[single-layer reflection]
(Chapter 5.5.4 in *Elements*)

A simple example

A simple example is that of a single layer of nickel metal on a thick substrate of silicon. Figure 5-SLR1 illustrates.

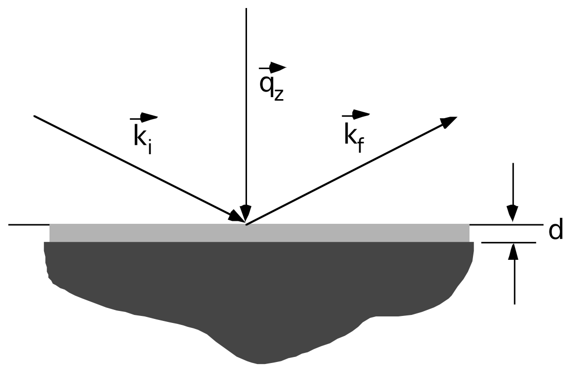

Figure 5-SLR1. *Reflection from a single layer on an infinite substrate.*

The algorithm sketched previously requires a computer to carry out the matrix multiplications for many-layered systems and in general situations having declared the variables complex. The case of Fig. 5-SLR1 is a tractable example, a single layer on an infinite substrate: nickel on silicon. Table 5-SLR1 summarizes the parameters.

Table 5-SLR1. Parameters of nickel and silicon

Material	Atomic density, ρ, at/cm^3	Coherent scattering length, b, Fm	Coherent scattering length, density, ρb, Å^{-2}	Critical wave number, q_{cr}, Å^{-1}	Thickness, d, Å
^{nat}Ni	9.143 x 10^{22}	10.3	9.417 x 10^{-6}	0.02176	100.
Si	5.00 x 10^{22}	4.149	2.073 x 10^{-6}	0.01021	Infinite

For the one-layer case, the matrix product has only a single factor,

$$\mathbf{M}(q) = \begin{pmatrix} \cos x & \frac{1}{\eta}\sin x \\ -\eta \sin x & \cos x \end{pmatrix} = \begin{pmatrix} s & t \\ u & v \end{pmatrix}, \qquad (5\text{-SLR1})$$

where

$$x = \eta\, dq/2 \qquad (5\text{-SLR2})$$

for the nickel layer and

$$a' = \frac{\eta_b t + u + i(v - \eta_b s)}{\eta_b t - u + i(v + \eta_b s)} = \frac{\left(\frac{\eta_b}{\eta} - \eta\right)\tan x + i(1 - \eta_b)}{\left(\frac{\eta_b}{\eta} + \eta\right)\tan x + i(1 + \eta_b)}, \tag{5-SLR3}$$

so that when the η's are real, that is, when $q > Max\left[q_{c\ \mathrm{layer}}, q_{c\ \mathrm{b}}\right]$,

$$R(q) = |a'|^2 = \frac{\left(\frac{\eta_b}{\eta} - \eta\right)^2 \tan^2 x + (1 - \eta_b)^2}{\left(\frac{\eta_b}{\eta} + \eta\right)^2 \tan^2 x + (1 + \eta_b)^2}. \tag{5-SLR4}$$

If there is no backing, that is, for a free-standing foil, $\eta_b = 1$ and

$$R(q) = \frac{1}{q^4} \frac{(16\pi\rho b)^2 \tan^2(\eta dq/2)}{(1 + \eta^2)^2 \tan^2(\eta dq/2) + 4\eta^2}. \tag{5-SLR5}$$

For the substrate alone, $d = 0$ and

$$R(q) = \frac{(1 - \eta_b)^2}{(1 + \eta_b)^2}. \tag{5-SLR6}$$

These expressions are valid for the nickel-only and nickel-on-silicon cases only when $q > q_{c\ \mathrm{Ni}} = 0.02176$ Å^{-1}.

When $q_{c\ \mathrm{b}} < q < q_{c\ \mathrm{Ni}}$, η and therefore x become pure imaginary,

$$\eta \to i\eta'' = \sqrt{\left|1 - \left(\frac{q_c}{q}\right)^2\right|}, \text{ etc., and } x \to ix'', \tag{5-SLR7}$$

so that

$$R(q) = \frac{\left(\frac{\eta_b}{\eta''} + \eta''\right)^2 \tanh^2 x'' + (1 - \eta_b)^2}{\left(\frac{\eta_b}{\eta''} - \eta''\right)^2 \tanh^2 x'' + (1 + \eta_b)^2}. \tag{5-SLR8}$$

When $q < q_{c\,\mathrm{b}}$, η_b also becomes pure imaginary,

$$\eta_b \to i\eta_b'', \tag{5-SLR9}$$

so that

$$a' = \frac{i\left(\dfrac{\eta_b''}{\eta''} - i\eta''\right)\tanh x + i\left(1 - i\eta_b''\right)}{i\left(\dfrac{\eta_b''}{\eta''} + i\eta''\right)\tanh x + i\left(1 + i\eta_b''\right)}, \tag{5-SLR10}$$

in which the numerator and denominator are complex conjugates, therefore

$$R(q) = \left|a'\right|^2 = 1. \tag{5-SLR11}$$

We leave the proof of these last results as an exercise for the reader.

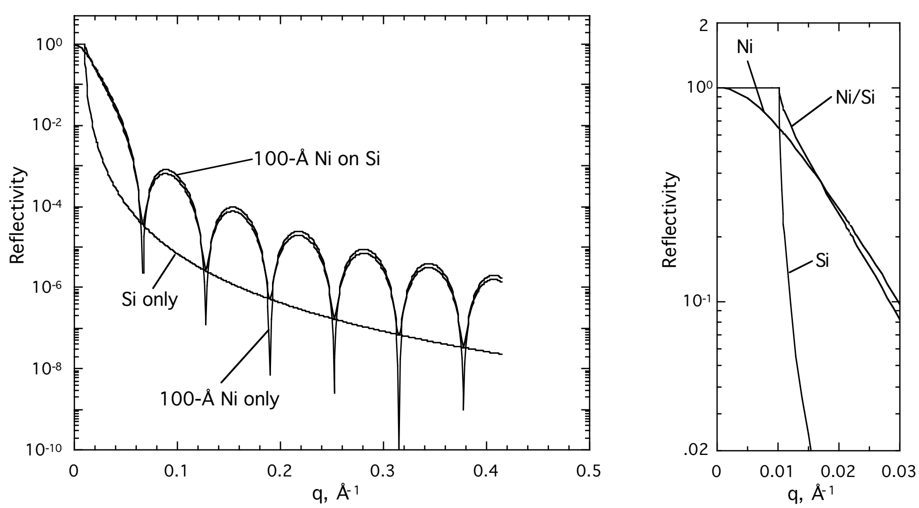

Figure 5-SLR2. *The reflectivity of a 100-Å nickel film on an infinitely thick silicon substrate. Smooth curve, substrate only. Upper curve, 100-Å nickel on silicon. Lower curve, 100-Å nickel alone. Right, expanded view of the low-q region.*

Figure 5-SLR2 shows the results of calculations using this formulation and the parameters of Table 5-SLR1, showing the reflectivity for the silicon substrate alone, the 100-Å nickel layer

alone, and the nickel layer on the substrate. The reflectivity for the substrate is the lower envelope of the reflectivity of the nickel layer on the substrate.