

6. INTERPRETATION OF DIFFRACTED INTENSITIES

with \mathbf{k}_0 denoting the wavevector of the neutron and \mathbf{r} its position relative to the nucleus. Then, for a nucleus of zero spin, the wavefunction of the scattered neutron is

$$\psi_s = -\frac{b}{r} \exp(ik_0 r).$$

b is the *bound nuclear scattering length* or *nuclear scattering amplitude*, and the negative sign ensures that b is positive for hard-sphere or potential scattering.

If the nucleus is free to recoil under the impact of the neutron, as in a gas, the scattering must be treated in the centre-of-mass system. The *free scattering length* is related to the bound scattering length b in condensed matter by

$$b_{\text{free}} = \frac{M}{m_n + M} b,$$

where M is the nuclear mass and m_n the mass of the neutron. For hydrogen, ^1H , the free scattering length is one half the bound scattering length, but the difference between the two rapidly diminishes for heavier nuclei.

In general, b is a complex quantity:

$$b = b_0 + b' + ib''. \quad (6.1.3.1)$$

b_0 is the scattering length associated with potential scattering, *i.e.* scattering in which the nucleus behaves like an impenetrable sphere. b' and b'' are the real and imaginary parts of the resonance scattering that takes place with the formation of a compound nucleus (nucleus plus neutron). Resonance scattering is only significant when the excitation energy of the neutron is close to an energy level of the compound nucleus. This occurs for relatively few nuclei, *e.g.* ^{113}Cd , ^{149}Sm , ^{157}Gd , ^{176}Lu , and b then varies rapidly with wavelength (Fig. 6.1.3.1). The phenomenon of resonance scattering has been used to phase neutron reflections (Schoenborn, 1975), but one difficulty is the strong absorption arising from the imaginary component b'' . For the majority of nuclei, the compound nucleus is not formed near resonance: the imaginary component is small, and the scattering length is independent of the neutron wavelength.

There is confusion in the literature regarding the appropriate signs for the real and imaginary parts of the scattering amplitude (Ramaseshan, Ramesh & Ranganath, 1975). The scattering-length curves in Fig. 6.1.3.1 have been drawn to be consistent with the structure-factor formulae in Volume A (*IT A*, 1983).

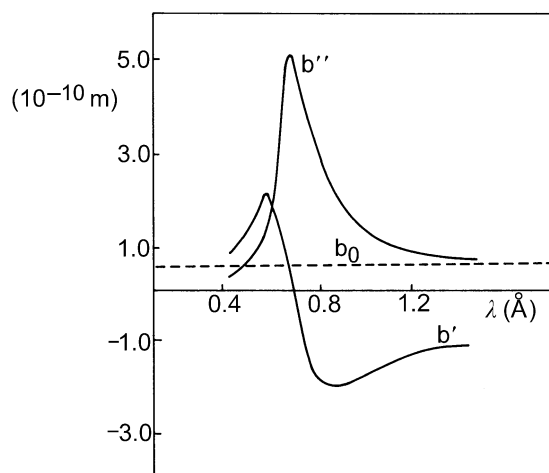


Fig. 6.1.3.1. Dependence on neutron wavelength of the coherent scattering length of ^{113}Cd . b_0 is the potential scattering component, and b' and b'' the real and imaginary components of the resonance scattering. The resonance wavelength is 0.68 Å.

Consider now the scattering from a nucleus with non-zero spin I . The neutron has spin $\frac{1}{2}$, and the spin of the combined nucleus–neutron system is either $I + \frac{1}{2}$ or $I - \frac{1}{2}$. Each spin state has its own scattering length, b_+ or b_- , and the weights of these states (for scattering unpolarized neutrons) are

$$w_+ = \frac{I + 1}{2I + 1} \quad (6.1.3.2a)$$

and

$$w_- = \frac{I}{2I + 1}. \quad (6.1.3.2b)$$

Values of b_+ and b_- have been determined experimentally for just a few nuclei with non-zero spin: ^1H , ^2H , ^{23}Na , ^{59}Co , ...

6.1.3.3. Scattering by a single atom

For a single element containing several isotopes, each isotope has its own characteristic scattering length(s). The mean value of the scattering length of the atom is obtained by averaging (where necessary) over the two spin states of the isotope:

$$\langle b \rangle_{\text{isotope}} = w_+ b_+ + w_- b_-,$$

where the angle brackets indicate a mean and w_+ and w_- are given by (6.1.3.2); $\langle b \rangle_{\text{isotope}}$ is then averaged over all isotopes, taking into account their relative abundance. The resultant quantity, $\langle b \rangle_{\text{isotopes}}^{\text{all}}$, is known as the *coherent scattering length* of the atom, denoted b_{coh} . b_{coh} plays the same role in neutron scattering as the atomic scattering factor f in X-ray scattering. Table 4.4.4.1 lists the coherent scattering lengths for the atoms in the Periodic Table.

The coherent scattering cross section of an atom is

$$\sigma_{\text{coh}} = 4\pi b_{\text{coh}}^2.$$

It represents that part of the *total scattering cross section*, σ_{tot} , that gives interference effects with other atoms. The total cross section is

$$\sigma_{\text{tot}} = 4\pi \langle b^2 \rangle_{\text{isotopes}}^{\text{all}},$$

and the *incoherent scattering cross section*, σ_{inc} , is the difference between σ_{tot} and σ_{coh} :

$$\sigma_{\text{inc}} = 4\pi [\langle b^2 \rangle - \langle b \rangle^2].$$

In incoherent scattering, there is no phase relationship between the waves scattered by different atoms. σ_{inc} for hydrogen is 40 times larger than σ_{coh} , but the proportion of coherent scattering is substantially increased by deuteration. The scattering from vanadium is almost entirely incoherent, and so it is useful as a container of polycrystalline samples.

6.1.3.4. Scattering by a single crystal

The scattering from a single crystal can be either elastic or inelastic. An elastic process is one in which there is no exchange of energy between the neutron and the target nucleus. In an inelastic process, energy exchange occurs, giving rise to the creation or annihilation of elementary excitations such as phonons [see Section 4.1.1 of Volume B (*IT B*, 1992)]. Here we shall be concerned only with elastic Bragg scattering.

If kinematic scattering conditions are assumed, the differential cross section, $(d\sigma/d\Omega)_{\text{coh,el}}$, giving the probability of coherent elastic scattering by a single crystal into the solid angle $d\Omega$, is

$$\left(\frac{d\sigma}{d\Omega} \right)_{\text{coh,el}} = N \frac{(2\pi)^3}{V} \sum_{\mathbf{h}} |F(\mathbf{h})|^2 \delta(\mathbf{H} - 2\pi\mathbf{h}). \quad (6.1.3.3)$$

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Here, N is the number of unit cells, each of volume V , $2\pi\mathbf{h}$ is a reciprocal-lattice vector, and $F(\mathbf{h})$ is the *nuclear structure factor* for Bragg scattering. \mathbf{H} is the scattering vector

$$\mathbf{H} = \mathbf{k} - \mathbf{k}_0,$$

where \mathbf{k} and \mathbf{k}_0 (with $k = k_0 = 2\pi/\lambda$) are the wavevectors of the scattered and incident beams, respectively, and the δ function indicates that the coherent elastic scattering is simply Bragg scattering. $F(\mathbf{h})$ is defined by

$$F(\mathbf{h}) = \sum_j b_{\text{coh}}^j \exp(i\mathbf{H} \cdot \mathbf{r}_j) \exp(-W_j),$$

in which b_{coh}^j is the coherent scattering length of the j th atom in the unit cell, \mathbf{r}_j is its equilibrium position with respect to the cell origin, and $\exp(-W_j)$ its Debye–Waller temperature factor.

The incoherent elastic scattering cross section is given by

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{inc,el}} = N \sum_j [\langle b_j^2 \rangle - \langle b_j \rangle^2] \exp(-2W_j).$$

Apart from the influence of the Debye–Waller temperature factor, this expression shows that the incoherent scattering is distributed uniformly throughout reciprocal space.