

Chapter 2

Neutron Scattering—A Non-destructive Microscope for Seeing Inside Matter

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How can we determine the relative positions and motions of atoms in a bulk sample of solid or liquid? Somehow we need to be able to see inside the sample with a suitable magnifying glass. It turns out that neutrons provide us with this capability. They have no charge, and their electric dipole moment is either zero or too small to measure. For these reasons, neutrons can penetrate matter far better than charged particles. Furthermore, neutrons interact with atoms via nuclear rather than electrical forces, and nuclear forces are very short range—on the order of a few femtometers (i.e., a few times 10^{-15} m). Thus, as far as the neutron is concerned, solid matter is not very dense because the size of a scattering center (i.e., a nucleus) is typically 100,000 times smaller than the distance between centers. As a consequence, neutrons can travel large distances through most materials without being scattered or absorbed. The attenuation, or decrease in intensity, of a beam of neutrons by aluminum, for example, is about 1% per millimeter compared with 99% per millimeter or more for X-rays. Figure 2.1 illustrates just how easily neutrons penetrate various materials compared with X-rays or electrons.

Like so many other things in life, the neutron's penetrating power is a double-edged sword. On the plus side, the neutron can penetrate deep within a sample even if it first has to pass through a container (such as would be required for a liquid or powder sample, for example, or if the sample had to be maintained at low temperature or high pressure). The corollary is that neutrons are only weakly scattered once they do penetrate. To make matters worse, available neutron beams have inherently low intensities. X-ray instruments at synchrotron sources can provide fluxes of 10^{18} photons per second per square millimeter compared with 10^4 neutrons per second per square millimeter in the same energy bandwidth even at the most powerful continuous neutron sources.

The combination of weak interactions and low fluxes make neutron scattering a signal-limited technique, which is practiced only because it provides information about the structure of materials that cannot be obtained in simpler, less expen-

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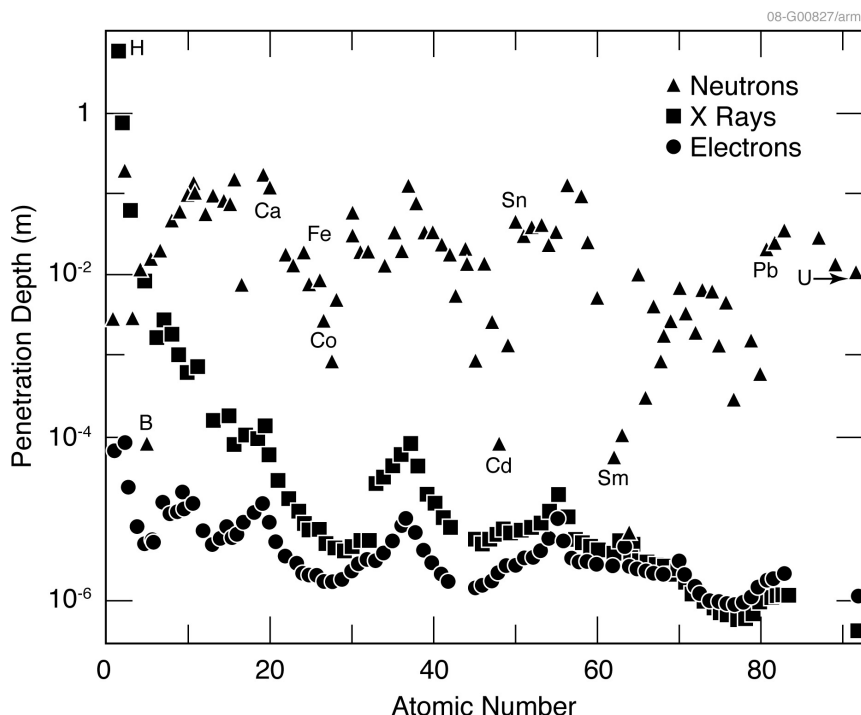


Fig. 2.1 The plot shows how deeply a beam of electrons, X-rays, or thermal neutrons penetrates a particular element in its solid or liquid form before the beam's intensity has been reduced by a factor $1/e$, which is about 37% of its original intensity. The neutron data are for neutrons having a wavelength of 0.14 nm

sive ways. This feature also means that no generic instrument can be designed to examine all aspects of neutron scattering. Instead a veritable zoo of instruments has arisen, each of which trades off the ability to resolve some details of the scattering in order to maintain sufficient scattered neutron intensity for a meaningful measurement.

In spite of its unique advantages, neutron scattering is only one of a battery of techniques for probing the structures of materials. All of the techniques, such as X-ray scattering, electron microscopy, and nuclear magnetic resonance (NMR), are needed if scientists are to understand the full range of structural properties of matter. In many cases, the different methods used to probe material structure give complementary information because the nature of the interactions between the probe and the sample are different.

To understand the neutron scattering technique, we first examine the *scattering by a single nucleus* and then *add up scattering from all of the nuclei* within the solid or liquid we are interested in. This allows us to describe phenomena like *neutron diffraction*, used to determine the atomic arrangement in a material, and

inelastic neutron scattering, which measures the vibrations of atoms. Minor modifications of the theory allows us to describe *Small-Angle Neutron Scattering (SANS)* that is used to study larger structures such as polymers and colloids, as well as *surface reflection* of neutrons (often called *reflectometry*) in which layered materials and interfaces are probed. The consequences of the neutron's magnetic moment can also be explored. It leads to *magnetic scattering* of neutrons as well as to the possibility of *polarized neutron beams* that can provide enhanced information about vector magnetization in materials.

2.1 Scattering by a Fixed Nucleus

The scattering of neutrons by nuclei is a quantum mechanical process. Formally, the process has to be described in terms of the wavefunctions of the neutron and the nucleus. Fortunately, the results of this calculation can be understood without going into all of the details involved. It is useful, though, to be able to switch to and fro between thinking about the *wavefunction of a neutron*—the squared modulus of which tells us the probability of finding a neutron at a particular point in space—and a particle picture of the neutron. This wave-particle duality is common in describing subatomic particles, and we will use it frequently, sometimes referring to neutrons as particles and sometimes as waves.

The neutrons used for scattering experiments usually have energies similar to those of atoms in a gas such as air. Not surprisingly, the velocities with which they move are similar to the velocities of gas molecules—a few kilometers per second. Quantum mechanics tells us that the wavelength of the neutron wave is inversely proportional to the speed of the neutron. For neutrons used in scattering experiment, the wavelength, λ , is usually between 0.1 and 1 nm. Often, we work in terms of the neutron wavevector \vec{k} , which is a vector of magnitude $2\pi/\lambda$ that points along the neutron's trajectory. The magnitude of the wavevector, \vec{k} , is related to the neutron velocity, v , by the equation

$$|\vec{k}| = 2\pi m v / h, \quad (2.1)$$

where h is Planck's constant and m is the mass of the neutron.

The scattering of a neutron by a free nucleus can be described in terms of a *cross section*, σ , measured in barns (1barn = 10^{-28} m²), that is equivalent to the effective area presented by the nucleus to the passing neutron. If the neutron hits this area, it is scattered isotropically, that is, with equal probability in any direction. The scattering is isotropic because the range of the nuclear interaction between the neutron and the nucleus is tiny compared with the wavelength of the neutron, so the nucleus essentially looks like a *point scatterer*.

Suppose that at an instant in time we represent neutrons incident on a fixed nucleus by a wavefunction $e^{i\vec{k}\cdot\vec{r}}$, in other words, a plane wave of unit amplitude.

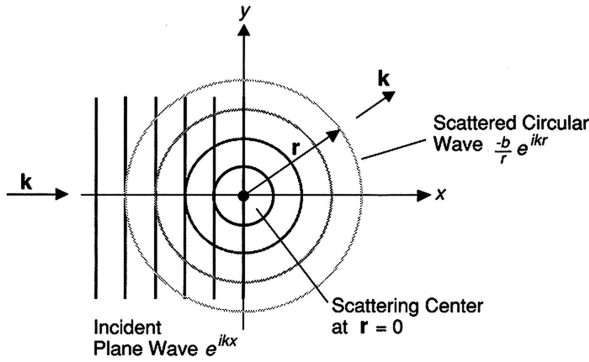


Fig. 2.2 A neutron beam incident on a single scattering center and traveling in the x direction can be represented by a plane wave e^{ikx} with unit amplitude. Because the neutron sees the scattering center (a nucleus) as a point, the scattering will be isotropic. As a result, the scattered neutron beam spreads out in spherical wavefronts (here drawn as circles) of amplitude b/r . The $1/r$ part of this amplitude factor, when squared to get neutron intensity, accounts for the $1/r^2$ decrease in intensity with distance that occurs as the scattered wavefront grows in size. Because we have taken the scattering center to be rigidly fixed, the scattering is elastic—that is, there is no change in the neutron's energy—so the incident and scattered wavevectors both have magnitude k

Note that the squared modulus of this wave function is unity for all positions \vec{r} so the neutron has the same probability of being found anywhere but has a definite momentum $mv = \hbar k/2\pi$. For a wave traveling in the x direction (i.e., for \vec{k} parallel to the x axis), the nodes of the wavefunction are straight wavefronts, as shown in Fig. 2.2.

The amplitude of the neutron wave scattered by the nucleus depends on the strength of the interaction between the neutron and the nucleus. Because the scattered wave is isotropic, its wavefunction can be written as $(-b/r)e^{ikr}$ if the scattering nucleus is at the origin of our coordinate system. The spherical wavefronts of the scattered neutrons are represented by the circles spreading out from the nucleus in Fig. 2.2. The factor $1/r$ in the wavefunction of the scattered neutron takes care of the inverse square law that applies to all wave motions: the intensity of the neutron beam, given by the square of the wavefunction, decreases as the inverse square of the distance from the source, in this case the scattering nucleus. The constant b , referred to as the **scattering length** of the nucleus, measures the strength of the interaction between the neutron and the nucleus. The minus sign means that b is a positive number for repulsive interaction between neutron and nucleus.

Because we have specified that the nucleus is fixed and because the energy of the neutron is too small to change the internal state of the nucleus, the scattering occurs without any change in the neutron's energy and is said to be **elastic**. Because the neutron's energy is unchanged by the collision, the same wavevector k appears in the incident and scattered wavefunctions. It turns out that the cross section, σ , is given by $\sigma = 4\pi b^2$ —as if the scattering length were half the radius of the nucleus as seen by the neutron. In the majority of cases of interest to neutron scatterers, b is a real energy-independent quantity that has to be determined by experiment or,

these days, simply looked up in a table called the *barn book*¹. The scattering length is not correlated with atomic number in any obvious systematic way and varies even from isotope to isotope of the same element. For example, hydrogen and deuterium, both of which interact weakly with X-rays because they only contain one electron, have neutron scattering lengths that are relatively large and quite different from one another. The differences in scattering length from one isotope to another can be used in various *isotope-labeling* techniques to increase the amount of information obtained from some neutron scattering experiments.

2.2 Scattering of Neutrons by Matter

To work out how neutrons are scattered by matter, we need to *add up the scattering from each individual nucleus*. The result of this lengthy quantum mechanical calculation is quite simple to explain and understand, even if the details are abstruse.

When neutrons are scattered by matter, the process can alter both the momentum and the energy of the neutrons and the matter. The scattering is not necessarily elastic as it is for a single fixed nucleus because the atoms in matter are free to move to some extent. They can therefore recoil during a collision with a neutron or, if they are moving when a neutron arrives, they can impart energy to the neutron. As is usual in a collision, the total energy and momentum are conserved: the energy, E , lost by the neutron in a collision is gained by the scattering sample. From Equation (2.1) it is easy to see that the amount of momentum given up by the neutron during its collision, the *momentum transfer*, is $\hbar \vec{Q}/2\pi = \hbar(\vec{k} - \vec{k}')/2\pi$, where \vec{k} is the wavevector of the incident neutrons and \vec{k}' is that of the scattered neutrons. The quantity $\vec{Q} = \vec{k} - \vec{k}'$ is known as the *scattering vector*, and the vector relation between \vec{Q} , \vec{k} , and \vec{k}' can be displayed pictorially in the so-called *scattering triangle* (Fig. 2.3). The angle 2θ shown in the scattering triangles is the angle through which the neutron is deflected during the scattering process. It is referred to as the *scattering angle*. For elastic scattering, for which $|\vec{k}| = |\vec{k}'|$, a little trigonometry applied to the triangles shows that $Q = 4\pi \sin \theta/\lambda$.

In all neutron scattering experiments, scientists measure the intensity of neutrons scattered by matter (per incident neutron) as a function of the variables Q and E . The scattered intensity, denoted $I(\vec{Q}, E)$, is often referred to colloquially as the *neutron-scattering law* for the sample material. In 1954, Van Hove [1] showed that the scattering law can be written in terms of time-dependent correlations between the positions of pairs of atoms in the sample. Van Hove's result implies that $I(\vec{Q}, E)$ is proportional to the Fourier transform of a function that gives the probability of finding two atoms a certain distance apart. It is the simplicity of the result that

¹ Thermal neutron cross-sections have been tabulated in a variety of places. The most accessible source these days is likely the NIST web site www.ncnr.nist.gov, which lists values tabulated in *Neutron News*, **3**(3) (1992), pp. 29–37. An alternative source is the *Neutron Data Booklet* (A. J. Dianoux and G. H. Lander Eds) published by the Institut Laue-Langevin, Grenoble, France. This can be ordered at <http://www-llb.cea.fr/menl/neutronlist/msg00063.html>.

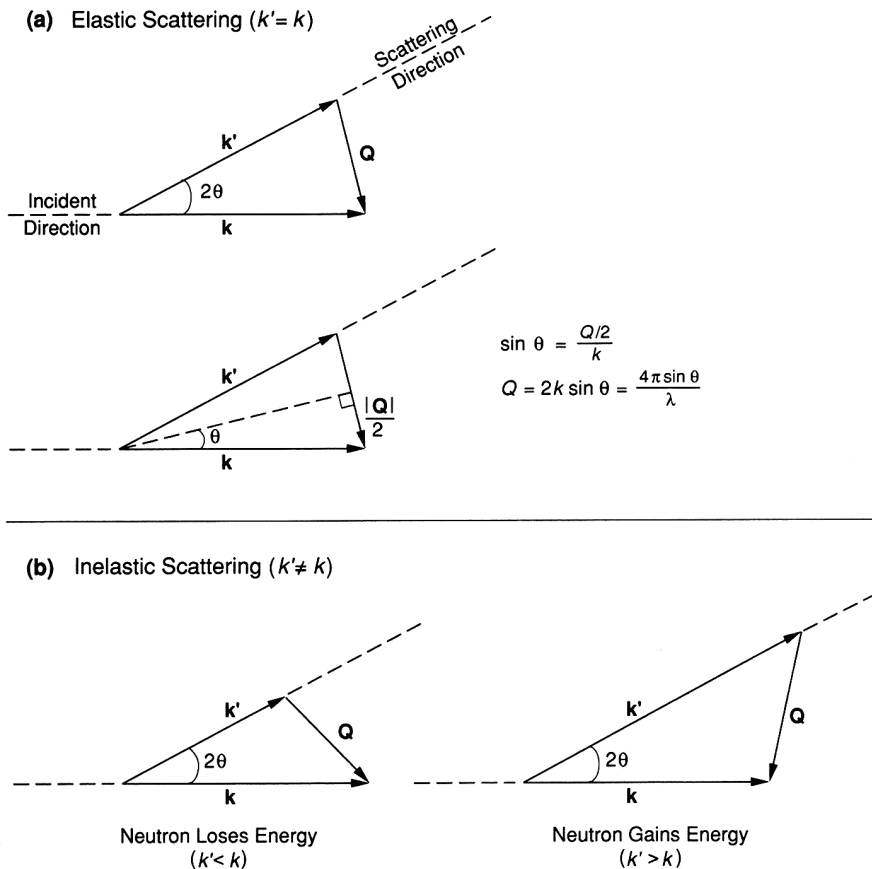


Fig. 2.3 Scattering triangles are depicted here for both **(a)** an elastic scattering event in which the neutron is deflected but does not gain or lose energy (so that $k' = k$) and **(b)** inelastic scattering in which the neutron either loses energy ($k' < k$) or gains energy ($k' > k$) during the interaction with the sample. In both elastic and inelastic scattering events, the neutron is scattered through the angle 2θ , and the scattering vector is given by the vector relationship $\vec{Q} = \vec{k} - \vec{k}'$. For elastic scattering, simple trigonometry shows (lower triangle in **(a)**) that $Q = 4\pi \sin \theta / \lambda$.

is responsible for the power of neutron scattering. If nature had been unkind and included correlations between triplets and quadruplets in the expression for the scattering law, neutron scattering would never have been used to probe the structure of materials.

Van Hove's work makes use of an observation made by Fermi that the actual interaction between a neutron and a nucleus may be replaced by an effective potential that is much weaker than the actual interaction. This so-called pseudo-potential causes the same scattering as the actual potential but is weak enough to be used in a perturbation treatment of scattering originally derived by Max Born. The Born

approximation [2] says that the probability of a neutron wave of wavevector \vec{k} being scattered by a potential $V(\vec{r})$ to become an outgoing wave of wavevector \vec{k}' is proportional to

$$\left| \int e^{i\vec{k}\cdot\vec{r}} V(\vec{r}) e^{-i\vec{k}'\cdot\vec{r}} d\vec{r} \right|^2 = \left| \int e^{i\vec{k}\cdot\vec{r}} V(\vec{r}) d\vec{r} \right|^2, \quad (2.2)$$

where the integration is over the volume of the sample. The potential $V(r)$ to be used in this equation is the Fermi pseudo-potential which, for an assembly of nuclei situated at positions \vec{r}_j , is given by

$$V(\vec{r}) = \frac{2\pi\hbar^2}{m} \sum_j b_j \delta(\vec{r} - \vec{r}_j), \quad (2.3)$$

where $\delta(\vec{r})$ is a Dirac delta function, which takes the value unity at position \vec{r} and is zero everywhere else. The b_j that appear in Equation (2.3) are the scattering lengths that we encountered earlier. Van Hove was able to show that the scattering law $I(\vec{Q}, E)$ could be written as

$$I(\vec{Q}, E) = \frac{1}{h} \frac{k'}{k} \sum_{i,j} b_i b_j \int_{-\infty}^{\infty} \left\langle e^{-i\vec{Q}\cdot\vec{r}_i(0)} e^{i\vec{Q}\cdot\vec{r}_j(t)} \right\rangle e^{-i(E/\hbar)t} dt. \quad (2.4)$$

In this equation, the nucleus labeled i is at position \vec{r}_i at time zero, while the nucleus labeled j is at position \vec{r}_j at time t . Equation (2.4) is a double sum over all of the positions of the nuclei in the sample, and the angular brackets $\langle \dots \rangle$ indicate that we need to do a thermodynamic average over all possible configurations that the sample could take. The steps in Van Hove's calculation are given in detail in several texts, for example, *The Theory of Thermal Neutron Scattering* by G. L. Squires [3].

The position vectors $\vec{r}_i(0)$ and $\vec{r}_j(t)$ are quantum mechanical position operators so, while Equation (2.4) looks simple, it is not as simple to evaluate in practice as one might imagine. To get a feeling for what the equation is telling us, we can try ignoring this subtlety and treat the vectors as classical quantities. In this case, the double sum in Equation (2.4) becomes

$$\sum_{i,j} b_i b_j \left\langle e^{-i\vec{Q}\cdot[\vec{r}_i(0) - \vec{r}_j(t)]} \right\rangle = \sum_{i,j} b_i b_j \int_{\text{sample}} \delta[\vec{r} - \vec{r}_i(0) + \vec{r}_j(t)] e^{-i\vec{Q}\cdot\vec{r}} d\vec{r}. \quad (2.5)$$

Let us suppose further that all of the nuclei in our sample have the same scattering length so that $b_i = b_j = b$. Then the right-hand side of Equation (2.5) becomes

$$Nb^2 \int_{\text{sample}} G(\vec{r}, t) e^{-i\vec{Q}\cdot\vec{r}}, \quad (2.6)$$

where

$$G(\vec{r}, t) = \frac{1}{N} \sum_{i,j} \delta(\vec{r} - [\vec{r}_i(0) - \vec{r}_j(t)]), \quad (2.7)$$

and N is the number of nuclei in the sample. Evidently, the function $G(\vec{r}, t)$ is zero unless the separation between nucleus i at time zero and nucleus j at time t is equal to the vector \vec{r} . Thus, the function tells us the probability that, within our sample, there will be a nucleus at the origin of our coordinate system at time zero *as well as* a nucleus at position \vec{r} at time t . For this reason, $G(\vec{r}, t)$ is called the **time-dependent pair correlation function** because it describes how the correlation between the positions of nuclei evolves with time.

In terms of $G(\vec{r}, t)$, Van Hove's scattering law can be written as

$$I(\vec{Q}, E) = \frac{Nb^2}{h} \frac{k'}{k} \int_{-\infty}^{\infty} dt \int_{\text{sample}} G(\vec{r}, t) e^{-i\vec{Q} \cdot \vec{r}} e^{-i(E/\hbar)t} d\vec{r}, \quad (2.8)$$

which allows us to see that the scattering law is proportional to the space and time Fourier transform of the time-dependent correlation function. This general result provides a unified description of all neutron scattering experiments. By inverting Equation (2.8)—easier said than done in many cases—we can obtain from neutron scattering information about both the equilibrium structure of matter and the way in which this structure evolves with time.

Even for a sample made up of a single isotope, all of the scattering lengths that appear in Equation (2.4) will not be equal. This occurs because the interaction between the neutron and the nucleus depends on the nuclear spin, and most isotopes have several nuclear spin states. Generally, however, there is no correlation between the spin of a nucleus and its position in a sample of matter. For this reason, the scattering lengths that appear in Equation (2.4) can be averaged without interfering with the thermodynamic average denoted by the angular brackets. Two averages come into play: the average value of b (denoted $\langle b \rangle$) and the average value of b^2 (denoted $\langle b^2 \rangle$). In terms of these quantities, the sum in Equation (2.4) can be averaged over the nuclear spin states to read

$$\sum_{i,j} \langle b_i b_j \rangle A_{ij} = \sum_{i,j} \langle b \rangle^2 A_{ij} + \sum_i (\langle b^2 \rangle - \langle b \rangle^2) A_{ii}, \quad (2.9)$$

where A_{ij} is shorthand for the integral in Equation (2.4). The first term is a sum over all pairs of nuclei in the sample. While i and j are occasionally the same nucleus, in general they are not because there are so many nuclei in the sample.

The first term in Equation (2.9) is **coherent scattering** in which neutron waves scattered from **different** nuclei interfere with each other. This type of scattering depends on the distances between atoms (through the integral represented by A_{ij})

and on the scattering vector \vec{Q} , and it thus gives information about the structure of a material. **Elastic coherent** scattering tells us about the *equilibrium structure*, whereas **inelastic coherent scattering** (with $E \neq 0$) provides information about the collective motions of the atoms, such as those that produce *phonons* or vibrational waves in a crystalline lattice. In the second type of scattering, **incoherent scattering**, represented by the second term in Equation (2.9), there is no interference between the waves scattered by different nuclei. Rather the intensities scattered from each nucleus just add up independently. Once again, one can distinguish between elastic and inelastic scattering. **Incoherent elastic scattering** is the same in all directions, so it usually appears as unwanted background in neutron scattering experiments. **Incoherent inelastic scattering**, on the other hand, results from the interaction of a neutron with the same atom at different positions and different times, thus providing information about atomic diffusion.

The values of the coherent and incoherent scattering lengths given by $b_{\text{coh}} = \langle b \rangle$ and $b_{\text{inc}} = \sqrt{\langle b^2 \rangle - \langle b \rangle^2}$ for different elements and isotopes do not vary in any systematic way across the periodic table. For example, hydrogen has a large incoherent scattering length (25.18 fm) and a small coherent scattering length (−3.74 fm). Deuterium, on the other hand, has a small incoherent scattering length (3.99 fm) and a relatively large coherent scattering length (6.67 fm).

The simplest type of coherent scattering to understand is **diffraction**. As the incident neutron wave arrives at each atom, the atomic site becomes the center of a scattered spherical wave that has a definite phase relative to all other scattered waves. As the waves spread out from a regular array of sites in a crystal, the individual disturbances will reinforce each other only in particular directions. These directions are closely related to the symmetry and spacing of the scattering sites. Consequently, one may use the directions in which constructive interference occurs and its intensity to deduce both the symmetry and the lattice constant of a crystal.

Even though diffraction is predominantly an elastic scattering process (i.e., one for which $E = 0$), most neutron diffractometers integrate over the energies of scattered neutrons. Accordingly, in the Van Hove formalism, rather than setting $E = 0$ in Equation (2.4), we integrate the equation over E to obtain the diffracted intensity. The integral over E gives us another Dirac delta function, this time $\delta(t)$, which tells us that the pair correlation function $G(\vec{r}, t)$ has to be evaluated at $t = 0$. For a sample containing a single isotope, the result is

$$I(\vec{Q}) = b_{\text{coh}}^2 \sum_{i,j} \left\langle e^{i\vec{Q} \cdot (\vec{r}_i - \vec{r}_j)} \right\rangle, \quad (2.10)$$

where the positions of the nuclei labeled i and j are now to be evaluated at the same instant. If the atoms in the crystal were stationary, the thermodynamic averaging brackets in Equation (2.10) could be removed because \vec{r}_i and \vec{r}_j would be constants. In reality, the atoms in a crystal oscillate about their equilibrium positions and spend only a fraction of the time at these positions. When this is taken into account, the thermodynamic averaging introduces another factor, so that

$$I(\vec{Q}) = b_{\text{coh}}^2 \sum_{i,j} e^{i\vec{Q} \cdot (\vec{r}_i - \vec{r}_j)} e^{-Q^2 \langle u^2 \rangle / 2} = \left| b_{\text{coh}} \sum_i e^{i\vec{Q} \cdot \vec{r}_i} \right|^2 e^{-Q^2 \langle u^2 \rangle / 2} \equiv S(\vec{Q}), \quad (2.11)$$

where $e^{-Q^2 \langle u^2 \rangle / 2}$ is called the **Debye–Waller factor** and $\langle u^2 \rangle$ is the average of the squared displacement of nuclei from their equilibrium lattice sites. Equation (2.11) gives the intensity that would be measured in a neutron scattering experiment with a real crystal. This quantity is often denoted by $S(\vec{Q})$ and called the **structure factor**.

Because there are so many atoms in a crystal, and each contributes a different phase factor to Equation (2.11), it is perhaps surprising that $S(\vec{Q})$ is non-zero for any value of \vec{Q} . We can determine the values of \vec{Q} that give non-zero values by consulting Fig. 2.4. Suppose \vec{Q} is perpendicular to a plane of atoms such as Scattering Plane 1 in this figure. If the value of \vec{Q} is an integral multiple of $2\pi/d$, where d is the distance between parallel neighboring planes of atoms (Scattering Planes 1 and 2 in the figure), then $\vec{Q} \cdot (\vec{r}_i - \vec{r}_j)$ is a multiple of 2π and $S(\vec{Q})$ is non-zero because each exponential term in the sum in Equation (2.11) is unity. Thus, for diffraction to occur, \vec{Q} must be perpendicular to a set of atomic planes. Using the relationship between Q , θ , and λ shown in Fig. 2.3, the condition for diffraction is easily rewritten as **Bragg’s Law** (discovered in 1912 by William and Lawrence Bragg, father and son [4]).

$$n\lambda = 2d \sin \theta. \quad (2.12)$$

Bragg’s law can also be understood in terms of the path-length difference between the waves scattered from neighboring planes of atoms (Fig. 2.4), and it is often taught that way in undergraduate physics classes, even though the planes of atoms do not really reflect neutrons like mirrors. For constructive interference to occur between the waves scattered from adjacent planes, the argument goes, the path-length difference must be a multiple of the wavelength, λ . Applying this condition to Fig. 2.4 immediately yields Equation (2.12).

Diffraction, or **Bragg scattering** as it is sometimes called, may occur for any set of planes that we can imagine in a crystal, provided the neutron wavelength, λ , and the angle θ satisfy Equation (2.12). To obtain diffraction from a set of planes, the crystal must be rotated to the correct orientation so that \vec{Q} is perpendicular to the scattering planes—much as a mirror is adjusted to reflect the sun at someone’s face. The signal that is observed in a neutron detector as the crystal is rotated in this way is called a **Bragg peak** because the signal appears only when the crystal is in the correct orientation. According to Equation (2.11), the intensity of the scattered neutrons is proportional to the square of the density of atoms in the atomic planes responsible for the scattering. Thus an observation of Bragg peaks allows us to deduce both the spacing of the planes and the density of atoms in the planes. To measure Bragg peaks corresponding to many different atomic planes, we have to pick the neutron wavelength and scattering angle to satisfy Bragg’s Law and then rotate the crystal until the Bragg diffracted beam falls on the detector.

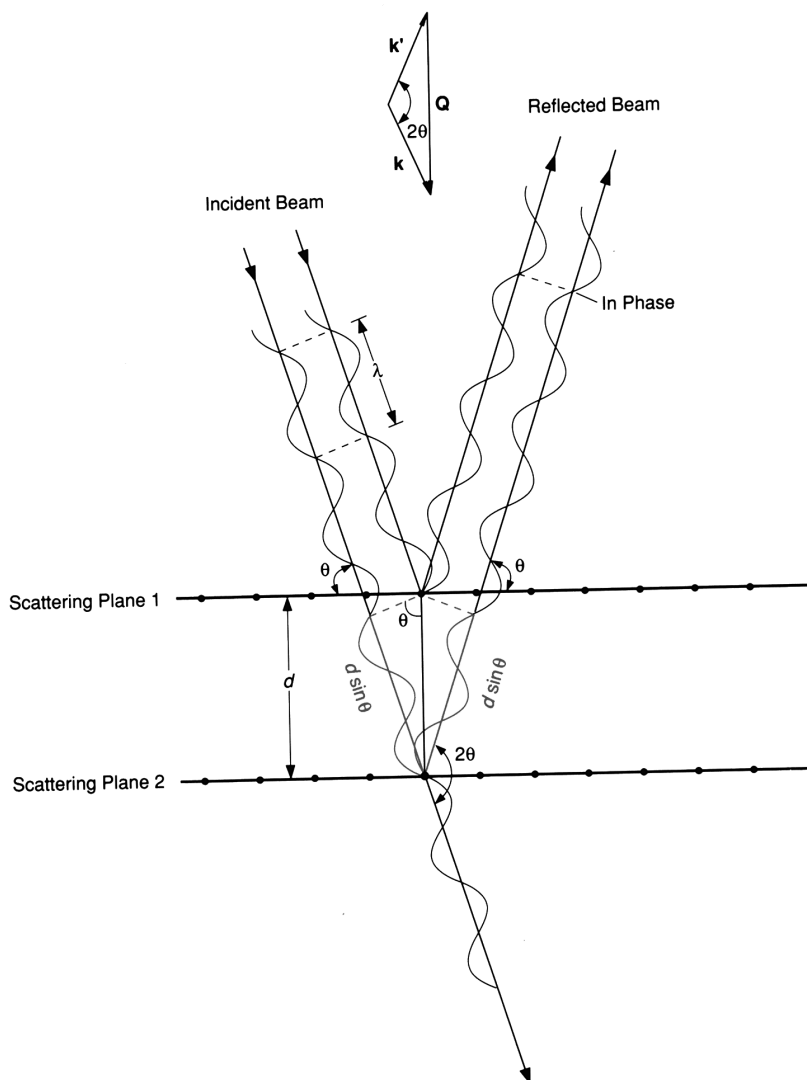


Fig. 2.4 Constructive interference occurs when the waves scattered from adjacent scattering planes of atoms remain in phase. This happens when the difference in distance traveled by waves scattered from adjacent planes is an integral multiple of wavelength. The figure shows the extra distance traveled by the wave scattered from Scattering Plane 2 is $2d \sin \theta$. When that distance is set equal to $n\lambda$ (where n is an integer), the result is Bragg's Law $n\lambda = 2d \sin \theta$. Primary scattering occurs when $n = 1$, but higher-order Bragg peaks are also observed for other values of n

To this point we have been discussing a simple type of crystal with one type of atom. However, the materials of interest to scientists almost invariably contain many different types of atoms. It is often not trivial to deduce the atomic positions even from a measurement of the intensities of many Bragg peaks because some of the exponential factors that contribute to $S(\vec{Q})$ are now complex and the phases of these quantities cannot be obtained directly from the measurement of Bragg scattering. $S(\vec{Q})$, given by Equation (2.11), is equal to the square of the modulus of a complex quantity, so the phase of this quantity simply cannot be obtained by measuring scattered intensities. This difficulty is referred to as the *phase problem* in diffraction. In practice, crystallographers generally have to resort to modeling the structure of crystals, shifting atoms around until they find an arrangement that accurately predicts the measured Bragg intensities when plugged into Equation (2.11). There are now many computer packages available to help them. One well known package is that by Larson and Von Dreele [5].

In diffraction experiments with single crystals, the sample must be correctly oriented to obtain Bragg scattering. On the other hand, polycrystalline powders, which consist of many randomly oriented single-crystal grains, will diffract neutrons whatever the relative orientation of the sample and the incident neutron beam. There will always be grains in the powder that are correctly oriented to diffract. However, many diffracting planes may “reflect” under the same or very similar angle, hence the need for high resolution (see Chapter 1 and Chapter 4). This observation is the basis of a widely used technique known as *neutron powder diffraction*.

In a *powder diffractometer at a reactor neutron source*, a beam of neutrons with a single wavelength is selected by a device called a *monochromator* and directed toward a powder sample. The monochromator is usually an assembly of single crystals—often made of either pyrolytic graphite, silicon, or copper—each correctly oriented to diffract a mono-energetic beam of neutrons toward the scattering sample. The neutrons scattered from a powder sample are counted by suitable neutron detectors and recorded as a function of the angles through which they were scattered by the sample. Each Bragg peak in a typical diffraction pattern (Fig. 2.5) corresponds to diffraction from atomic planes with different interplanar spacings, d .

In a *powder diffractometer at a pulsed neutron source*, the sample is irradiated by a pulsed beam of neutrons with a wide spectrum of energies. Scattered neutrons are recorded in banks of detectors located at different scattering angles, and the time at which each scattered neutron arrives at the detector is also recorded. At a particular scattering angle, the result is a diffraction pattern very similar to that measured at a reactor, but now the independent variable is the neutron’s *time of flight* rather than the scattering angle. The time of flight is easily deduced from the arrival time of the neutron because we know when the pulse of neutrons left the source. Because the neutron’s time of flight is inversely proportional to its velocity, it is linearly related to the neutron wavelength.

At both reactors and pulsed sources, powder diffraction patterns can be plotted as a function of the interplanar separations, d , by using Bragg’s law to derive the value of d from the natural variables—scattering angle at a reactor and neutron wavelength at a pulsed source. Using these patterns, the atomic structure of a polycrystalline sample may be deduced by using Equation (2.11) and shifting the atoms

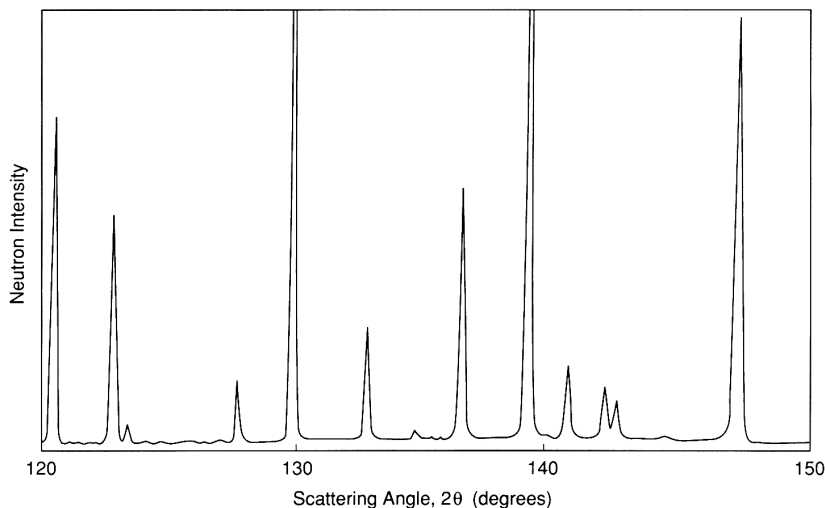


Fig. 2.5 A typical powder diffraction pattern obtained at a reactor neutron source gives the intensity, or number of neutrons, as a function of the scattering angle 2θ . Each peak represents neutrons that have been scattered from a particular set of atomic planes in the crystalline lattice

around until a good fit to the experimental pattern is obtained. In practice, one needs to account carefully for the shape of the Bragg peaks in carrying out this refinement. These shapes result from the fact that the diffractometers really use a small range of wavelengths or scattering angles rather than a single value as we have assumed—an effect called *instrumental resolution*. The simultaneous refinement of the atomic positions to obtain a powder diffraction pattern that is the same as the measured pattern is often referred to as *Rietveld analysis*, after the inventor of the technique [6].

2.3 Probing Larger Structures

We have seen already in our discussion of diffraction that elastic scattering at a scattering vector $Q = (4\pi/\lambda) \sin \theta$ results from periodic modulations of the neutron scattering lengths with period $d = 2\pi/Q$. Combining these two expressions gives us Bragg's Law (Equation (2.12)). In the case of a crystal, d was interpreted as the distance between the planes of atoms. To measure structures that are larger than typical interatomic distances, we need to arrange for Q to be small, either by increasing the neutron wavelength, λ , or by decreasing the scattering angle. Because we do not know how to produce copious fluxes of very-long-wavelength neutrons, we always need to use small scattering angles to examine larger structures such as polymers, colloids, or viruses. For this reason, the technique is known as *small-angle neutron scattering*, or SANS.

For SANS, the scattering wavevector, Q , is small, so the phase factors in Equation (2.11) do not vary greatly from one nucleus to its neighbor. For this reason,

the sum in Equation (2.11) can be replaced by an integral and the structure factor for SANS can be written as

$$S(\vec{Q}) = \left| \int_{\text{sample}} \rho(\vec{r}) e^{i\vec{Q} \cdot \vec{r}} d\vec{r} \right|^2, \quad (2.13)$$

where $\rho(\vec{r})$ is a spatially varying quantity called the **scattering length density** calculated by summing the coherent scattering lengths of all atoms over a small volume (such as that occupied by a single molecule) and dividing by that volume. In many cases, samples measured by SANS can be thought of as particles with a constant scattering length density, ρ_p , which are dispersed in a uniform medium with scattering length density ρ_m . Examples include pores in rock, colloidal dispersions, biological macromolecules in water, and many more. The integral in Equation (2.13) can, in this case, be separated into a uniform integral over the whole sample and terms that depend on the difference, $(\rho_p - \rho_m)$, a quantity often called the **contrast factor**. If all of the particles are identical and their positions are uncorrelated, Equation (2.13) becomes

$$S(\vec{Q}) = N_p (\rho_p - \rho_m)^2 \left| \int_{\text{particle}} e^{i\vec{Q} \cdot \vec{r}} d\vec{r} \right|^2, \quad (2.14)$$

where the integral is now over the volume of one of the particles and N_p is the number of particles in the sample. The integral of the phase factor $e^{i\vec{Q} \cdot \vec{r}}$ over a particle is called the **form factor** for that particle. For many simple particle shapes, the form factor can be evaluated analytically [7], whereas for complex biomolecules, for example, it has to be computed numerically. Usually, the intensity one sees plotted for SANS is normalized to the sample volume so that $S(Q)$ is reported in units of cm^{-1} (as compared with Equation (2.14), which has units of length squared).

Equation (2.14) allows us to understand an important technique used in SANS called **contrast matching**. The total scattering is proportional to the square of the scattering contrast between the particle and the matrix in which it is embedded. If we embed the particle in a medium whose scattering length density is equal to that of the particle, the latter will not scatter—it will be invisible.

Suppose that the particles we are interested in are spherical eggs rather than uniform spheres: they have a core (the yolk) and a shell (the white) whose scattering lengths are different. If such particles are immersed in a medium whose scattering length density is equal to that of the egg white, then a neutron scattering experiment will only “see” the yolk. The form factor in Equation (2.14) will be evaluated by integrating over this central region only. On the other hand, if the dispersing medium has the scattering length density of the yolk, only the egg white will be visible: the form factor will be that of a thick hollow shell. The scattering patterns will be different in the two cases, and from two experiments, we will discover the structure of both the coating and the core of the particle.

Variation of the scattering length density of the matrix is often achieved by choosing a matrix that contains hydrogen (such as water). By replacing different fractions of the hydrogen with deuterium atoms, a large range of scattering length densities can be achieved for the matrix. Both DNA and typical proteins can be contrast matched by water containing different fractions of deuterium. *Isotopic labeling* of this type can also be applied to parts of molecules in order to highlight them for neutron scattering experiments.

2.4 Inelastic Scattering

In reality, atoms are not frozen in fixed positions inside a crystal. Thermal energy causes them to oscillate about their lattice sites and to move around inside a small volume with the lattice site as its center. Since an atom can contribute to the constructive interference of Bragg scattering *only* when it is located exactly at its official position at a lattice site, this scattering becomes weaker the more the atoms vibrate and the less time they spend at their official positions. The factor by which the Bragg peaks are attenuated because of the atomic motion is called the *Debye–Waller factor*. It was introduced above in connection with Equation (2.11).

Although such weakening of the scattering signal is the only effect of the thermal motions of atoms on elastic Bragg scattering, it is not the only way to use neutrons to study atomic motions. In fact, one of the great advantages of neutrons as a probe of condensed matter is that they can be used to measure details of atomic and molecular motions by measuring *inelastic scattering* in which the neutron exchanges energy with the atoms in a material.

Atoms in a crystal lattice behave a bit like coupled pendulums—if we displace one pendulum, the springs that couple the pendulums together will cause the neighboring pendulums to move as well and a wave-like motion propagates down the line of pendulums. The frequency of the motion depends on the mass of the pendulums and the strength of the spring constants coupling them. Similar waves pass through a lattice of atoms connected by the binding forces that are responsible for the cohesion of matter. Of course, in this case, the atomic vibrations occur in three dimensions and the whole effect becomes a little hard to visualize. Nevertheless, it is possible to prove that any atomic motion in the crystal can be described by a superposition of waves of different frequencies and wavelengths traveling in different directions. These lattice waves are known as *phonons*. Their energies are quantized so that each phonon has an energy $h\nu$, where ν is the frequency of atomic motion associated with the phonon. Just as in the pendulum analogy, the frequency of the phonon depends on the wavelength of the distortion, the masses of the atoms, and the stiffness of the “springs”, or binding forces, that connect them.

When a neutron is scattered by a crystalline solid, it can absorb or emit an amount of energy equal to a quantum of phonon energy, $h\nu$. This gives rise to *inelastic coherent scattering* in which the neutron energy before and after the scattering differ by an amount, E —the same quantity that appeared in Equation (2.8)—equal

to the phonon energy. In most solids ν is a few terahertz (THz), corresponding to phonon energies of a few meV (1 THz corresponds to an energy of 4.18 meV). Because the thermal neutrons used for neutron scattering also have energies in the meV range, scattering by a phonon causes an appreciable fractional change in the neutron energy, allowing accurate measurement of phonon frequencies.

For inelastic scattering, the neutron has different velocities, and thus different wavevectors, before and after it interacts with the sample. To determine the phonon energy and the scattering vector, \vec{Q} , we need to determine the neutron wavevector before and after the scattering event. Different methods are used to accomplish this at reactor and pulsed neutron sources. At reactors the workhorse instruments for this type of measurement are called *three-axis spectrometers*. They work by using assemblies of single crystals both to set the incident neutron wavevector and to analyze the wavevector of the scattered neutrons. Each measurement made on a three-axis spectrometer—usually taking several minutes—records the scattered neutron intensity at a single wavevector transfer and a single energy transfer. To determine the energy of a phonon, a sequence of measurements is usually made at a constant value of the wavevector transfer. The peak that is obtained during this *constant-Q* scan yields the energy of the phonon. Constant-Q scans were invented by B. N. Brockhouse [8], one of the co-winners with C. Shull in 1994 of the Nobel Prize for their work on neutron scattering. At pulsed spallation sources, there is no real equivalent of the three-axis spectrometer and constant-Q scans cannot be performed using hardware. Rather, the time-of-flight technique is used with a large array of detectors and various cuts through the data in (\vec{Q}, E) space are performed after the experiment using appropriate computer software.

2.5 Magnetic Scattering

So far we have discussed only the interaction between neutrons and atomic nuclei. But there is another interaction between neutrons and matter—one that results from the fact that the neutron has a magnetic moment. Just as two bar magnets either attract or repel one another, the neutron experiences a force of magnetic origin whenever it moves in a magnetic field, such as that produced by unpaired electrons in matter.

Ferromagnetic materials, such as iron, are magnetic because the moments of their unpaired electrons tend to align spontaneously. For many purposes, such materials behave as if small magnetic moments were located at each atomic site with all the moments pointing in the same direction. These moments give rise to *magnetic Bragg scattering* of neutrons in the same manner as the nuclear interactions. Because the nuclear and magnetic interactions experienced by the neutron are of similar magnitude, the corresponding Bragg reflections are also of comparable intensity.

One difference between the two types of scattering, however, is that the magnetic interaction, unlike the nuclear interaction is not isotropic. The magnetic interaction

is dipolar, just like that between two bar magnets. And just like two bar magnets, the strength of the interaction between the neutron and a nucleus depends on the relative orientations of their magnetic moments and the line joining their centers. For neutrons, the dipolar nature of the magnetic interaction means that only the component of the sample's magnetization, which is perpendicular to the scattering vector, \vec{Q} , is effective in scattering neutrons. Neutron scattering is therefore sensitive to the spatial distribution of both the direction and the magnitude of magnetization inside a material.

The anisotropic nature of the magnetic interaction can be used to separate nuclear and magnetic Bragg peaks in ferromagnets, for which both types of Bragg peaks occur at the same values of \vec{Q} . If the electronic moments can be aligned by an applied magnetic field, magnetic Bragg peaks for which \vec{Q} is parallel to the induced magnetization vanish, leaving only the nuclear component. On the other hand, an equivalent Bragg peak for which \vec{Q} is perpendicular to the magnetization will manifest both nuclear and magnetic contributions.

2.6 Polarized Neutrons

Usually, a neutron beam contains neutrons with magnetic moments pointing in all directions. If we measured the number of neutrons with moments parallel and antiparallel to a given direction—say an applied magnetic field—we would find equal populations. However, various special techniques can generate a polarized neutron beam, that is, one where the majority of neutron moments are in the same direction. The polarization of such a beam, once it is created, can be maintained by applying a small, slowly varying magnetic field (a milli-Tesla is enough) parallel to the neutron moments. Such a field is called a *guide field*.

There are several ways to polarize neutron beams: Bragg diffraction from suitable magnetized crystals [9], reflection from magnetized mirrors made of CoFe or from supermirrors [10], and transmission through polarized ^3He [11], for example. Each of these methods selects neutrons whose magnetic moments are either aligned parallel or antiparallel to an applied magnetic field and removes other neutrons from the beam in some way. If the neutron moments are parallel to the applied field, they are said to be “*up*”: if the moments are antiparallel they are said to be “*down*”. An “*up*” polarizer will not transmit “*down*” neutrons, and a “*down*” polarizer blocks “*up*” neutrons. Thus, by placing “*up*” polarizers before and after a sample, the neutron scattering law can be measured for those scattering processes in which the direction of the neutron moments are not changed by the scattering process. To measure the other combinations—such as “*up*” neutron being flipped to “*down*” neutrons—requires either a combination of “*up*” and “*down*” polarizers or a *flipper*, a device that can change a neutron spin from “*up*” to “*down*” or vice versa. Various types of flippers have been developed over the years, but the most common these days are direct-current coils (often called Mezei flippers) and adiabatic rf flippers [12].

If flippers are inserted on either side of a sample, we can measure all of the neutron-spin-dependent scattering laws—up to down, up to up, and so forth—simply by turning the appropriate flipper on or off. This technique, known as *polarization analysis*, is useful because some scattering processes flip the neutron's magnetic moment, whereas others do not. Scattering from a sample that is magnetized provides a good example. It turns out that magnetic scattering will flip the neutron's moment if the magnetization responsible for the scattering is perpendicular to the magnetic field used to maintain the neutron's polarization at the sample position. If the scattering magnetization is parallel to the guide field, no flipping of the neutron spin occurs. Thus, polarization analysis can be used to determine the direction of the magnetic moments in a sample that is responsible for particular contributions to the neutron scattering pattern.

Incoherent scattering (cf. Equation (2.9)) that arises from the random distribution of nuclear spin states in materials provides another example of the use of polarization analysis. Most isotopes have several nuclear spin states, and the scattering cross section for neutrons varies with the spin states of both the nucleus and the neutron. The random distribution of nuclear spins in a sample gives rise to incoherent scattering of neutrons as we have described above. It turns out that two-thirds of the neutrons scattered by this incoherent process have their spins flipped, whereas the moments of the remaining third are unaffected. This result is independent of the isotope that is responsible for the scattering and of the direction of the magnetic guide field at the sample. Although incoherent scattering can also arise if the sample contains a mixture of isotopes of a particular element, neither this second type of incoherent scattering nor coherent scattering flip the neutron's spin. Polarization analysis thus becomes a useful tool for sorting out these different types of scattering, allowing nuclear coherent scattering to be distinguished from magnetic scattering and nuclear spin-incoherent scattering.

The polarization of neutron beams can also be used to improve the resolution of neutron spectrometers using a technique known as *neutron spin echo* [13]. If the magnetic moment of a neutron is somehow turned so that it is perpendicular to an applied magnetic field, the neutron moment starts to precess around the field direction, much like the second hand on a stopwatch rotates about the spindle in the center of the watch. This motion of the neutron moment is called *Larmor precession*. The sense of the precession—clockwise or anticlockwise—depends on the sense of the magnetic field, and the rate of precession is proportional to the magnitude of the applied magnetic field. If a neutron is sent through two identical regions in which the magnetic fields are equal but oppositely directed, it will precess in one direction in the first field and in the opposite direction in the second field. Because the fields are equal in strength, the number of forward rotations will be equal to the number of backward rotations. This is the phenomenon of spin echo, first discovered by Hahn for nuclear spins [14]. If the neutron's speed changes between these field regions—because it is inelastically scattered, for example—the number of forward and backward rotations will not be equal. In fact, the difference will be proportional to the change in the neutron's speed. By measuring the final polarization of the neutron beam, we can obtain a sensitive measure of the change of neutron speed

and hence the change in its energy, E , caused by a scattering event. Spin echo spectrometers based on this method provide the best energy resolution obtainable with neutrons—they can measure neutron energy changes less than a nano-electron-volt.

2.7 Reflectometry

So far we have described only experiments in which the structure of bulk matter is probed. One may ask whether neutrons can provide any information about the structure at or close to the surfaces of materials. At first sight, one might expect the answer to be a resounding “No!” After all, one of the advantages of neutrons is that they can penetrate deeply into matter without being affected by the surface. Furthermore, because neutrons interact only weakly with matter, large samples are generally required. Because there are far fewer atoms close to the surface of a sample than in its interior, it seems unreasonable to expect neutron scattering to be sensitive to surface structure.

In spite of these objections, it turns out that neutrons are sensitive to surface structure when they impinge on surfaces at sufficiently low angles. In fact, for smooth, flat surfaces, reflection of neutrons occurs for almost all materials at angles of incidence, α_i (defined for neutrons as the angle between the incident beam and the surface), less than a **critical angle**, denoted γ_c . Surface reflection of this type is **specular**; that is, the angle of incidence, α_i , is equal to the angle of reflection, α_r , just as it is for a plane mirror reflecting light. In this case, the wavevector transfer, \vec{Q} , is perpendicular to the material surface, usually called the z direction, and is given by (refer to the scattering triangle Fig. 2.3)

$$Q_z = k_{iz} - k_{rz} = \frac{2\pi}{\lambda}(\sin \alpha_i + \sin \alpha_r) = \frac{4\pi \sin \alpha_i}{\lambda}, \quad (2.15)$$

where k_{iz} is the z component of the incident neutron wavevector and k_{rz} is the z component of the reflected neutron wavevector. There is no change of the neutron wavelength on reflection, so the process is elastic and the modulus of the neutron wavevector is not changed. Just like light incident on the surface of a pond, some of the neutron energy is reflected and some is transmitted into the reflecting medium with a wavevector given by $n \cdot k$ where n is the **refractive index** of the material and k the incident wavevector. The kinetic energy of the neutron before it strikes the surface is just $\hbar^2 k^2 / 2m$ (m is the neutron mass), while the kinetic energy inside the medium is $\hbar^2 n^2 k^2 / 2m$. The difference is just the neutron scattering potential of the medium given by Equation (2.3), averaged over the sample volume. Conservation of energy immediately tells us that the refractive index is given by

$$n = 1 - \rho \lambda^2 / 2\pi, \quad (2.16)$$

where ρ is the scattering length density we introduced earlier in connection with Eqn (2.13). Because the surface cannot change the component of the neutron's

velocity parallel to the surface, we can also use the conservation of energy to write down the z -component of the neutron's wavevector inside the medium, k_{tz} :

$$k_{tz}^2 = k_{iz}^2 - 4\pi\rho. \quad (2.17)$$

Critical external reflection of neutrons occurs when the transmitted wavevector reaches zero, allowing us to express the critical angle as $\gamma_c = \sin^{-1}(\lambda\sqrt{\rho/\pi})$. For a strongly reflecting material, such as nickel, the critical angle measured in degrees is roughly equal to the wavelength in nanometers—well under a degree for thermal neutrons. As the angle of incidence increases above the critical angle, fewer of the incident neutrons are reflected by the surface. In fact, reflectivity, $R(Q_z)$ —the fraction of neutrons reflected by the surface—obeys the same law, discovered by Fresnel, that applies to the reflection of light: reflectivity decreases as the fourth power of the angle of incidence at sufficiently large grazing angles.

However, Fresnel's law applies to reflection of radiation from smooth, flat surfaces of a homogeneous material. If there is a variation of the scattering length density close to the surface—for example, if there are layers of different types of material—the neutron reflectivity measured as a function of the angle of incidence shows a more complicated behavior. Approximately, we may write [15]

$$R(Q_z) = \frac{16\pi^2}{Q_z^4} \left| \int \frac{d\rho(z)}{dz} e^{iQ_z z} dz \right|^2, \quad (2.18)$$

where the pre-factor is the Fresnel reflectivity mentioned above. Equation (2.18) tells us that the reflectivity depends on the gradient of the average scattering length density perpendicular to the surface (i.e., in the z direction). If we have a layered material, this gradient will have spikes at the interfaces between layers and one may use a measurement of the reflectivity to deduce the thickness, sequence, and scattering length densities of layers close to the surface. This method is usually referred to as **neutron reflectometry**. Often, the reflectivity is analyzed using a more complicated formula than Equation (2.18), one in which the scattering length density, averaged over dimensions parallel to the surface, is split into thin layers and each density is refined until the measurement can be fitted. This method is called the **Parratt formalism** [16] and has been programmed into a number of widely available software packages. A certain amount of caution is needed in computing $\rho(z)$, however, Equation (2.18) has the same phase problem as we discussed for diffraction, and this means that $\rho(z)$ cannot be uniquely obtained from a single reflectivity curve. Indeed, remarkably different versions of $\rho(z)$ can yield very similar values of $R(Q_z)$.

In some ways, surface reflection is very different from conventional neutron scattering. After all, Van Hove's assumption in deriving Equation (2.4) was that neutron scattering was weak enough to be described by a perturbation theory—the Born Approximation—yet critical reflection from a surface is anything but a weak process because all of the incident neutrons are reflected at angles of incidence below γ_c . At large enough angles of incidence, the scattering is weak enough for the Born Approximation to apply, but between the so-called critical edge and these large

angles, a different theory called the Distorted Wave Born Approximation (DWBA) is needed. It turns out that the effect of surface roughness on neutron reflection, for example, is different from the result one gets from Equation (2.18), and only the DWBA can account for the observed experimental effects.

Reflectometry has been applied to soft matter [17]—where deuterium contrast enhancement can often be used to highlight particular layers—as well as to man-made multilayer structures of metals and alloys. In the latter case, *polarized neutron reflectometry* provides a powerful tool for determining the depth profile of *vector magnetization* close to the surface of a sample [18].

2.8 Conclusion

The conceptual framework for neutron scattering experiments was established over 50 years ago by Van Hove, who showed that the technique measures a time-dependent pair correlation function between scattering centers—either nuclei or magnetic moments. Because thermal neutrons have wavelengths similar to interatomic distances in matter and energies similar to those of excitations in matter, neutrons turn out to be a useful probe of both static structure and dynamics. The weak interaction between neutrons and matter is both a blessing and a curse. On the positive side, it is what allows us to describe scattering experiments so completely by the Born approximation and therefore to interpret the data we obtain in an unambiguous manner. It also permits us to contain interesting samples in relatively massive containers so that we can do neutron scattering experiments at a variety of temperatures and pressures. On the negative side of the balance sheet, the weak interaction of neutrons means that the scattering signals we measure are small—of the more than 10^{18} neutrons produced per second in the best research reactors, less than 1 in 10^{10} are used in a typical experiment and very few of these ever provide useful information! The weak interaction also means that we need to start out with a copious supply of neutrons if we are ever to have a chance of recording any that are scattered, and this, in turn, means that we are obliged to centralize the production of neutrons at a few specialized laboratories, restricting access to a technique that has been extremely useful in scientific fields from condensed matter physics to chemistry and from biology to engineering. But, in spite of all these penalties of a signal-limited technique, neutron scattering continues to occupy an important place among the panoply of tools available to study materials structure because it can often provide information that cannot be obtained in any other way. Were it not so, the technique would long have followed the dodo.

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