[modeling reflectivity]
(Chapter 5.5.3 in *Elements*)

Modeling the reflectivity

Extracting the scattering length density profile from the measured reflectivity as a function of wave vector transfer (the glancing angle) is impossible in the absence of phase information of the reflection amplitude, which is a complex number (Majkrzak and Berk 1995), while measurements provide only its magnitude (squared). The conventional method of extracting the SCD profile is by a cut-and-try method. We follow the Majkrzak and Berk (1995), carrying the effect of a thick backing behind the unknown layers.

The modeling approach of Ankner and Majkrzak (1992) rests on the observation that neutrons incident on one layer of material are reflected and transmitted, the reflected neutrons are incident from below on the layer above, and the transmitted neutrons are incident on the layer below, proceeding through the layered material. Figure 5-MR-1 illustrates. The thickness of the j^{th} layer is d_j, where the scattering length density is $\rho_j b_j$. As shown, the scattering length density at the incident end, $z = 0$, is 0 (vacuum) and at the exit side is $\rho_b b_b$.

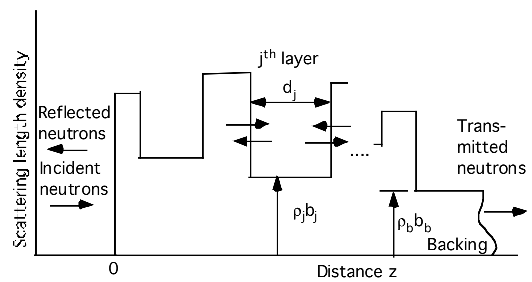

Figure 5-MR.1. Scattering length density as a function of depth in a layered material.

In a multilayer structure, the amplitudes of the reflected wave a' and of the transmitted wave A, where the amplitude of the incident wave is defined to be $a = 1$, are related by the matrix formula

$$\begin{pmatrix} A \\ i\eta_b A \end{pmatrix} = \prod_{j=1}^{N} \begin{pmatrix} \cos\vartheta_j & \frac{1}{\eta_j}\sin\vartheta_j \\ -\eta_j \sin\vartheta_j & \cos\vartheta_j \end{pmatrix} \begin{pmatrix} 1+a' \\ i(1-a') \end{pmatrix}, \qquad \text{(5-MR1)}$$

where N is the number of layers and

$$\vartheta_j = \frac{1}{2} q \eta_j d_j . \qquad \text{(5-MR2)}$$

Here, η's are not the refractive indices, but rather are

$$\eta_j = \sqrt{1-16\pi\rho_j b_j/q^2} = \sqrt{1-q_{cj}^2/q^2} \ . \tag{5-MR3}$$

The extended product of 2x2 *layer transfer matrices* is itself a 2x2 matrix, the *overall transfer matrix,*

$$\mathbf{M}(q) = \prod_{j=1}^{N} \begin{pmatrix} \cos\vartheta_j & \frac{1}{\eta_j}\sin\vartheta_j \\ -\eta_j \sin\vartheta_j & \cos\vartheta_j \end{pmatrix} = \begin{pmatrix} s(q) & t(q) \\ u(q) & v(q) \end{pmatrix}. \tag{5-MR4}$$

All elements of $\mathrm{M}(q)$ and the η_j are real numbers when all the scattering lengths are positive which are not true in general. Actual calculations must be computed carrying out complex-number calculations. Eliminating the amplitude of the transmitted (refracted) wave, *A* in Eq. 5-MR1 gives the reflected-wave amplitude

$$a' = \frac{\eta_b t + u + i(v-\eta_b s)}{\eta_b t - u + i(v+\eta_b s)}, \tag{5-MR5}$$

in which all, in general, are complex numbers. The directly measurable reflectivity is a real number,

$$R = |a'|^2, \tag{5-MR6}$$

which is the reflectivity as a function of *q*, to be compared with experiment.

Let us consider the result when all quantities are real, as discussed by Majkrzak and Berk [1995]. In that case, those authors note that the reflectivity comes out easily if first one computes

$$2\left(\frac{1+R}{1-R}\right) = 2\left(\frac{1+|a'|^2}{1-|a'|^2}\right) = \eta_b^2 s^2 + \eta_b^2 t^2 + u^2 + v^2 \equiv \Sigma + (\eta_b^2 - 1)(s^2+t^2), \tag{5-MR7}$$

where Σ is the trace of the matrix product,

$$\Sigma = tr\left[\mathbf{M}^T\mathbf{M}\right], \tag{5-MR8}$$

which depends on the properties of the layers only, not of the substrate. Solving the bilinear form for R, one finds

$$R = \frac{\Sigma + (\eta_b^2 - 1)(s^2 + t^2) - 2}{\Sigma + (\eta_b^2 - 1)(s^2 + t^2) + 2}. \qquad (5\text{-MR9})$$

It must be that $\Sigma + (\eta_b^2 - 1)(s^2 + t^2) \geq 2$ in order that $R > 0$. Moreover, the reflectivity achieves a plateau when $\Sigma + (\eta_b^2 - 1)(s^2 + t^2)$ becomes very large, that is, $R \to 1$. One can properly anticipate that this occurs when $q < q_{cj}$ for any layer, including the substrate. Therefore in practical cases when absorption is negligible, and the coherent scattering lengths are real, there is always a plateau, although perhaps not a distinct critical edge.

References

Ankner, J. F. and C. F. Majkrzak (1992). Subsurface profile refinement for neutron specular reflectivity. *Neutron Optical Devices and Applications*, Proc. SPIE—The International Society for Optical Engineering, 1738, 259-69.