5.3. Dynamical theory of neutron diffraction

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5.3.1. Introduction

Neutron and X-ray scattering are quite similar both in the geometry of scattering and in the orders of magnitude of the basic quantities. When the neutron spin is neglected, *i.e.* when dealing with scattering by perfect non-magnetic crystals, the formalism and the results of the dynamical theory of X-ray scattering can be very simply transferred to the case of neutrons (Section 5.3.2). Additional features of the neutron case are related to the neutron spin and appear in diffraction by magnetic crystals (Section 5.3.3). The low intensities available, coupled with the low absorption of neutrons by most materials, make it both necessary and possible to use large samples in standard diffraction work. The effect of extinction in crystals that are neither small nor bad enough to be amenable to the kinematical approximation is therefore very important in the neutron case, and will be discussed in Section 5.3.4 together with the effect of crystal distortion. Additional possibilities arise in the neutron case because the neutrons can be manipulated from outside through applied fields (Section 5.3.5). Reasonably extensive tests of the predictions of the dynamical theory of neutron diffraction have been performed, with the handicap of the very low intensities of neutron beams as compared with X-rays: these are described in Section 5.3.6. Finally, the applications of the dynamical theory in the neutron case, and in particular neutron interferometry, are reviewed in Section 5.3.7.

5.3.2. Comparison between X-rays and neutrons with spin neglected

5.3.2.1. *The neutron and its interactions*

An excellent introductory presentation of the production, properties and scattering properties of neutrons is available (Scherm & Fåk, 1993, and other papers in the same book). A stimulating review on neutron optics, including diffraction by perfect crystals, has been written by Klein & Werner (1983). X-rays and neutrons are compared in terms of the basic quantities in Table 4.1.3.1 of *IT* C (1999), where Chapter 4.4 is devoted to neutron techniques.

The neutron is a massive particle for which the values relevant to diffraction are: no electric charge, rest mass $m = 1.675 \times 10^{-27}$ kg, angular momentum eigenvalues along a given direction $\pm\hbar/2$ (spin $\frac{1}{2}$) and a magnetic moment of -1.913 nuclear magneton, meaning that its component along a quantization direction z can take eigenvalues $\mu_z = \mp 0.996 \times 10^{-26}$ A m^2. The de Broglie wavelength is $\lambda = h/p$ where h is Planck's constant ($h = 2\pi\hbar = 6.625 \times 10^{-34}$ J s) and p is the linear momentum; $p = mv$ in the non-relativistic approximation, which always applies in the context of this chapter, v being the neutron's velocity. The neutron's wavelength, λ, and kinetic energy, E_c, are thus related by $\lambda = h/(2mE_c)^{1/2}$, or, in practical units, $\lambda\ [\text{Å}] = 9.05/(E_c\ [\text{meV}])^{1/2}$. Thus, to be of interest for diffraction by materials, neutrons should have kinetic energies in the range 10^0 to 10^2 meV. In terms of the velocity, $\lambda\ [\text{Å}] = 3.956/(v\ [\text{km s}^{-1}])$.

Neutron beams are produced by nuclear reactors or by spallation sources, usually pulsed. In either case they initially have an energy in the MeV range, and have to lose most of it before they can be used. The moderation process involves inelastic interactions with materials. It results in statistical distributions of energy, hence of velocity, close to the Maxwell distribution characteristic of the temperature T of the moderator. Frequently used moderators are liquid deuterium (D_2, *i.e.* $^2H_2$) at 25 K, heavy water (D_2O) at room temperature and graphite allowed to heat up to 2400 K; the corresponding neutron distributions are termed cold, thermal and hot, respectively.

The interaction of a neutron with an atom is usually described in terms of scattering lengths or of scattering cross sections. The main contribution corresponding to the nuclear interaction is related to the strong force. The interaction with the magnetic field created by atoms with electronic magnetic moments is comparable in magnitude to the nuclear term.

5.3.2.2. *Scattering lengths and refractive index*

The elastic scattering amplitude for scattering vector $\mathbf{s}$, $f(\mathbf{s})$, is defined by the wave scattered by an object placed at the origin when the incident plane wave is $\Psi_i = A\exp[i(\mathbf{k}_0 \cdot \mathbf{r} - \omega t)]$, written as $\Psi_s = A[f(\mathbf{s})/r]\exp[i(kr - \omega t)]$ with $k = |\mathbf{k}_0| = |\mathbf{k}_0 + \mathbf{s}| = 2\pi/\lambda$. In the case of the strong-force interaction with nuclei, the latter can be considered as point scatterers because the interaction range is very small, hence the scattering amplitude is isotropic (independent of the direction of $\mathbf{s}$). It is also independent of λ except in the vicinity of resonances. It is conventionally written as $-b$ so that most values of b, called the scattering length, are positive. A table of experimentally measured values of the scattering lengths b is given in *IT* C for the elements in their natural form as well as for many individual isotopes. It is apparent that the typical order of magnitude is the fm (femtometer, *i.e.* 10^{-15} m, or fermi), that there is no systematic variation with atomic number and that different isotopes have very different scattering lengths, including different signs. The first remark implies that scattering amplitudes of X-rays and of neutrons have comparable magnitudes, because the characteristic length for X-ray scattering (the scattering amplitude for forward scattering by one free electron) is $R = 2.8$ fm, the classical electron radius. The second and third points explain the importance of neutrons in structural crystallography, in diffuse scattering and in small-angle scattering. Scattering of neutrons by condensed matter implies the use of the bound scattering lengths, as tabulated in *IT* C. The 'free' scattering length, used in some presentations, is obtained by multiplying the bound scattering lengths by $A/(A+1)$, where A is the mass of the nucleus in atomic units.

A description in terms of an interaction potential is possible using the Fermi pseudo-potential, which in the case of the nuclear interaction with a nucleus at $\mathbf{r}_0$ can be written as $V(\mathbf{r}) = (h^2/2\pi m)b\delta(\mathbf{r} - \mathbf{r}_0)$, where δ denotes the three-dimensional Dirac distribution.

Refraction of neutrons at an interface can be conveniently described by assigning a refractive index to the material, such that the wavenumber in the material, k, is related to that in a vacuum, k_0, by $k = nk_0$. Here

$$n = \left(1 - \frac{\lambda^2}{\pi V}\sum_i b_i\right)^{1/2},$$

where the sum is over the nuclei contained in volume V. With typical values, n is very close to 1 and $1 - n = (\lambda^2/2\pi V)\sum_i b_i$ is typically of the order of 10^{-5}. This small value, in the same range as for X-rays, gives a feeling for the order of magnitude of key quantities of the dynamical theory, in particular the Darwin width 2δ as discussed in Chapter 5.1. It also makes total external reflection possible on materials for which $\sum_i b_i > 0$: this is the basis for the neutron guide tubes now installed in most research reactors, as well as for reflectometry.

The notations prevailing in X-ray and in neutron crystallography are slightly different, and the correspondence is very simple: X-ray atomic scattering factors and structure factors are numbers. When

references