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# 2.9. Neutron reflectometry

By G. S. Smith and C. F. Majkrzak

## 2.9.1. Introduction

The neutron reflectivity of a surface is defined as the ratio of the number of neutrons elastically and specularly reflected to the number of incident neutrons. When measured as a function of neutron wave-vector transfer, the reflectivity curve contains information regarding the profile of the in-plane average of the scattering-length density (or simply scattering density) normal to that surface. The concentration of a given atomic species at a particular depth can then be inferred. Although similar information can often be extracted from X-ray reflectivity data, an additional sensitivity is gained by using neutrons in those cases where elements with nearly the same number of electrons or different isotopes (especially hydrogen and deuterium) need to be distinguished. Furthermore, if the incident neutron beam is polarized and the resultant polarization of the reflected beam analysed, it is possible to determine, in both magnitude and direction, the in-plane magnetic moment depth profile. This latter capability is greatly facilitated by the simple correlation of the relative counts of neutron spin-flip and non-spin-flip scattering to magnetic moment orientation and by the relatively high instrumental polarization and spin-flipping efficiencies possible with neutrons. These properties make neutron reflectivity a powerful tool for the study of surface layers and interfaces.

## 2.9.2. Theory of elastic specular neutron reflection

Consider the glancing (small-angle) reflection of a neutron plane wave characterized by a wave vector $\mathbf{k}_i$ from a perfectly flat and smooth surface of infinite lateral extent, as depicted schematically in Fig. 2.9.2.1. Although the density of the material can, in general, vary as a function of depth [along the direction ($z$) of the surface normal], it is assumed that there are no in-plane variations of the density. If the scattering is also elastic, so that the neutron neither gains nor loses energy (*i.e.* $|\mathbf{k}_i| = |\mathbf{k}_f| = k = 2\pi/\lambda$, where the subscripts $i$ and $f$ signify initial and final values, respectively, and $\lambda$ is the neutron wavelength), then the component of the neutron wave vector parallel to the surface must be conserved. In this case, the magnitude of the wave-vector transfer is $Q = |\mathbf{Q}| = |\mathbf{k}_f - \mathbf{k}_i| = 2k\sin(\theta) = 2k_z$, where the angles of incidence and reflection, $\theta$, are equal, and the scattering is said to be *specular*. Since at low values of $Q$ the neutrons are strongly scattered from the surface (*i.e.* the magnitude of the reflectivity approaches 1), the neutron wave function is significantly distorted from its free-space plane-wave form. The first Born approximation normally applied in the description of high-$Q$ crystal diffraction is therefore not valid for the analysis of low-$Q$ reflectivity measurements, and a more accurate, dynamical treatment is required.

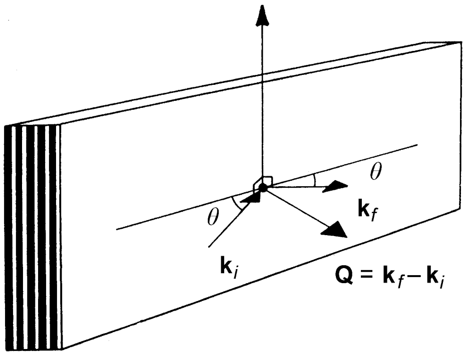

Fig. 2.9.2.1. Schematic diagram of reflection geometry.

Because the in-plane component of the neutron wave vector is a constant of the motion in the specular elastic reflection process described above, the appropriate equation of motion is the one-dimensional, time-independent, Schrödinger equation (see, for example, Merzbacher, 1970)

$$\psi''(z) + k_z^2\psi(z) = 0, \qquad (2.9.2.1)$$

where $\psi$ is the neutron wave function [which in free space is proportional to $\exp(ik_{0z}z)$, where $k_{0z}$ is the magnitude of the $z$ component of the neutron wave vector in vacuum]. If the infinite planar boundary from which the neutron wave reflects separates vacuum from a medium in which the neutron potential energy is $V_1$, conservation of the neutron's total energy requires that

$$k_{0z}^2 = k_{1z}^2 + \frac{2mV_1}{\hbar^2}, \qquad (2.9.2.2)$$

where $\hbar$ is Planck's constant divided by $2\pi$ and $m$ is the neutron mass. If $2\pi/Q$ has a magnitude much greater than interatomic distances in the medium, then the medium can be treated as if it were a continuum. In this limit, the potential energy $V_1$ can be expressed as (see, for example, Sears, 1989)

$$V_1 = \frac{2\pi\hbar^2\overline{Nb}}{m}, \qquad (2.9.2.3)$$

where $\overline{Nb} = \sum N_i b_i$, $i$ represents the $i$th atomic species in the material, $N_i$ is the number density of that species and $b_i$ is the coherent neutron scattering length for the $i$th atom (which is in general complex if absorption or an effective absorption such as isotopic incoherent scattering exists; magnetic contributions are not accounted for here but will be considered below). The quantity $\overline{Nb} \equiv \rho$ is the effective scattering density. Substituting the expression for $V_1$ given in equation (2.9.2.3) into (2.9.2.2) yields

$$k_{1z}^2 = k_{0z}^2 - 4\pi\rho(z). \qquad (2.9.2.4)$$

In order to calculate the reflectivity, continuity of the wave function and its first derivative (with respect to $z$) are imposed. These boundary conditions are a consequence of restrictions on current densities required by particle and momentum conservation. In general, given a sample with layers of varying potentials where the boundaries of the $j$th layer are at $z_{oj}$ and $z_{oj} + \delta_j$, and the potential, $V_j$, is constant over that layer, it can be shown that (see, for example, Yamada, Ebisawa, Achiwa, Akiyoshi & Okamoto, 1978)

$$\begin{aligned}\begin{pmatrix}\psi_j(z_{oj}+\delta_j)\\ \psi'_j(z_{oj}+\delta_j)\end{pmatrix} &= \mathbf{M}_j\begin{pmatrix}\psi_j(z_{oj})\\ \psi'_j(z_{oj})\end{pmatrix}\\ &= \begin{pmatrix}\psi_{j+1}(z_{oj}+\delta_j)\\ \psi'_{j+1}(z_{oj}+\delta_j)\end{pmatrix},\end{aligned} \qquad (2.9.2.5)$$

where

$$\mathbf{M}_j = \begin{pmatrix}\cos(k_{jz}\delta_j) & (1/k_{jz})\sin(k_{jz}\delta_j)\\ -k_{jz}\sin(k_{jz}\delta_j) & \cos(k_{jz}\delta_j)\end{pmatrix}, \qquad (2.9.2.6)$$

and $k_{jz}$ is the magnitude of the neutron wave vector in the $j$th layer [equation (2.9.2.4)].

The first equality in (2.9.2.5) relates the wave function at one boundary within the $j$th layer to the next boundary within the $j$th layer, whereas the second equality represents the continuity of the wave function and its derivative across the boundary between the $j$th and $(j+1)$th layers. When a neutron plane wave is incident on a multilayer sample, we can take the incident amplitude as unity, set up the coordinate system to have $z = 0$ at the air/sample interface, and write the wave function in air as the sum of the incident and reflected waves,

$$\psi_{\text{incident}}(z) = \exp(ik_{0z}z) + R\exp(-ik_{0z}z), \qquad (2.9.2.7)$$

and the wave function in the substrate as a purely transmitted wave,

$$\psi_{\text{substrate}}(z) = T\exp(ik_{sz}z), \qquad (2.9.2.8)$$

where $k_{sz}$ is the magnitude of the $z$ component of the neutron wave vector in the substrate. By combining equations (2.9.2.5) through (2.9.2.8), we obtain a working equation for calculating the reflectivity:

$$\begin{pmatrix} T \\ ik_{sz}T \end{pmatrix} \exp(ik_{sz}\Delta) = M_N M_{N-1}\ldots M_1 \begin{pmatrix} (1+R) \\ ik_{0z}(1-R) \end{pmatrix}, \qquad (2.9.2.9)$$

where $\Delta = \sum \delta \equiv$ total film thickness. The experimentally measured reflection and transmission coefficients $|R|^2$ and $|T|^2$ can be computed from (2.9.2.9). The procedure outlined above can be applied in piece-wise continuous fashion to arbitrary, smooth potentials, $\rho(z)$, which are approximated to any desired degree of accuracy by an appropriate number of consecutive rectangular slabs, each having its own uniform scattering density, $\rho_j$, and thickness, $\delta_j$, as depicted in Fig. 2.9.2.2.

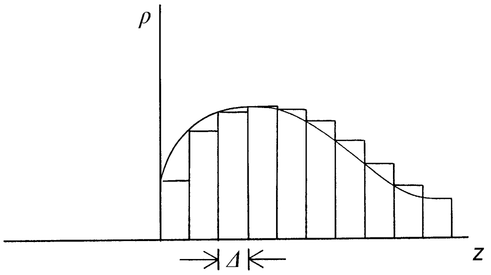

Fig. 2.9.2.2. Arbitrary scattering density profile represented by slabs of uniform potential.

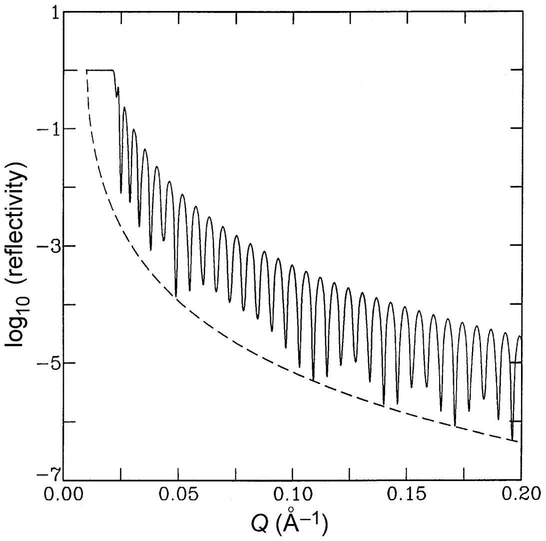

Fig. 2.9.2.3. Neutron reflectivities calculated for an infinite Si substrate (dashed line) and 1000 Å Ni film on an Si substrate (solid line).

If $k_{0z}^2 < 4\pi\rho_{\text{substrate}}$, then $k_z$ becomes imaginary in the substrate, and total external reflection occurs. In addition, for a single layer deposited on the substrate, the reflectivity will oscillate with a periodicity characteristic of the layer thickness. Fig. 2.9.2.3 compares the ideal Fresnel reflectivity corresponding to an infinite silicon substrate and that of a 1000Å nickel film deposited on silicon. For a barrier of finite thickness, tunnelling phenomena can also be observed (see, for instance, Merzbacher, 1970; Buttiker, 1983; Nuñez, Majkrzak & Berk, 1993; Steinhauser, Steryl, Scheckenhofer & Malik, 1980).

With the matrix method described above, the reflectivity of any model scattering-density profile can be calculated with quantitative accuracy over many orders of magnitude. Unfortunately, the inverse computation of an unknown scattering density profile corresponding to a given reflectivity curve can be exceedingly difficult, in part due to the the lack of phase information on $R(Q)$, which forces one to use highly non-linear relations between $|R(Q)|^2$ and $\rho(z)$. Often, parameterized model scattering-density profiles are fit to the experimental data (Felcher & Russell, 1991). Recently, several authors have described model-independent methods for obtaining $\rho(z)$ from measured reflectivity curves (Zhou & Chen, 1993; Pedersen & Hamley, 1994; Berk & Majkrzak, 1995).

### 2.9.3. Polarized neutron reflectivity

Reflectivity measurements with polarized neutrons can reveal the in-plane magnetization-vector depth profile in magnetic thin films and multilayers. The interaction between the neutron and atomic magnetic moments is dependent upon their relative orientations. Two important yet simple selection rules apply in the case where the neutron polarization axis (defined by an applied magnetic field at the sample position) is perpendicular to **Q**. Any component of the in-plane magnetization parallel to this quantization axis gives rise to non-spin-flip (NSF) neutron scattering, which interferes with scattering due to the nuclear potential: any perpendicular magnetic component creates spin-flip (SF) scattering, which is purely magnetic. Consequently, the atomic magnetic moment's direction can be inferred by measuring the two NSF ($++$, $--$) and two SF ($+-$, $-+$) reflectivities (where $+-$ refers to a reflection measurement in which the incident neutron magnetic moment is parallel to the applied field and only neutrons with their magnetic moment antiparallel to the applied field are measured, *etc.*), in addition to its absolute magnitude (which is proportional to a magnetic scattering density $\rho_M = Np$, where $p$ is a magnetic scattering length). The matrix formalism described earlier to obtain the reflectivity in the non-polarized-beam case can be extended to treat polarized beams as well. The resulting transfer matrix is, however, in the latter instance a $4 \times 4$ matrix relating two spin-dependent reflectivities and transmissions for each of two possible incident-neutron spin states. The matrix elements are given in Felcher, Hilleke, Crawford, Haumann, Kleb & Ostrowski (1987), and more detailed discussions of the method of polarized neutron reflectometry can be found in Majkrzak (1991) and Majkrzak, Ankner, Berk & Gibbs (1994).

### 2.9.4. Surface roughness

Up to this point, we have only considered reflection from smooth, flat surfaces. In reality, however, all surfaces have microscopic or mesoscopic imperfections such as steps, facets and rough hills and valleys. In this case, the potential must be represented by a three-dimensional function instead of the simple one-dimensional example discussed above. In addition, the roughness may not be confined to the outer surface or substrate, but the imperfections may propagate through several layers. This roughness at the interfaces modifies the specularly reflected beam and adds a diffuse component to the scattered beam (*i.e.* neutrons scattered at angles other than the incident angle). Theories based on the distorted-wave, Born approximation have been developed to describe this type of scattering (Nevot & Croce, 1980; Sinha, Sirota, Garroff & Stanley, 1988; Pynn, 1992; Sears, 1993; Holy, Kubena, Ohlidal, Lischka & Plotz, 1993; de Boer, 1994) for a microscopically rough surface. These theories give results consistent with the earlier work (Nevot & Croce, 1980) for the modification to the specular scattering due to a single rough surface. The reader is referred to Sinha, Sirota, Garroff & Stanley (1988) and Pynn (1992) for a more complete discussion of diffuse scattering.

In order to fit the specular scattering from a rough surface, two simple methods have been employed. First, using the matrix method discussed above, the rough interface can be modelled as a smoothly varying scattering density approximated as a series of steps. This has the advantage that complex interfaces that are combinations of rough surfaces and intermixed layers can be approximated. The other method is to extend the results of Nevot to each successive interface while iteratively calculating the reflection amplitude. This method works well for simple interfaces of Gaussian roughness and is faster, in general, than the matrix method, since fewer calculations are needed for each interface. However, this latter technique suffers from frequently yielding unphysical answers (*i.e.* surface widths greater than adjacent layer thicknesses). Both of these methods are inadequate, in that there is no way to separate the effects of graded interfaces from rough surfaces. This can only be done with a simultaneous examination of both the diffuse and specular scattering.

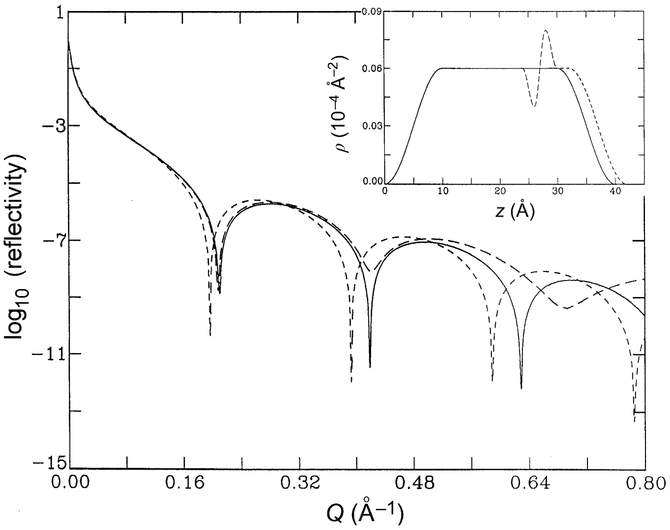

Fig. 2.9.6.1. Calculated neutron reflectivity curves corresponding to the three density profiles in the inset (*i.e.* solid line in density profile corresponds to solid line in reflectivity plot). Note that in the density plots the solid and long-dash curves coincide except at the oscillation on top of the plateau, whereas the solid and short-dashed curves coincide except at the trailing edge between 30 and 42 Å.

### 2.9.5. Experimental methodology

Neutron reflectivity measurements can be carried out in two principal ways: either (1) with a monochromatic incident beam of narrow angular divergence in the plane of reflection (defined by $\mathbf{k}_i$ and $\mathbf{k}_f$, where $\lambda$ is constant, and $Q$ is varied by changing the glancing angle of incidence, $\theta$, relative to the sample surface; or (2) using a pulsed polychromatic incident beam, also of narrow angular divergence at fixed $\theta$, and obtaining data over a range of $Q$ values simultaneously by performing time-of-flight analysis on the reflected neutrons. For either method, the instrumental resolution is simply given as

$$\left(\frac{\Delta Q}{Q}\right)^2=\left(\frac{\Delta\lambda}{\lambda}\right)^2+\left(\frac{\Delta\theta}{\theta}\right)^2, \qquad (2.9.5.1)$$

where $\Delta\theta$ is the angular divergence of the reflected beam, and $\Delta\lambda$ is the wavelength spread. In the case of a steady-state source,

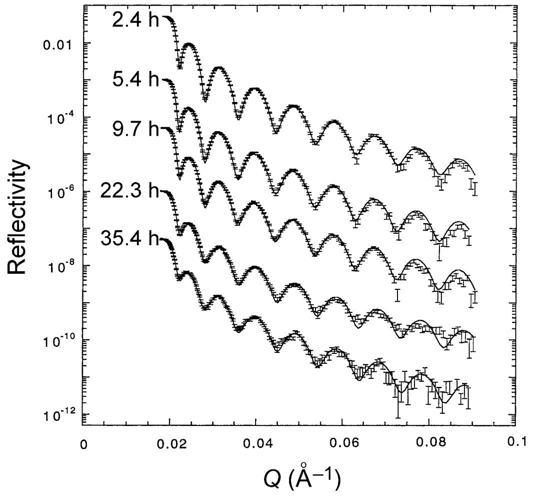

Fig. 2.9.7.1. Measured neutron reflectivities from boron bilayers [from Smith *et al.* (1992)].

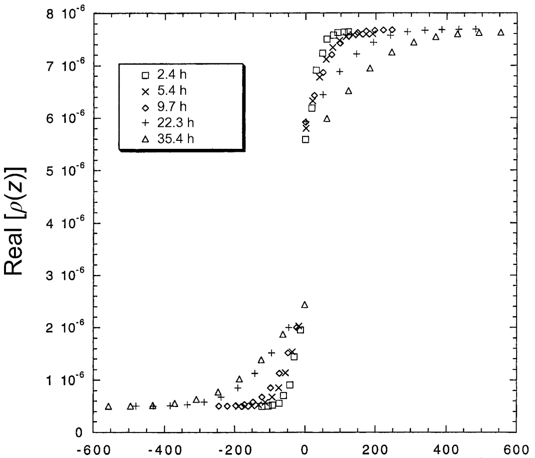

Fig. 2.9.7.2. The fitted real part of the scattering density profiles for the measured reflectivities of Fig. 2.9.7.1. Note the pinning of the concentration of $^{10}$B at the interface [after Smith *et al.* (1992)].

the wavelength resolution is determined by the monochromator, whereas the timing and moderator characteristics determine the wavelength resolution on a time-of-flight instrument. Although the second term in equation (2.9.5.1) is standard in scattering, it has a unique characteristic, in that the angular divergence of the reflected beam determines the resolution. This is the case because the sample is a $\delta$-function scatterer, so that the angle of the incident beam can be determined precisely by knowing the reflected angle (Hamilton, Hayter & Smith, 1994). For a more complete description of both types of neutron reflectometry instrumentation, see Russell (1990).

### 2.9.6. Resolution in real space

From Fig. 2.9.2.3, the period $\delta Q$ of the reflectivity oscillation (in the region where the Born approximation becomes valid, sufficiently far away from the critical angle) is inversely proportional to the thickness $t$ of the film. That is, $2\pi/(\delta Q) = t$. Consequently, in order to be able to resolve reflectivity oscillations for a film of thickness $t$, the instrumental $Q$ resolution $\Delta Q$ [from equation (2.9.5.1)] must be approximately $2\pi/t$ or smaller. With sufficiently good instrumental resolution, even the thickness of a film with non-abrupt interfaces can be accurately determined, as demonstrated by the hypothetical case depicted in Fig. 2.9.6.1 (where the instrumental resolution is taken to be perfect): an overall film-thickness difference of 2 Å (between 42 and 40 Å films) is clearly resolved at a $Q$ of about 0.2 $\text{Å}^{-1}$. In practice, differences even less than this can be distinguished. Note, however, that to 'see' more detailed features in the scattering-density profile (such as the oscillation on top of the plateau shown for the long-dash profile in the inset of Fig. 2.9.6.1), other than the overall film thickness, it can be necessary to make reflectivity measurements at values of $Q$ corresponding to $2\pi$/(characteristic dimension of the feature).

### 2.9.7. Applications of neutron reflectometry

#### 2.9.7.1. *Self-diffusion*

One of the simplest, yet powerful, examples of the use of neutron reflectivity is in the study of self-diffusion. Most techniques to measure diffusion coefficients rely on chemical and mechanical methods to measure density profiles after a sample

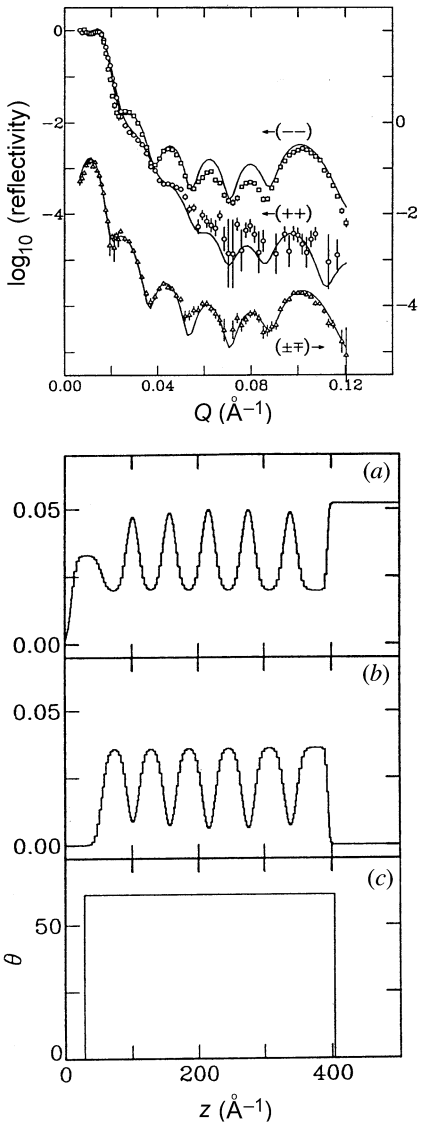

Fig. 2.9.7.3. Co/Cu(111) spin-dependent reflectivities (top). Nuclear (Nb) and magnetic (Np) scattering densities (bottom). Also shown is the (constant) moment direction [after Schreyer *et al.* (1993)].

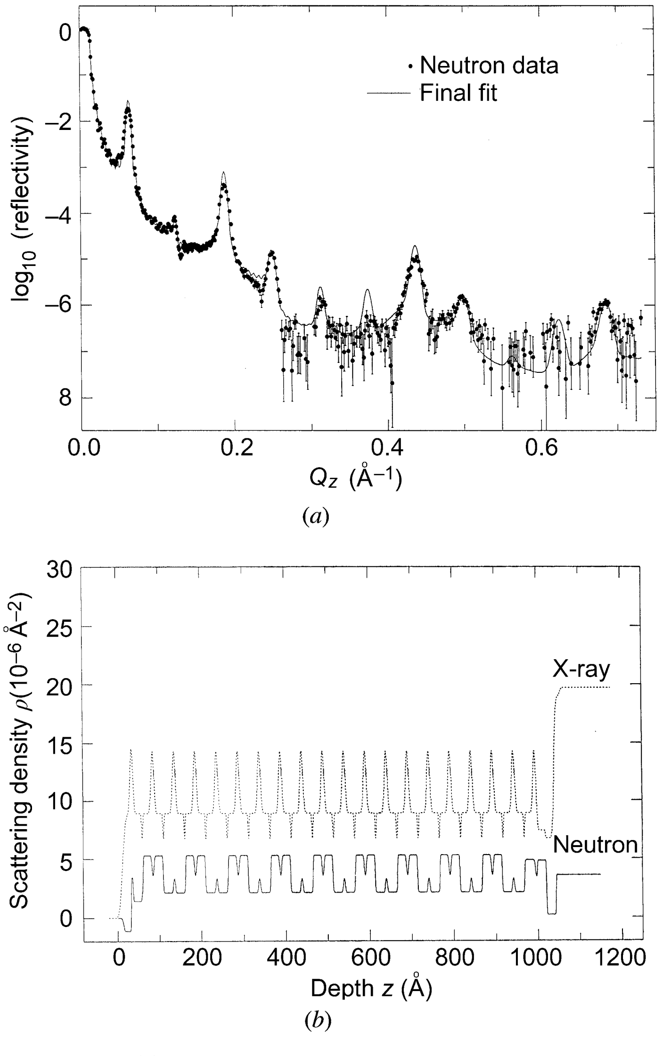

Fig. 2.9.7.4. (*a*) Measured neutron reflectivity for the Langmuir–Blodgett multilayer described in the text along with the fit. (*b*) Both corresponding neutron and X-ray scattering density profiles. The X-ray reflectivity is more sensitive to the high-$Z$ barium in the head groups whereas the neutron reflectivity can distinguish mixing between adjacent hydrogenated and deuterated hydrocarbon tails [after Wiesler *et al.* (1995)].

has been annealed. Then a model for the diffusion is assumed, and the coefficients are calculated. Using standard techniques, researchers are unable to detect the movement of an atom through a sample of like atoms. However, using single bilayers of amorphous $^{10}$B and $^{11}$B, it was shown (Smith, Hamilton, Fitzsimmons, Baker, Hubbard, Nastasi, Hirvonen & Zocco, 1992) through neutron-reflectivity measurements that the diffusion of boron in boron could be measured by studying the density profile (see Figs. 2.9.7.1 and 2.9.7.2) of one isotope in the other as a function of annealing time. Also, because of the sensitivity of the technique to the interfacial density profile, it was found that standard Fickian diffusion models could not explain the measured density profiles.

### 2.9.7.2. *Magnetic multilayers*

In order to understand interlayer coupling mechanisms, it is necessary to know what the magnetic superstructure is for a given nonmagnetic spacer layer thickness and/or applied field strength. Fig. 2.9.7.3 shows the spin-dependent reflectivities for a Co/Cu (111) multilayer along with the nuclear (Nb) and magnetic (Np) scattering-density profiles deduced from the data of Schreyer, Zeidler, Morawe, Metoki, Zabel, Ankner & Majkrzak (1993). In this specific case, the in-plane ferromagnetic Co layers are themselves coupled ferromagnetically across the nonmagnetic Cu, all at a constant angle.

### 2.9.7.3. *Hydrogenous materials*

There are a substantial number of applications of neutron reflectometry in the study of hydrogenous films and multilayers, including diblock copolymer, surfactant, Langmuir–Blodgett, self-assembled monolayer, and lipid bilayer films. Reviews of the extensive research that has already been done have been written by Russell (1990) and Penfold & Thomas (1990). Only one specific example will be given here.

Fig. 2.9.7.4 shows neutron reflectivity data and the corresponding density profile for a Langmuir–Blodgett film composed of alternating bilayers of deuterated and hydrogenated stearic acid [after Wiesler, Feigin, Majkrzak, Ankner, Berzina & Troitsky (1995)]. Also shown in Fig. 2.9.7.4 is the scattering-density profile for the same sample as seen by X-rays. It is obvious that the X-rays are more sensitive to the high-$Z$ barium in the head group, whereas the neutrons are especially good at distinguishing the degree of mixing between adjacent hydrogenated and deuterated hydrocarbon tails. This is a good example of the complementary nature of neutron and X-ray reflectivities.

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