Scattering of neutrons and x radiation in the range 10–300 Å by periodic structures with rough boundaries

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A theory is derived for real multilayer neutron and x-ray mirrors in the approximation of slight scattering. The results explain the experimental data available and can be used to fabricate reflecting elements with optimum characteristics.

Despite the extensive theoretical and experimental studies of multilayer x-ray and neutron mirrors for the wavelength range 1–300 Å (Refs. 1–5), we lack a theory that gives a satisfactory description of the real structures. Common features in this wavelength range are a small optical density of all materials, $|\epsilon - 1| \ll 1$, and the existence, at the boundaries between layers, of irregularities which may be comparable in size to the wavelength. For x radiation, the situation is complicated by the substantial absorption which is characteristic of all materials in this range. In general, we must consider structures with absorbing layers with rough boundaries.

In the present paper we use the customary assumption that the jump in ϵ at the interfaces is small, and we also make use of the circumstance that the most important goal for practical applications is an appropriate description of good optical systems, so that we can restrict the analysis to the case in which the resultant intensity of the radiation scattered diffusively by the multilayer structure is much weaker than the intensity of the radiation propagating in the specular direction. Since the laws for combining the diffuse and specular components may differ, this condition does not necessarily have to be satisfied in the scattering by a single boundary.

Making use of the small value of the jump in ϵ, we can find the scattering indicatrix of the radiation for scattering from a surface with a rough boundary with arbitrary characteristics in the Born approximation. Assuming a Gaussian distribution of irregularities, we can write the average intensity of the radiation into the element of solid angle $d\Omega$ as follows:

$$< \frac{dT}{d\Omega} > = \frac{k_0^5 I_0}{q_z^2 k_{1z}} |\chi_0|^2 \exp(-q_z^2 \sigma^2)\{\delta(\mathbf{p})$$

$$+ 2\pi \int_0^\infty \rho J_0(p\rho)[\exp[q_z^2 \sigma^2 \psi(\rho)] - 1]\,d\rho\} \quad , \tag{1}$$

where $\chi_0 = (1-\epsilon)/4\pi$ is the dielectric constant of the medium, $\mathbf{q} = \mathbf{k}_1 - \mathbf{k}_2$, $\mathbf{k}_1$ and $\mathbf{k}_2$ are the wave vectors of the incident and scattered waves, $k_0 = |k_1|$, q_z and $\mathbf{p}$ are the projections of the vector $\mathbf{q}$ onto the normal to the surface and onto the XY plane, I_0 is the intensity of the incident wave, $\delta(\mathbf{p})$ is the Dirac δ-function, $\psi(\rho)$ is the correlation function of the roughness irregularities, and σ^2 is the variance.

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Since the solution is found in the approximation of single scattering, expression (1) agrees (within a factor) with the result found by the Kirchhoff method.[6] It can be seen from expression (1) that as the correlation radius l decreases, the first term, which represents the specular component of the reflection, does not change, while the second, representing the diffuse component, decreases; i.e., the small-scale irregularities match the impedances of the media at the interface. This circumstance can be exploited to describe the wave propagation in a multilayer structure with rough boundaries.

Ignoring the small-scattering loss, we can treat the multilayer structure as consisting of layers between which the profile of ϵ is smooth. The reflection coefficient for the specular component, for s-polarized radiation, is found by the truncated-equation method[7] to be

$$R = \left| \frac{k_0^2 a_1 \varphi_0 \tan \gamma L}{\delta \tan \gamma L + i q_0 \gamma} \right|^2 , \tag{2}$$

where $\gamma = (1/q_0)\sqrt{k_0^4 a_1^2 \varphi_0^2 - \delta^2}$ is the field-decay rate, $\delta = k_0^2(a_0 - \sin^2\theta) - (q_0^2/4)$, $a_0 = \epsilon_1(d_1/d) + \epsilon^2(d_2/d)$ and $a_1 = ((\epsilon_1 - \epsilon_2)/\pi) \sin(\pi d_1/d)$ are the amplitudes of the zeroth and first harmonics in the expansion of the dielectric constant of a structure without a roughness in a Fourier series, $d_{1,2}$ are the thicknesses of the layers with dielectric constants $\epsilon_{1,2}$, d is the period of the structure, $q_0 = 2\pi/d$, θ is the angle at which the radiation is incident, $L = Nd$ is the thickness of the structure, and $\varphi_0 = \exp(-\frac{1}{2}q_0^2\sigma^2)$. For the reflection of p-polarized radiation, we would have an analogous expression with the substitution $a_1 \rightarrow a_1 \cos 2\theta$. A more complicated question is the range of applicability of this expression. To answer it, we need to examine the interaction of the waves scattered in the multilayer structure. Here we can distinguish two limiting cases: that in which the irregularities at the interfaces repeat each other (correlated irregularities) and that in which the irregularities at the boundaries are statistically independent.

The scattering loss in a structure with uncorrelated irregularities can be found through an incoherent addition of the scattering components of the various layers. The result will obviously be approximately equal to the product of the integrated (over all momenta $\mathbf{p}$) intensity of the diffuse component from one surface by the number of scattering boundaries. The angular dependence of the scattering intensity must not depend on $N_{\rm eff}$. It can be shown that in the case of correlated interfacial irregularities, the diffuse component adds up coherently; i.e., the intensity is proportional to $N_{\rm eff}^2$. It can be seen from the phase relations, however, that the directions of the effective increase in intensity should coincide with the directional pattern of an ideal structure and that the width of the main lobe in the pattern is inversely proportional to the number of effectively reflecting layers, $\sim 1/N_{\rm eff} \sim \gamma d$. The integrated loss intensity is thus proportional to $N_{\rm eff}$, as in the first case. A rigorous solution yields $J \simeq q_0^2\sigma^2$ for the integrated intensity of the scattered radiation in the case of large-scale irregularities ($\mu = k_0^2 a_1 l^2 \gg 1$) and $J \simeq 2\pi k_0^2 a e^2 q_0^2 \sigma^2$, in the opposite limit ($\mu \ll 1$). This result determines the requirement that the scattering be slight: $J \ll 1$. The integrated intensity of the scattered radiation is proportional to $N_{\rm eff}^2$ when the width of the scattering pattern for scattering from one surface is much smaller than the width of the directional pattern of the multilayer stucture: $k_0^2 l^2 \gg N_{\mathrm{eff}}$. This condition, which determines the range of parameters for which the Kirchhoff approximation holds, is more restrictive than the condition which is ordinarily used, $k_0 l \gg 1$.

These expressions can explain the observed amplitude, frequency, and angular characteristics of multilayer elements. In addition, these expressions can be used to compensate for or to make use of the structural irregularities which are unavoidable in this range. In particular, it follows from expression (2) that a better spectral and angular resolution can be achieved with structures with interfacial irregularities under the condition $(\mathrm{Im}\,a_1)^2 < (\mathrm{Re}\,a_1)^2$.

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