

6.1. INTENSITY OF DIFFRACTED INTENSITIES

magnetized by an external field. The ‘flipping ratio’ then becomes

$$R = \frac{1 + 2Py \sin^2 \rho + y^2 \sin^2 \rho}{1 - 2Pe y \sin^2 \rho + y^2 \sin^2 \rho}, \quad (6.1.2.22)$$

with $y = (\gamma r_e)M(\mathbf{k})/F(\mathbf{k})$, ρ being the angle between the magnetization direction and the scattering vector. The solution to this equation is

$$y = \{P \sin \rho (Re + 1) \pm [P^2 \sin^2 \rho (Re + 1)^2 - (R - 1)^2]^{1/2}\} \times [(R - 1) \sin \rho]^{-1}; \quad (6.1.2.23)$$

the relative signs of $F(\mathbf{k})$ and $M(\mathbf{k})$ are determined by whether R is greater or less than unity. The uncertainty in the sign of the square root in (6.1.2.23) corresponds to not knowing whether $F(\mathbf{k}) > M(\mathbf{k})$ or *vice versa*.

6.1.2.6. Rotation of the polarization of the scattered neutrons

Whenever the neutron spin direction is not parallel to the magnetic interaction vector $\mathbf{Q}(\mathbf{k})$, the direction of polarization is changed in the scattering process. The general formulae for the scattered polarization are given by Blume (1963). The result for most cases of interest can be inferred by calculating the components of the scattered neutron’s spin in the x , y , and z directions for a neutron whose spin is initially parallel to z . For simplicity, y is taken parallel to \mathbf{k} ; x and z define a plane that contains $\mathbf{Q}(\mathbf{k})$. From (6.1.2.18),

$$\begin{aligned} S_x &= \frac{1}{2} \{ [Q_z(\mathbf{k}) + F'(\mathbf{k})] Q_x^*(\mathbf{k}) \\ &\quad + [Q_z^*(\mathbf{k}) + F'^*(\mathbf{k})] Q_x(\mathbf{k}) \} / N \\ S_y &= \frac{1}{2i} \{ [Q_z(\mathbf{k}) + F'(\mathbf{k})] Q_x^*(\mathbf{k}) \\ &\quad - [Q_z^*(\mathbf{k}) + F'^*(\mathbf{k})] Q_x(\mathbf{k}) \} / N \\ S_z &= \frac{1}{2} \{ [Q_z(\mathbf{k}) + F'(\mathbf{k})] [Q_z^*(\mathbf{k}) + F'^*(\mathbf{k})] \} / N \\ N &= |Q_z(\mathbf{k}) + F'(\mathbf{k})|^2 + |Q_x(\mathbf{k})|^2. \end{aligned} \quad (6.1.2.24)$$

It is clear from this set of equations that S_x and S_y are zero if $Q_x(\mathbf{k}) = 0$. Three simple cases may be taken as examples of the use of (6.1.2.24):

(a) A magnetic reflection from a simple antiferromagnet for which $\mathbf{Q}(\mathbf{k})$ is real, $F(\mathbf{k}) = 0$; under these conditions,

$$\begin{aligned} S_x &= Q_x(\mathbf{k})[Q_z(\mathbf{k})]/|\mathbf{Q}(\mathbf{k})|^2 \\ S_y &= 0 \\ S_z &= \frac{1}{2} [Q_z(\mathbf{k})^2 - Q_x(\mathbf{k})^2]/|\mathbf{Q}(\mathbf{k})|^2, \end{aligned}$$

showing that the direction of polarization is turned through an angle 2φ in the xy plane where φ is the angle between $\mathbf{Q}(\mathbf{k})$ and the initial polarization direction.

(b) A satellite reflection from a magnetic structure described by a *circular helix* for which $Q_x(\mathbf{k}) = iQ_z(\mathbf{k})$, $F'(\mathbf{k}) = 0$; in this case,

$$\begin{aligned} S_x &= 0 \\ S_y &= Q_z^2(\mathbf{k})/|\mathbf{Q}(\mathbf{k})|^2 = \frac{1}{2} \\ S_z &= 0 \end{aligned}$$

and the scattered polarization is parallel to the scattering vector independent of its initial direction.

(c) A mixed magnetic and nuclear reflection from a Cr_2O_3 -type antiferromagnet for which $\mathbf{Q}(\mathbf{k})$ is imaginary, $\mathbf{Q}(\mathbf{k}) = -\mathbf{Q}^*(\mathbf{k})$, $F(\mathbf{k})$ is real. Then,

$$\begin{aligned} S_x &= Q_x(\mathbf{k})Q_z(\mathbf{k})/[F'(\mathbf{k})^2 + |\mathbf{Q}(\mathbf{k})|^2] \\ S_y &= iF(\mathbf{k})Q_x(\mathbf{k})/[F'(\mathbf{k})^2 + |\mathbf{Q}(\mathbf{k})|^2] \\ S_z &= \frac{1}{2} [|Q_z(\mathbf{k}) + F'(\mathbf{k})|^2 - |Q_x(\mathbf{k})|^2] \\ &\quad \times [F'(\mathbf{k})^2 + |\mathbf{Q}(\mathbf{k})|^2]^{-1} \end{aligned}$$

so that in this case the final polarization has components along all three directions.

6.1.3. Nuclear scattering of neutrons (By B. T. M. Willis)

6.1.3.1. Glossary of symbols

b	Bound nuclear scattering length
b_{free}	Free nuclear scattering length
b_0	Potential scattering length
b', b''	Real and imaginary parts of resonant scattering length
b_{coh}	Coherent scattering length
$F(\mathbf{h})$	Structure factor for nuclear Bragg scattering
$2\pi\mathbf{h}$	Reciprocal-lattice vector
\mathbf{H}	Scattering vector ($= \mathbf{k} - \mathbf{k}_0$)
I	Nuclear spin
\mathbf{k}	Wavevector of scattered neutron
\mathbf{k}_0	Wavevector of incident neutron
M	Nuclear mass
m_n	Neutron mass
N	Number of unit cells in crystal
V	Volume of unit cell
W_j	Exponent of temperature factor $\exp(-W_j)$ of j th atom
w_+	Weight of spin state $I + \frac{1}{2}$
w_-	Weight of spin state $I - \frac{1}{2}$
σ_{coh}	Coherent scattering cross section
σ_{inc}	Incoherent scattering cross section
σ_{tot}	Total scattering cross section ($= \sigma_{\text{coh}} + \sigma_{\text{inc}}$)

$\left(\frac{d\sigma}{d\Omega}\right)_{\text{coh,el}}$ Differential coherent elastic scattering cross section

$\left(\frac{d\sigma}{d\Omega}\right)_{\text{inc,el}}$ Differential incoherent elastic scattering cross section

The nucleus is the fundamental unit involved in the scattering of neutrons by atoms. For magnetic materials, electronic scattering takes place as well (see Section 6.1.2). Apart from these two main interactions, there are a number of subsidiary ones (Shull, 1967) that are extremely weak and can be ignored in nearly all diffraction studies.

In this section, we discuss the neutron–nucleus interaction only, starting from scattering by a single nucleus, then scattering by an atom, and finally scattering by a single crystal. For a more detailed account, see Bacon (1975).

6.1.3.2. Scattering by a single nucleus

The nuclear forces giving rise to the scattering of neutrons have a range of 10^{-14} to 10^{-15} m. This is much smaller than the wavelength of thermal neutrons, and so (from elementary diffraction theory) the neutron wave scattered by the nucleus is spherically symmetrical. Unlike magnetic scattering, there is no ‘form-factor’ dependence of nuclear scattering on the scattering angle.

The incident neutron beam can be represented by the plane wave

$$\psi_0 = \exp(i\mathbf{k}_0 \cdot \mathbf{r}),$$