CHAPTER III

NEUTRON DIFFRACTION

A detailed survey of the principles and uses of neutron diffraction is given in the book by Bacon.[19] A brief survey of the principles employed in this work will be given in this chapter.

The wavelength λ associated with a particle of mass m and velocity v is

$$\lambda = \frac{h}{mv} \tag{5}$$

Neutrons which have attained thermal equilibrium in a reactor at a temperature T will have a mean kinetic energy given by

$$\frac{1}{2} m \bar{v}^2 = \frac{3}{2} kT \tag{6}$$

where $\bar{v}^2$ is the mean square velocity.

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(19)   Bacon, G.E., <u>Neutron Diffraction</u>, Oxford University Press 1962

Combination of equation (5) and (6) gives the wavelength corresponding to the root mean square velocities as

$$\lambda = \frac{h}{\sqrt{3mkT}} \quad (7)$$

The wavelength corresponding to $20\,°C$ is ~ 1.5 Å, which is just the right wavelength for diffraction by crystalline solids.

The intensity of a beam of unpolarized neutrons, scattered at an angle Θ by a powder sample in the form of a vertical circular cylinder fully bathed in the neutron beam, is given by the relation.

$$I \propto jFA(\theta)\, e^{-2B\sin^2\theta/\lambda^2} / \sin\theta \sin 2\theta \quad (8)$$

The formula is made up of the following parts:

(1) The multiplicity factor j is the number of cooperating planes of the same form for the particular reflection being measured.

(2) The structure factor F (hkl) for each set of planes indicated by the Miller indices h, k and 1 can be expressed in term

of the atomic scattering factor b_r of coordinates X_r, Y_r and z_r in the unit cell as

$$F(hkl) = \sum_{r} b_r \exp 2\pi i (hx_r + ky_r + lz_r) \tag{9}$$

The summation is over one unit cell.

(3) A (θ), the absorption factor, varies very slowly with angle, and for most materials can be ignored.

(4) The temperature factor, $\exp(-2B \sin^2\theta/\lambda^2)$ can only apply strictly to monatomic cubic crystals, but reasonable agreement can usually be obtained for polyatomic crystal. Values of the functions $\exp(-2B \sin^2\theta/\lambda^2)$ are tabulated in the International Tables for X-ray Crystallography, Volume 2.[20]

(5) The geometrical factors, $1/\sin 2\theta$ which is known as the Lorentz factor, is a measure of the duration that a particular plane will be in a reflecting position. The $1/\sin\theta$ is a measure of fraction of the radiation scattered at an angle θ .

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(20) Macqillavry, C.H. and Rieck, G.D., (Ed.), International
Tables for X-ray Crystallography, Vol II, The Kynoch Press,
Birmingham (England) 1967

III. 1   Nuclear Scattering of Neutrons

The fundamental scattering body in nuclear scattering is the nucleus, and this leads to the immediate result that, since the dimensions of the nucleus are small compared with wavelength of the incident thermal neutrons, the scattering is then isotropic, and there is no form factor fall-off with $\sin\theta/\lambda$. The neutron scattering power of a nucleus is usually expressed in terms of a scattering length b which take both positive and negative values, and different values for different isotopes. The scattering length b for nickel, manganese and germanium are shown in table 3 (from Bacon[16])

III. 2   Magnetic Scattering of Neutrons

In addition to its mass, a neutron possesses a spin ½, and a   magnetic moment of 1.9 nuclear magnetons. The interaction of this moment with that of a magnetic atom produces an additional magnetic scattering of the neutron. Since the magnetic scattering is due to the unpaired electrons, and not the nucleus, the magnetic scattering amplitude ,p, exhibits a form factor fall-off with $\sin\theta/\lambda$. The magnetic form factor used for manganese is shown in figure 2 (from 20 a)

The magnetic scattering amplitude p is defined as

$$ p = \left(\frac{e^2 \gamma}{m c^2} \right) S f $$

(10)

(20 a) Webster, P.J., Ph.D. Thesis, Sheffield University, (1968)

Elements	Atomic Number	Specific Nucleus	Scattering length (b) $(10^{-12}$ cm)
Manganese	25	Mn^{55}	− 0.36
Nickel	28	−	1.03
		Ni^{58}	1.44
		Ni^{60}	0.30
		Ni^{62}	− 0.87
Germanium	32	−	0.84

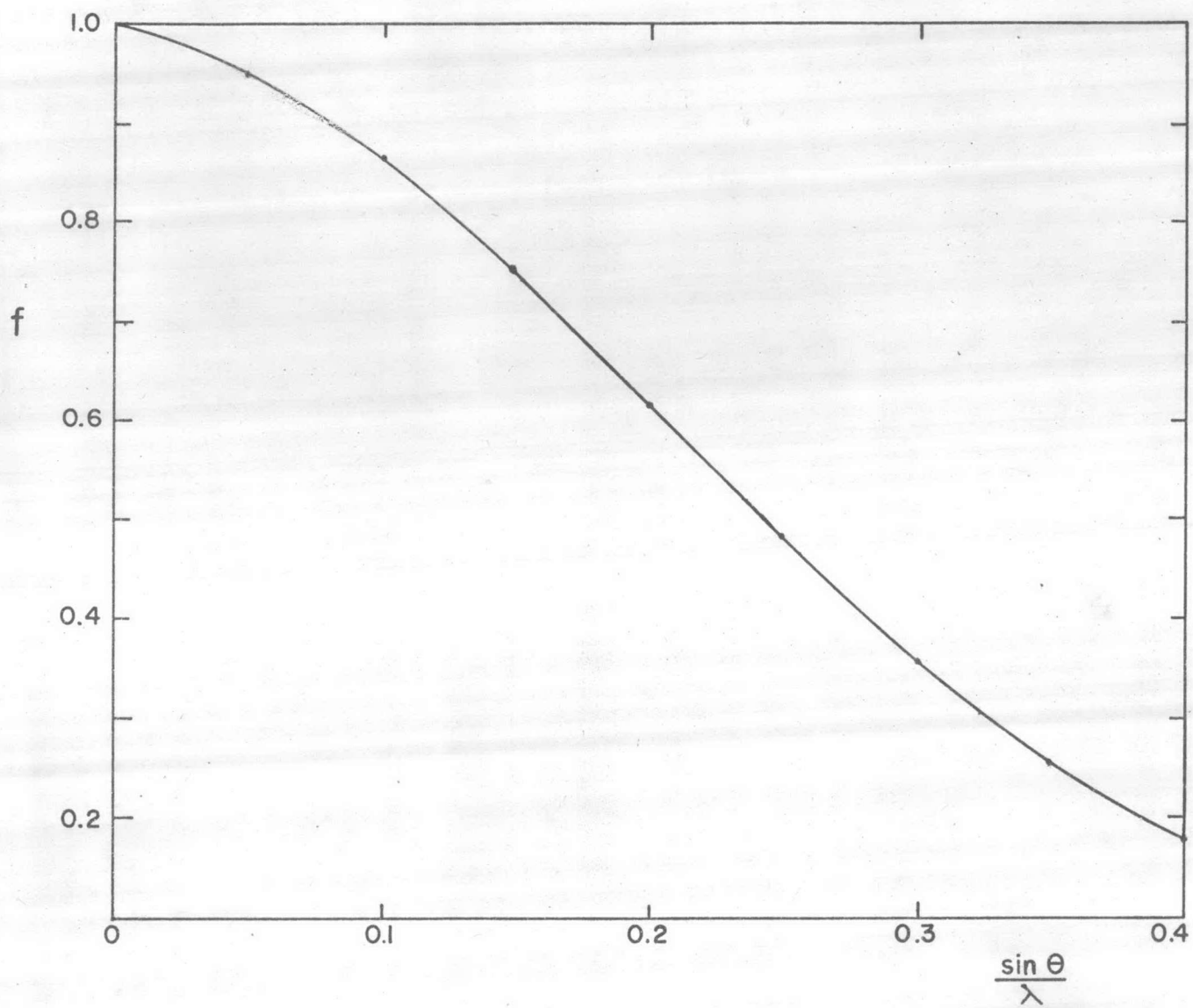Table 3   Neutron scattering length for manganese, nickel and germanium.

Fig. 2 Magnetic form factor of manganese. (From 20a)

where e and m are the electronic charge and mass respectively,
γ is the magnetic moment of the neutron, S is the spin quantum
number and f is the magnetic form factor. In term of the Bohr
magneton number of the atomic magnetic moment, the magnetic scatter-
ing amplitude can be expressed as

$$p = 0.269 \, \mu_B f \times 10^{-12} \, em \tag{11}$$

where μ_B is the magnitude of the atomic magnetic moment in Bohr
magneton.

In ordered magnetic crystals the magnetic moments are oriented
in a regular manner and coherent Bragg reflections occur. The total
scattering cross-section $d\sigma$ of an unpolarized neutron beam is

$$d\sigma = b^2 + q^2 p^2 \tag{12}$$

where q is the magnetic interaction vector defined by

$$q = \underline{\epsilon}(\underline{\epsilon} \cdot \underline{x}) - \underline{x} \tag{13}$$

$\in$ is a unit scattering vector normal to the reflecting planes,
and $\underline{x}$ is a unit vector in the direction of the magnetic moment.
Consequently,

$$q^2 = 1 - (\in \cdot \underline{x})^2 = \sin^2\alpha \tag{14}$$

where α is the angle between $\in$ and $\underline{x}$.

The total scattering intensity for any reflection is obtained
by calculating the total structure factor F for the unit cell.
The nuclear structure factor F_n is given by

$$F_n(hkl) = \sum_r b_r \exp 2\pi i(hx_r + ky_r + lz_r) \tag{15}$$

and the magnetic structure factor F_m by

$$F_m(hkl) = \sum_r p_r \exp 2\pi i(hx_r + ky_r + lz_r) \tag{16}$$

The resultant intensity is proportional to F^2 which is given by

$$F^2 = F_n^2 + q^2 F_m^2 \tag{17}$$

Thus if q^2 is known for a particular reflection, the orientation of the magnetic moment may be in principle be determined. However, for polycrystalline materials only a mean value of q^2 from all reflecting planes of the same form is obtained, and the most that can be calculated is the orientation of the moments with respect to the unique axis. If no unique axis exists, as in a cubic crystal for example, it is impossible to determine the moment orientations from measurements on polycrystalline sample using unpolarized neutrons, and q^2 takes a mean value of $2/3$.

In antiferromagnetic materials the magnetic unit cell can be either equal or larger than the chemical unit cell, in the latter case the magnetic and nuclear diffraction peaks are not superimposed. In ferromagnetic materials the magnetic and chemical unit cells are usually the same size and the magnetic and nuclear peaks are superimposed at the same Bragg angle. The magnetic and nuclear contributions to the diffraction peaks may be determined by three methods. The best method is to vary q^2. This may be done by applying a magnetic field, sufficiently large to saturate the sample along or perpendicular to the scattering vector. In the first case $q^2 = 0$, and in the second $q^2 = 1$, and the difference between the two diffraction patterns is the magnetic scattering. If suitable magnetic field is not available, measurements may be made above and below the Curie temperature, but this method suffers from the disadvantage that other parameters may

change with temperature, and corrections have to be applied. The

third method is to compare the intensities of diffraction lines

at low and high angles. At low angle the magnetic contribution

may be large, but there is a rapid fall off in magnetic contribution

with angle due to the magnetic form factor, and high angle lines have

virtually no magnetic component. The disadvantage of this method is

that intensities cannot be measured as accurately at high angle.