Possibility of solving the inverse problem of diffractive scattering with dynamic effects

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The complex reflection coefficient of a crystal can be reconstructed from the angular distribution of diffractive reflection under conditions such that dynamic scattering of x rays in a defective crystal layer is important.

One of the fundamental problems in the theory of inverse diffraction problems is that of determining how the complex reflection coefficient of a crystal [this coefficient depends on a structure factor $\sigma(z)$ and on the elastic displacements $\vec{u}(z)$ of the lattice sites] varies along the thickness z by working from the angular distribution of the Bragg reflection of x rays.[1–5] This problem reduces to the successive solution of two subproblems:

1) reconstructing the phase of the reflected wave or of the amplitude reflection coefficient from experimental data on diffractive scattering of x rays;

2) calculating the complex reflection coefficient from the angular distribution of the amplitude reflection coefficient.

The solution of the first of these problems in the Born approximation of the theory of diffractive x-ray scattering is described in detail in Refs. 1 and 2. Examples of the practical application of the theory to thin heteroepitaxial structures, in which the thickness of the defective crystal layer satisfies $T \ll \Lambda_{\rm ex}$, where $\Lambda_{\rm ex}$ is the x-ray extinction length, were given in Ref. 2. Dynamic effects of diffractive x-ray scattering become important at $T \gtrsim \Lambda_{\rm ex}$ and complicate the relationship between the complex reflection coefficient and the amplitude reflection coefficient. It is important to note,[1] however, that the solutions of the first of these problems in the Born case and in the dynamic case of diffractive x-ray scattering are the same. Accordingly, if we wish to extend the existing theory[1] to thicker crystal structures, we need to develop a solution method which goes beyond the scope of the Born approximation of the theory of diffractive x-ray scattering.

It is convenient to use a method based on recurrence relations which relate the amplitude reflection coefficients $R(q,z_N)$ and $R(q,z_{N+1})$ at two different depths z_N and z_{N+1} in the crystal $(z_{N+1} > z_N)$:

$$R(q, z_N) = r_N(q, z_N) + R(q, z_{N+1})/\beta_N(q, z_N), \tag{1}$$

where $q = q' + i\mu_0$, q' is the normalized deviation from the Bragg condition for the ideal crystal, μ_0 is the normal absorption coefficient, and $\tau_N(q,z_N)$ is the reflection coefficient of a thin, isolated crystal layer $\Delta = z_{N+1} - z_N$. It follows from the general theory of diffractive x-ray scattering that $\beta_N(q,z)$ satisfies the equation

$$-i\frac{d\beta_N(q,z)}{dz}=(q-\alpha)\beta_N(q,z)+\sigma(z)[2r_N(q,z)\beta_N(q,z)+R(q,z_{N+1})], \qquad (2)$$

with the boundary condition $\beta_{N+1}(q,z_{N+1})=1$ and with $z_N \leqslant z \leqslant z_{N+1}$. Here $\alpha=d(\vec{h}\vec{u})/dz$, $\vec{h}$ is the diffraction vector, $\vec{u}(z)$ is the displacement of the reflection plane, and $\sigma(z)$ is proportional to the absolute value of the structure factor. If $\Delta \ll \Lambda_{ex}$, one can show that a calculation of $\tau_N(q,z_N)$ in the Born approximation of the theory of diffractive x-ray scattering has an error $\sim\Delta^3 \ll 1$. If the first term in square brackets in Eq. (2) is ignored, one can calculate $\beta_N(q,z_N)$ within an error $\sim\Delta^2 \ll 1$.

The amplitude reflection coefficients $R(q,z_{N+1})$, thought of as functions in the complex q plane, are analytic in the upper half-plane, so the corresponding Fourier transforms are nonzero only at[1] $z>z_N$. One can show that when $R(q,z_{N+1})$ is divided by $\beta_N(q,z_N)$, this property is retained, so the Fourier transform of the second term in (1) is nonzero at $z>z_{N+1}$, while the Fourier transform of $\tau_N(q,z_N)$ gives us the profile of the complex reflection coefficient on the interval $z_N<z<z_{N+1}$. An important assertion follows: The Fourier transforms of the amplitude reflection coefficients in the Born and dynamic cases are the same in a layer which is sufficiently close to the surface.

We thus obtain the following algorithm for solving the second problem involved in determining the complex reflection coefficient from the angular distribution of the amplitude reflection coefficient:

1) Break the crystal structure up into sublayers of thickness $\Delta \ll \Lambda_{ex}$.

2) Calculate the Fourier transform of the given amplitude reflection coefficient at the surface of the structure, i.e., $R(q,0)$, and thereby determine the fragment of the profile of the complex reflection coefficient in the first sublayer.

3) Work from the distribution of the complex reflection coefficient $\sigma(z)\times\exp[-i\varphi(z)]$, where $\varphi(z)=\vec{h}\vec{u}(z)$, in the first sublayer to calculate the amplitudes $\tau_1(q,z_1)$ and $\beta_1(q,z_1)$ in the Born approximation. Then calculate the amplitude reflection coefficient $R(q,z_1)$ from Eq. (1). In other words, calculate the reflection coefficient corresponding to a structure "from which the first sublayer has been removed."

4) Repeat the process, starting with step 2, until all sublayers of the defective layer have been removed. Join the fragments of the complex reflection coefficient calculated in this manner for the various sublayers, and construct the complete profile of the complex reflection coefficient over thickness of the defective crystal.

As an example of the use of this algorithm we have carried out a numerical simulation for a step profile of the complex reflection coefficient, corresponding to a structure consisting of a substrate and a near-surface crystalline layer with an altered lattice constant and a thickness $T=1.6\Lambda_{ex}$. The direct problem of dynamic diffractive x-ray scattering was solved. The angular distribution of the amplitude reflection coefficient at the surface of the crystal, $R(q,0)$, was calculated. The profile of the complex reflection coefficient was then reconstructed in accordance with the algorithm outlined above. This profile was then compared with the original, given profile; it was also compared with the profile reconstructed in the Born approximation (Fig. 1). We see

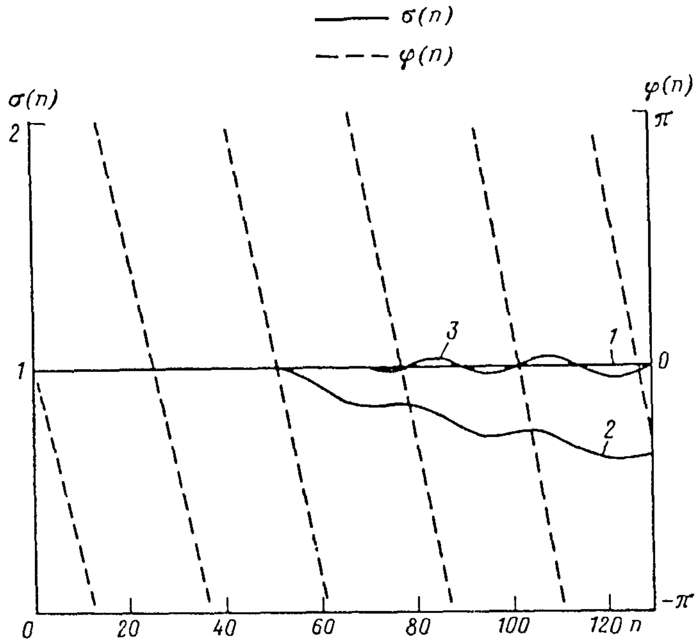

FIG. 1. Profile of the complex reflection coefficient of a crystal with a defective layer. Here $z_N = (T/128)n$, where $n = 0, 1, 2, \dots, 128$. 1—Model profile; 2—theoretical profile in the Born approximation; 3—theoretical profile in the dynamics case.

that the solution of the inverse problem of diffractive x-ray scattering with dynamic effects is closer than the Born approximation to the actual solution. The parasitic beats seen on both reconstructed profiles of the complex reflection coefficient at large thicknesses, $z > T/2$, apparently result from a buildup of rounding errors associated with the use of discrete Fourier transforms. These beats essentially disappear when one uses methods for stabilizing the solution of ill-posed problems.[6]

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