diffraction experiments are carried out as a function of time and use a large part of the neutron energy spectrum. For protein crystallography, this wavelength range might cover from 1 to 5 Å, depending on the unit-cell size and the moderator used. This is particularly advantageous and allows the collection of data in a quasi-Laue fashion (Schoenborn, 1992*a*) without the drawback of spot overlap normally encountered in Laue patterns. Data are collected in a stroboscopic fashion, synchronized to the pulsed nature of the source, with each separately recorded time frame producing a Laue pattern from a narrow, gradually increasing wavelength band. The summation of all time frames will produce a true Laue pattern. The collection and analysis of these quasi-Laue patterns (time frames) will eliminate spot overlap and yield a greatly improved peak-to-background ratio, since the integrated background is produced only by the small wavelength band responsible for a particular diffraction peak.

6.2.2.5. *Data-collection considerations*

Single-event-counting multiwire chambers with centroid-finding electronics (introduced in Section 6.2.1.4) are well suited for the type of time-sliced data collection that is mandatory for spallation neutron instruments. For large, high-resolution, multi-segmented detectors collecting about 100 time slices per cycle, data memories in the order of 100 million pixels are required. The number of time slices that needs to be collected to produce the optimum peak-to-background ratio depends on the characteristics (wavelength bandwidth) of the coupled or decoupled moderator.

Data-integration techniques are similar to those for the classic reactor case (Section 6.2.1.5), but contain a time (wavelength) dimension and no crystal stepping. The crystal is stationary and the reflection is 'scanned' as a function of time by the wavelength band. Time-dependent reflection overlap, caused by long pulse decay (particularly observed in fully coupled moderators), can be a problem. Such overlaps can be minimized by using a partially coupled moderator (Schoenborn *et al.*, 1999).

6.2.3. Summary

In the preceding sections, a brief overview has been presented of (i) the two main types of neutron sources and (ii) some of the primary components required to prepare a neutron beam for a neutron-scattering instrument. It has been assumed that as well as macromolecular crystallography, membrane and fibre diffraction, small-angle neutron scattering (see Chapter 19.4) is of interest. From a structural-biology user perspective, the advantages and disadvantages of reactor-based and spallation-source-based facilities are difficult to assess, since only very limited use of spallation sources has been documented. Direct comparisons between the performances of neutron-scattering instruments and sources are difficult, and would undoubtedly change as facilities are progressively upgraded (Carpenter & Yelon, 1986; Richter & Springer, 1998). Calculations show, however, that the use of time-of-flight techniques with partially coupled moderators on a spallation neutron source is ideal for structural-biology diffraction studies and promises to yield an effective gain of an order of magnitude in intensity (Schoenborn, 1996). When the protein crystallographic diffraction instrument now being built at LANSCE is completed in 2000, a more meaningful comparison will be possible between a premier spallation-source-based instrument and comparable reactor-based instruments.

In summary, the neutron source plays a pivotal role in the design and utility of an experiment in macromolecular crystallography, membrane and fibre diffraction, and small-angle neutron scattering. However, innovative design of the scattering instrument using the latest technology (*e.g.* image plates or large MWPCs) can partially offset certain negative impacts of the source and make an enormous difference to the instrument as a user facility. In general, neutron sources are national or regional facilities and consequently carry special requirements for user access. Therefore, a local, well equipped, medium-flux neutron source may be more suitable to test potential experiments and the premier international facility should be used only where required.