International Tables for Crystallography (2006). Vol. C, Section 4.4.2.7.3, pp. 442–443.

4.4.2.6.4. *Zeeman polarizer*

The reflection width of perfect silicon crystals for thermal neutrons and the Zeeman splitting ($\Delta E = 2\mu B$) of a field of about 10 kGs are comparable and therefore can be used to polarize a neutron beam. For a monochromatic beam (energy E_0) in a strong magnetic field region, the result of the Zeeman splitting will be a separation into two polarized subbeams, one polarized along **B** with energy $E_0 + \mu B$, and the other polarized antiparallel to **B** with energy $E_0 - \mu B$. The two polarized beams can be selected by rocking a perfect crystal in the field region B (Forte & Zeyen, 1989).

4.4.2.7. *Spin-orientation devices*

Polarization is the state of spin orientation of an assembly of particles in a target or beam. The beam polarization vector **P** is defined as the vector average of this spin state and is often described by the density matrix $\rho = \frac{1}{2}(1 + \sigma \mathbf{P})$. The polarization is then defined as $\mathbf{P} = \mathrm{Tr}(\rho\sigma)$. If the polarization vector is inclined to the field direction in a homogenous magnetic field, **B**, the polarization vector will precess with the classical Larmor frequency $\omega_L = |\gamma| B$. This results in a precessing spin polarization. For most experiments, it is sufficient to consider the linear polarization vector in the direction of an applied magnetic field. If, however, the magnetic field direction changes along the path of the neutron, it is also possible that the direction of **P** will change. If the frequency, Ω, with which the magnetic field changes is such that

$$\Omega = \mathrm{d}(\mathbf{B}/|\mathbf{B}|)/\,\mathrm{d}t \ll \omega_L, \qquad (4.4.2.19)$$

then the polarization vector follows the field rotation adiabatically. Alternatively, when $\Omega \gg \omega_L$, the magnetic field changes so rapidly that **P** cannot follow, and the condition is known as non-adiabatic fast passage. All spin-orientation devices are based on these concepts.

4.4.2.7.1. *Maintaining the direction of polarization*

A polarized beam will tend to become depolarized during passage through a region of zero field, since the field direction is ill defined over the beam cross section. Thus, in order to keep the polarization direction aligned along a defined quantization axis, special precautions must be taken.

The simplest way of maintaining the polarization of neutrons is to use a guide field to produce a well defined field **B** over the whole flight path of the beam. If the field changes direction, it has to fulfil the adiabatic condition $\Omega \ll \omega_L$, *i.e.* the field changes must take place over a time interval that is long compared with the Larmor period. In this case, the polarization follows the field direction adiabatically with an angle of deviation $\Delta\theta \leq 2\arctan(\Omega/\omega_L)$ (Schärpf, 1980).

Alternatively, some instruments (*e.g.* zero-field spin-echo spectrometers and polarimeters) use polarized neutron beams in regions of zero field. The spin orientation remains constant in a zero-field region, but the passage of the neutron beam into and out of the zero-field region must be well controlled. In order to provide a well defined region of transition from a guide-field region to a zero-field region, a non-adiabatic fast passage through the windings of a rectangular input solenoid can be used, either with a toroidal closure of the outside field or with a μ-metal closure frame. The latter serves as a mirror for the coil ends, with the effect of producing the field homogeneity of a long coil but avoiding the field divergence at the end of the coil.

4.4.2.7.2. *Rotation of the polarization direction*

The polarization direction can be changed by the adiabatic change of the guide-field direction so that the direction of the polarization follows it. Such a rotation is performed by a spin turner or spin rotator (Schärpf & Capellmann, 1993; Williams, 1988).

Alternatively, the direction of polarization can be rotated relative to the guide field by using the property of precession described above. If a polarized beam enters a region where the field is inclined to the polarization axis, then the polarization vector **P** will precess about the new field direction. The precession angle will depend on the magnitude of the field and the time spent in the field region. By adjustment of these two parameters together with the field direction, a defined, though wavelength-dependent, rotation of **P** can be achieved. A simple device uses the non-adiabatic fast passage through the windings of two rectangular solenoids, wound orthogonally one on top of the other. In this way, the direction of the precession field axis is determined by the ratio of the currents in the two coils, and the sizes of the fields determine the angle φ of the precession. The orientation of the polarization vector can therefore be defined in any direction.

In order to produce a continuous rotation of the polarization, *i.e.* a well defined precession, as required in neutron spin-echo (NSE) applications, precession coils are used. In the simplest case, these are long solenoids where the change of the field integral over the cross section can be corrected by Fresnel coils (Mezei, 1972). More recently, Zeyen & Rem (1996) have developed and implemented optimal field-shape (OFS) coils. The field in these coils follows a cosine squared shape that results from the optimization of the line integral homogeneity. The OFS coils can be wound over a very small diameter, thereby reducing stray fields drastically.

4.4.2.7.3. *Flipping of the polarization direction*

The term 'flipping' was originally applied to the situation where the beam polarization direction is reversed with respect to a guide field, *i.e.* it describes a transition of the polarization direction from parallel to antiparallel to the guide field and *vice versa*. A device that produces this 180° rotation is called a π flipper. A $\pi/2$ flipper, as the name suggests, produces a 90° rotation and is normally used to initiate precession by turning the polarization at 90° to the guide field.

The most direct wavelength-independent way of producing such a transition is again a non-adiabatic fast passage from the region of one field direction to the region of the other field direction. This can be realized by a current sheet like the Dabbs foil (Dabbs, Roberts & Bernstein, 1955), a Kjeller eight (Abrahams, Steinsvoll, Bongaarts & De Lange, 1962) or a cryoflipper (Forsyth, 1979).

Alternatively, a spin flip can be produced using a precession coil, as described above, in which the polarization direction makes a precession of just π about a direction orthogonal to the guide field direction (Mezei, 1972). Normally, two orthogonally wound coils are used, where the second, correction, coil serves to compensate the guide field in the interior of the precession coil. Such a flipper is wavelength dependent and can be easily tuned by varying the currents in the coils.

Another group of flippers uses the non-adiabatic transition through a well defined region of zero field. Examples of this type of flipper are the two-coil flipper of Drabkin, Zabidarov, Kasman & Okorokov (1969) and the line-shape flipper of Korneev & Kudriashov (1981).

Historically, the first flippers used were radio-frequency coils set in a homogeneous magnetic field. These devices are wavelength dependent, but may be rendered wavelength independent by replacing the homogeneous magnetic field with a gradient field (Egorov, Lobashov, Nazarento, Porsev & Serebrov, 1974).

In some devices, the flipping action can be combined with another selection function. The wavelength-dependent magnetic wiggler flipper proposed by Agamalyan, Drabkin & Sbitnev (1988) in combination with a polarizer can be used as a polarizing monochromator (Majkrzak & Shirane, 1982). Badurek & Rauch (1978) have used flippers as choppers to pulse a polarized beam.

In neutron resonance spin echo (NRSE) (Gähler & Golub, 1987), the precession coil of the conventional spin-echo configuration is replaced by two resonance spin flippers separated by a large zero-field region. The radio-frequency field of amplitude B_1 is arranged orthogonal to the DC field, B_0, with a frequency $\omega = \omega_L$, and an amplitude defined by the relation $\omega_1 \tau = \pi$, where τ is the flight time in the flipper coil and $\omega_1 = \gamma B_1$. In this configuration, the neutron spin precesses through an angle π about the resonance field in each coil and leaves the coil with a phase angle φ. The total phase angle after passing through both coils, $\varphi = 2\omega L/v$, depends on the velocity v of the neutron and the separation L between the two coils. Thus, compared with conventional NSE, where the phase angle comes from the precession of the neutron spin in a strong magnetic field compared with a static flipper field, in NRSE the neutron spin does not precess, but the flipper field rotates. Effectively, the NRSE phase angle φ is a factor of two larger than the NSE phase angle for the same DC field B_0. Furthermore, the resolution is determined by the precision of the RF frequencies and the zero-field flight path L rather than the homogeneity of the line integral of the field in the NSE precession coil.

4.4.2.8. *Mechanical choppers and selectors*

Thermal neutrons have relatively low velocities (a 4 Å neutron has a reciprocal velocity of approximately $1000\,\mu\text{s}\,\text{m}^{-1}$), so that mechanical selection devices and simple flight-time measurements can be used to make accurate neutron energy determinations.

Disc choppers rotating at speeds up to 20 000 revolutions per minute about an axis that is parallel to the neutron beam are used to produce a well defined pulse of neutrons. The discs are made from absorbing material (at least where the beam passes) and comprise one or more neutron-transparent apertures or slits. For polarized neutrons, these transparent slits should not be metallic, as the eddy currents in the metal moving in even a weak guide field will strongly depolarize the beam. The pulse frequency is determined by the number of apertures and the rotation frequency, while the duty cycle is given by the ratio of open time to closed time in one rotation. Two such choppers rotating in phase can be used to monochromate and pulse a beam simultaneously (Egelstaff, Cocking & Alexander, 1961). In practice, more than two choppers are generally used to avoid frame overlap of the incident and scattered beams. The time resolution of disc choppers (and hence the energy resolution of the instrument) is determined by the beam size, the aperture size and the rotation speed. For a realistic beam size, the rotation speed limits the resolution. Therefore, in modern instruments, it is normal to replace a single chopper with two counter-rotating choppers (Hautecler *et al.*, 1985; Copley, 1991). The low duty cycle of a simple disc chopper can be improved by replacing the single slit with a series of slits either in a regular sequence (Fourier chopper) (Colwell, Miller & Whittemore, 1968; Hiismäki, 1997) or a pseudostatistical sequence (pseudostatistical chopper) (Hossfeld, Amadori & Scherm, 1970), with duty cycles of 50 and 30%, respectively.

The Fermi chopper is an alternative form of neutron chopper that simultaneously pulses and monochromates the incoming beam. It consists of a slit package, essentially a collimator, rotating about an axis that is perpendicular to the beam direction (Turchin, 1965). For optimum transmission at the required wavelength, the slits are usually curved to provide a straight collimator in the neutron frame of reference. The curvature also eliminates the 'reverse burst', *i.e.* a pulse of neutrons that passes when the chopper has rotated by 180°.

A Fermi chopper with straight slits in combination with a monochromator assembly of wide horizontal divergence can be used to time focus a polychromatic beam, thus maintaining the energy resolution while improving the intensity (Blanc, 1983).

Velocity selectors are used when a continuous beam is required with coarse energy resolution. They exist in either multiple disc configurations or helical channels rotating about an axis parallel to the beam direction (Dash & Sommers, 1953). Modern helical channel selectors are made up of lightweight absorbing blades slotted into helical grooves on the rotation axis (Wagner, Friedrich & Wille, 1992). At higher energies where no suitable absorbing material is available, highly scattering polymers [poly(methyl methacrylate)] can be used for the blades, although in this case adequate shielding must be provided. The neutron wavelength is determined by the rotation speed, and resolutions, $\Delta\lambda/\lambda$, ranging from 5% to practically 100% ($\lambda/2$ filter) can be achieved. The resolution is fixed by the geometry of the device, but can be slightly improved by tilting the rotation axis or relaxed by rotating in the reverse direction for shorter wavelengths. Transmissions of up to 94% are typical.

4.4.3. Resolution functions (By R. Pynn and J. M. Rowe)

In a *Gedanken* neutron scattering experiment, neutrons of wavevector $\mathbf{k}_I$ impinge on a sample and the wavevector, $\mathbf{k}_F$, of the scattered neutrons is determined. A number of different types of spectrometer are used to achieve this goal (*cf.* Pynn, 1984). In each case, finite instrumental resolution is a result of uncertainties in the definition of $\mathbf{k}_I$ and $\mathbf{k}_F$. Propagation directions for neutrons are generally defined by Soller collimators for which the transmission as a function of divergence angle generally has a triangular shape. Neutron monochromatization may be achieved either by Bragg reflection from a (usually) mosaic crystal or by a time-of-flight method. In the former case, the mosaic leads to a spread of $|k_I|$ while, in the latter, pulse length and uncertainty in the lengths of flight paths (including sample size and detector thickness) produce a similar effect. Calculations of instrumental resolution are generally lengthy and lack of space prohibits their detailed presentation here. In the following paragraphs, the concepts involved are indicated and references to original articles are provided.

In resolution calculations for neutron spectrometers, it is usually assumed that the uncertainty of the neutron wavevector does not vary spatially across the neutron beam, although this reasoning may not apply to the case of small samples and compact spectrometers. To calculate the resolution of the spectrometer in the large-beam approximation, one writes the measured intensity I as

references