International Tables for Crystallography (2006). Vol. C, Figure 2.9.2.2, p. 127.

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

The first equality in (2.9.2.5) relates the wave function at one boundary within the jth layer to the next boundary within the jth layer, whereas the second equality represents the continuity of the wave function and its derivative across the boundary between the jth 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, ρ_j, and thickness, δ_j, as depicted in Fig. 2.9.2.2.

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).

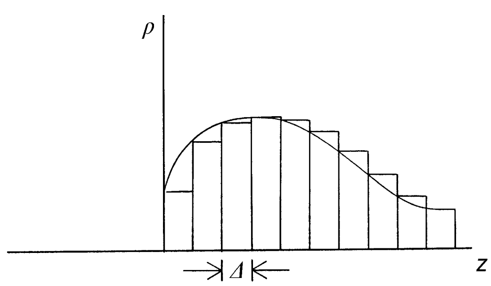

Fig. 2.9.2.2. Arbitrary scattering density profile represented by slabs of uniform potential.

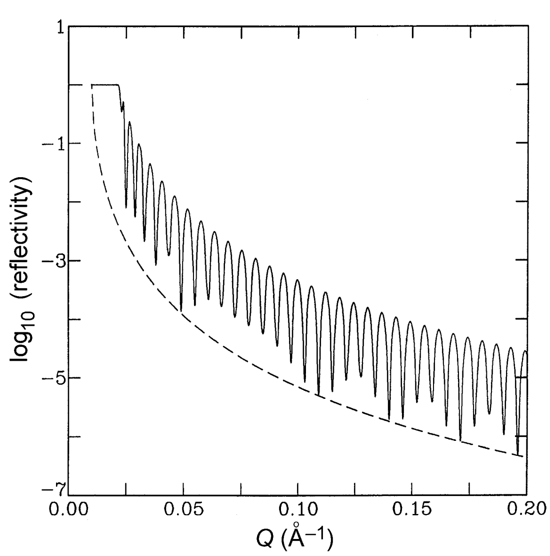

Fig. 2.9.2.3. Neutron reflectivities calculated for an infinite Si substrate (dashed line) and 1000 Å Ni film on an Si substrate (solid line).

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 $\mathbf{Q}$. 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 4×4 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).

references