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On the Theory of Reflectivity by an X-Ray Multilayer Mirror

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A general theory of reflectivity by a perfect X-ray multilayer mirror based on the usage of a recurrent relation is developed. The reflectivity is described by the well-known Fresnel formulae which take into account jumps of susceptibility at the boundary between the layers. The analytical solution in the frame of the most general dynamical approach is found and the condition of application of the kinematical approximation is discussed. Special attention is paid to the periodic multilayer structure containing two layers of different materials with more than one pair of these layers in the period.

1. Introduction

The reflection of light at the boundary of two optically inhomogeneous media is the most widely used effect in optics. Different interference instruments, polarizers, focusing lenses, and coatings are used in different spheres of life and science [1]. In recent years large success was achieved in the technology of creating a multilayer system with a very small thickness of the layers of about nm. The semiconductor monocrystal superlattice opens a new branch of technology – quantum tunneling devices [2]. The synthetic multilayer structure is an excellent tool for the preparation of X-ray beams with desired characteristics. The latter problem is essentially important for the use of synchrotron radiation sources [3, 4]. An interesting application of multilayer structures for decreasing the electronic reflectivity background in studying the coherent nuclear scattering of γ -radiation (Mössbauer effect) was discussed recently [5, 6].

The theory of reflectivity of a multilayer structure is in general based on an iteration procedure with the use of a recurrent formula which connects the reflection amplitudes of X-ray waves in two nearest layers. This formula is a direct consequence of the Fresnel formulae, namely, the law of penetration and reflection of radiation at the boundary of two homogeneous media. In this way only a computer simulation is possible. On the other hand, considering the periodic multilayer structure, the so-called X-ray multilayer mirror, it is possible to find the analytical solution of the problem. The main purpose of this paper is to present this analytical solution in a most general case taking into account multiple reflections and a nonzero boundary condition.

In Section 2 the basic formulation of the problem of X-ray multilayer structure reflectivity is given and the computer simulation is described. The analytical solution is presented in Section 3. The probabilities of penetration and reflection by one cell of the periodic structure are discussed in Section 4. Section 5 contains comments on the role of defects. A numerical example is presented in the last section.

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2. Fresnel Formulae and the Recurrent Relation

Let us consider an artificial system which consists of plane parallel layers of different materials with abrupt boundaries between them. The layers are homogeneous along the surface which is parallel to the (X, Y) plane of the rectangular coordinate system so that the change of the material occurs only along the Z-direction perpendicular to the surface. Let a plane monochromatic wave of X-rays fall on the system and have a wave vector k in the plane (X, Z) with positive k_x and k_z components (see Fig. 1). At the boundaries the plane wave is refracted and reflected. As a result two plane waves exist in each layer, a refracted one and a reflected one. These waves have just the same k_x components of the wave vector in all the layers but the k_z components have opposite signs in the two waves and, moreover, they differ from one layer to another. Thus, the electric field vector in the layer with number m has the form

$$\boldsymbol{E}_{m}(\boldsymbol{x}, \boldsymbol{z}, t) = \boldsymbol{E}(\boldsymbol{x}, t) \left[\boldsymbol{E}_{tm} \exp\left(i\boldsymbol{k}_{zm}\boldsymbol{z}\right) + \boldsymbol{E}_{tm} \exp\left(-i\boldsymbol{k}_{zm}\boldsymbol{z}\right) \right], \tag{1}$$

where $E(x, t) = \exp(ik_x x - i\omega t)$, E_{tm} and E_{rm} are the amplitudes of refracted and reflected waves in the middle of the layer and the coordinate z is measured from the middle line of the layer (see Fig. 1).

Inside the layer these waves do not interact with each another. Each of them is the solution of the Maxwell equation in a homogeneous medium with susceptibility $\chi_m = \varepsilon_m - 1$. This equation determines the value of k_z as

$$k_{zm} = \sqrt{\left(\frac{2\pi}{\lambda}\right)^2 \left(1 + \chi_m(\omega)\right) - k_x^2}.$$
(2)

Here λ is the wavelength of radiation. Let θ be the angle between the direction of the incident wave and the surface (see Fig. 1), then

$$k_x = K \cos \theta$$
, $k_{zm} = K \sqrt{\sin^2 \theta + \chi_m}$; $K = 2\pi/\lambda$. (3)



Fig. 1. Geometrical parameters of the theory

As follows from (3), k_z differs in different layers due to different values of susceptibility χ_m . The susceptibility is very small for X-rays (about 10⁻⁵), therefore the reflectivity will be sufficient only for small enough values of the angle θ (of about tens of mrad).

Maxwell's equation determines only the wave vector and the wave amplitudes remain free. They are determined by the boundary conditions. Let us consider first the more simple case of σ -polarized radiation when the amplitudes E_{tm} and E_{rm} have only a y-component perpendicular to the scattering plane. Below the layers will be numbered from the bottom of the structure to the top in the direction of the reflected wave (see Fig. 1). The conditions of continuity for the electric and magnetic fields at the boundary between the layers with numbers 1 and 2 can be written as

$$E_{t_2}C_2 + E_{r_2}C_2^{-1} = E_{t_1}C_1^{-1} + E_{r_1}C_1,$$

$$k_{z_2}(E_{t_2}C_2 - E_{r_2}C_2^{-1}) = k_{z_1}(E_{t_1}C_1^{-1} - E_{r_1}C_1).$$
(4)

Here and below $C_m = \exp(ik_{zm}D_m/2)$, where D_m is the thickness of the *m*-th layer, and the amplitudes in each layer are determined for the middle line of the layer.

Let us assume the amplitudes E_{t2} and E_{r1} to be known and the amplitudes E_{t1} and E_{r2} to be found. The solution of this problem can be written in the form

$$E_{r2} = r_{22}^{(1)}E_{t2} + t_{21}E_{r1}, \qquad E_{t1} = t_{12}E_{t2} + r_{11}^{(2)}E_{r1}, \qquad (5)$$

where

$$r_{22}^{(1)} = \frac{k_{22} - k_{21}}{k_{21} + k_{22}} C_2^2 = F_{21} C_2^2, \qquad t_{12} = \frac{2k_{22}}{k_{21} + k_{22}} C_1 C_2, \qquad (6)$$

and the formulae for t_{21} and $r_{11}^{(2)}$ are obtained from (6) by permutation of the indexes 1 and 2.

Thus, we introduce a 2×2 matrix. The nondiagonal elements of this matrix describe the penetration of the waves from one layer to another through the boundary (the refraction effect). The diagonal elements describe the reflection of the waves when the waves remain in the layer as a result of reflection from another layer with number given by the upper index. These formulae are the well-known Fresnel formulae [7] which are written in a form convenient for us. We note that the formulae remain true when we increase the indexes by an arbitrary number *m*. In the case of π -polarized radiation it is convenient to consider the magnetic field vector instead of the electric one [7]. In this case all the consideration remains valid if we replace (6) by

$$r_{22}^{(1)} = \frac{\varepsilon_1 k_{z2} - \varepsilon_2 k_{z1}}{\varepsilon_2 k_{z1} + \varepsilon_1 k_{z2}} C_2^2, \qquad t_{12} = \frac{2\varepsilon_1 k_{z2}}{\varepsilon_2 k_{z1} + \varepsilon_1 k_{z2}} C_1 C_2, \tag{7}$$

where $\varepsilon_m = 1 + \chi_m$ is the dielectric function in the *m*-th layer.

If we are interested only in the reflectivity of the multilayer structure, then we can use these formulae in another form, namely, in terms of the reflection amplitude $R_m = E_{rm}/E_{tm}$. Indeed, (5) can be rewritten as

$$E_{11} = \frac{t_{12}}{1 - r_{11}^{(2)} R_1} E_{12}, \qquad R_2 = r_{22}^{(1)} + \frac{t_{21} t_{12} R_1}{1 - r_{11}^{(2)} R_1}.$$
(8)

This formula gives the expression for R_2 through R_1 and the characteristics of the boundary between layers 1 and 2, so it is a recurrent formula. It gives the simple solution of the computer simulation of an arbitrary multilayer structure by means of multiple use from the 'lower layer' with number 0 (substrate) where $R_0 = 0$ to the 'upper layer' that is the air above the structure. If the structure has N layers, then $R_1 = r_{11}^{(0)}$ and using (7) N times we obtain $R_{N+1} = R_{tot}$ as the relation of the electric field amplitude reflected by all layers to the amplitude of the incident wave $R_{tot} = E_r/E_t$. The reflectivity is $P(\theta) = |R_{tot}(\theta)|^2$.

We note that (8) coincides completely with the well-known Parratt recurrent formula [8] for $R'_m = R_m C_m^2$,

$$R'_{2} = C_{2}^{4} \frac{F_{21} + R'_{1}}{1 + F_{21}R'_{1}}.$$
(9)

Although the Parratt formula is more simple we shall use our notations which are more convenient for our analytical consideration (see the following section).

The susceptibility $\chi(\omega)$ is a complex quantity in the X-ray regions of frequencies,

$$\chi = \chi' + i\chi'' = \frac{\lambda}{2\pi} \sum_{a} N_a [-2\lambda r_0 (Z_a + \Delta f'_a) + i\sigma_a], \qquad (10)$$

where the *a* sum is over atom sorts, N_a is the number of atoms of *a*-th sort in a unit volume, $r_0 = e^2/mc^2$, Z_a is the number of electrons in the atom, $\Delta f'_a$ the resonant dispersion error, and σ_a the absorption cross-section. The real part χ' of the susceptibility is negative, while the imaginary part χ'' is positive and has much smaller magnitude than the real one, $\chi'' \ll |\chi'|$. Since $\chi = 0$ in air, it follows from (3) and (6) that there is some region of angle θ values near zero where k_{zm} is imaginary even if the medium is non-absorbing. It is the region of total external reflection. The limiting angle of total reflection is about $\theta_e = |\sqrt{|\chi'|}$.

If $\theta > \theta_c$, then the reflectivity decreases with the increase of θ . Additional peaks can arise in the periodic multilayer structure which we shall call the multilayer mirror (MLM) at angles if the phases of waves reflected by different cells of the MLM differ by an even multiple of π . If D is the thickness of the cell, then the condition of Bragg peaks is $2D \sin \theta = n\lambda$. In the following sections we shall consider the Bragg peaks of MLM in more detail.

3. Reflectivity by a Perfect Multilayer Mirror

Let us consider two cells of MLM. The amplitudes of refracted and reflected waves in the first layer of each cell are connected by relations similar to (5),

$$E_{r2} = rE_{t2} + \bar{t}E_{r1}, \qquad E_{t1} = tE_{t2} + \bar{r}E_{r1}, \qquad (11)$$

but here the indexes 1 and 2 number the cells from the bottom to the top of the MLM and the probabilities of penetration and reflection of the waves do not depend on the number of cells because all the cells are identical. Now we introduce once again the reflection amplitude $R_m = E_{cm}/E_{tm}$ in the first layer of each cell and (11) immediately leads us to the recurrent formula

$$R_{n+1} = r + \frac{t\bar{t}R_n}{1 - \bar{r}R_n} \tag{12}$$

with constant coefficients.

A relation of such type has been considered earlier in the theory of X-ray diffraction in a semiconductor superlattice [9 to 11] and the analytical solution has been found with the

$$R_n = \frac{rA_n}{A_n - \sqrt{t\bar{t}A_{n-1}}}.$$
(13)

With the use of this expression (12) transforms to

$$\frac{A_{n+1}}{A_{n+1} - \sqrt{t\bar{t}A_n}} = \frac{2vA_n - A_{n-1}}{2vA_n - A_{n-1} - \sqrt{t\bar{t}A_n}},$$
(14)

where

$$v = \frac{1 + t\bar{t} - r\bar{r}}{2\sqrt{t\bar{t}}} = \cos(\psi/2).$$
(15)

It can be seen directly that (14) becomes valid if

$$A_{n+1}(v) = 2vA_n(v) - A_{n-1}(v).$$
(16)

Thus, we pass from (12) to a more simple equation, i.e. the recurrent relation for Chebyshev's polynomials [12]. The detailed analysis shows that in the case of arbitrary boundary condition we must choose A_n in the form

$$A_n(v) = (r - R_0) U_{n-1}(v) + \sqrt{t\bar{t}} R_0 U_n(v), \qquad (17)$$

where $U_n(v)$ are Chebyshev's polynomials of second kind which can be determined by the recurrent relation (16) and the following terms:

$$U_{-2} = -1$$
, $U_{-1} = 0$, $U_0 = 1$. (18)

Equations (13) and (17) are useful due to the analytical expression of Chebyshev's polynomial

$$U_{n-1}(v) = \frac{\sin(n \arccos v)}{\sqrt{1-v^2}} = \frac{\sin(n\psi/2)}{\sin(\psi/2)}.$$
(19)

Here the complex phase ψ is determined by (15). To obtain the equation for R_n in a more convenient form we introduce the second phase φ by the relation

$$t\bar{t} = \exp\left(i\varphi\right). \tag{20}$$

Now by use of (15), (17), (19), and (20) the formula for R_n can be written in the form

$$R_{n} = r \frac{r - R_{0}f_{-} - (r - R_{0}f_{+})\exp(in\psi)}{f_{+}(r - R_{0}f_{-}) - f_{-}(r - R_{0}f_{+})\exp(in\psi)},$$
(21)

where

$$f_{\pm} = 1 - \exp(i[\varphi \pm \psi]/2), \qquad \exp(\pm i\psi/2) = \nu \mp \sqrt{\nu^2 - 1}.$$
 (22)

The functions f_{\pm} can be expressed directly via the parameters of penetration and reflection by the cell using (15) and (20),

$$f_{\pm} = a \pm \sqrt{a^2 - r\bar{r}}, \qquad a = 1 - v \sqrt{t\bar{t}} = \frac{1}{2} (1 - t\bar{t} + r\bar{r}).$$
 (23)

5 physica (b) 187/1

Our formula for R_n has a such structure that the limiting value of reflectivity for very large values of *n* is clear. The physical nature of the subject under consideration demands the phase ψ to have a positive imaginary part, so exp (*in* ψ) vanishes and we have

$$R_{\infty} = \frac{r}{f_{+}} = \frac{r}{a + \sqrt{a^{2} - r\bar{r}}} \,. \tag{24}$$

This expression does not depend on R_0 and this fact is very clear from the physical point of view. It is easy to see, the formula for R_{∞} is very similar to Darwin's formula in the dynamical theory of symmetrical Bragg X-ray diffraction by thick absorbing crystals [13], because this approach is the dynamical theory of reflectivity by a multilayer mirror. We note that in the case under consideration the parameters are related to a complex cell and have not so simple expressions as in the Darwin theory. For this reason the approach considered may be called the generalized dynamical theory.

It is interesting to consider also a more simple kinematical theory of MLM reflectivity. This theory ignores multiple reflections, so it uses the approximate recurrent formula

$$R_{n+1} = r + t\bar{t}R_n. \tag{25}$$

With account of (20) the solution can be obtained directly by summing up the geometrical progression

$$R_n = r \frac{1 - \exp(in\varphi)}{1 - \exp(i\varphi)} + R_0 \exp(in\varphi).$$
⁽²⁶⁾

This can also be obtained from the accurate formula (21) in the approximation $\psi = \varphi$ as it follows from (15) if multiple reflection is ignored. The more simple kinematical approximation is good enough in cases of small reflectivity by one cell and a small number of cells in the MLM. However, in the angular regions of the Bragg peaks it can give a non-physical reflectivity which exceeds unity in the limit of a large number of cells and slightly absorbing matter while the accurate formula (21) is correct in all cases.

For the evaluation of the accuracy of the kinematical approximation inside the Bragg peaks we can use the ideas of the dynamical theory of X-ray diffraction. So in the kinematical approximation the maximum number of cells is limited by the absorption $n_{\rm abs} = 1/\varphi''$, where φ'' is the imaginary part of φ . On the other hand, for the dynamical reflectivity (extinction effect) to arise we need a number of cells $n_{\rm ext} = 1/\sqrt{|r\bar{r}|}$. The reflectivity by MLM with a large number of cells remains kinematical if $n_{\rm abs} \ll n_{\rm ext}$. For numerical calculation we need the accurate formula only near the most strong Bragg peaks while in the whole angular region where the kinematical approximation gives a small value of reflectivity, it is correct.

The simplest real MLM has a substrate below and air above the periodic structure. Let χ_s be the susceptibility of the substrate. Then

$$R_0 = \frac{k_{z1} - k_{zs}}{k_{z1} + k_{zs}} C_1^2, \qquad k_{zs} = K \sqrt{\sin^2 \theta + \chi_s}.$$
(27)

To take into account the top boundary we must exclude the boundary between the last layer with the number N and the first layer of the cell and include the boundary between the last layer and air. As a result the total reflectivity of the multilayer mirror is determined

On the Theory of Reflectivity by an X-Ray Multilayer Mirror

by the following formulae:

$$R_{\text{tot}} = r_{AA}^{(N)} + \frac{t_{AN} t_{NA} R_l}{1 - r_{NN}^{(A)} R_l}, \qquad R_l = \frac{R_n - r_{11}^{(N)}}{t_{1N} t_{N1} + r_{NN}^{(1)} (R_n - r_{11}^{(N)})},$$
(28)

where we use the index A for air and the probabilities of penetration and reflection are determined by the general formulae (6) with $k_{zA} = K \sin \theta$, $C_A = 1$.

4. Reflectivity by One Cell

The cells of the multilayer mirror must have at minimum two layers of different materials and consequently two boundaries. Let us make use of (5) twice, for two boundaries between layers 1 and 2 and between layers 2 and 3 (see Fig. 1), and then exclude the middle layer 2. As a result we obtain

$$E_{r3} = r_{33}^{(1)}E_{t3} + t_{31}E_{r1}, \qquad E_{t1} = t_{13}E_{t3} + r_{11}^{(3)}E_{r1}, \qquad (29)$$

where

$$r_{33}^{(1)} = r_{33}^{(2)} + t_{32}t_{23}\frac{r_{22}^{(1)}}{1 - r_{22}^{(3)}r_{22}^{(1)}}, \qquad t_{13} = t_{23}\frac{t_{12}}{1 - r_{22}^{(3)}r_{22}^{(1)}}.$$
(30)

The formulae for t_{31} and $r_{11}^{(3)}$ can be obtained from (30) by permutation of the indexes 1 and 3. It is easy to see, these formulae have the structure of recurrent formulae. Moreover, the problem can be formulated in terms of four recurrent procedures for calculating the four scattering parameters of the cell.

For this purpose let us introduce the new notations

$$r_n = r_{n+1\,n+1}^{(n)}, \quad \bar{r}_n = r_{nn}^{(n+1)}, \quad t_n = t_{nn+1}, \quad \bar{t}_n = t_{n+1\,n},$$
 (31)

and the recurrent relations

$$R_{n} = r_{n} + \frac{\bar{t}_{n} t_{n} R_{n-1}}{1 - \bar{r}_{n} R_{n-1}}, \qquad T_{n} = T_{n-1} \frac{t_{n}}{1 - \bar{r}_{n} R_{n-1}},$$

$$\bar{R}_{n} = \bar{r}_{m} + \frac{t_{m} \bar{t}_{m} \bar{R}_{n-1}}{1 - \bar{r}_{m} \bar{R}_{n-1}}, \qquad \bar{T}_{n} = \bar{T}_{n-1} \frac{\bar{t}_{m}}{1 - r_{m} \bar{R}_{n-1}},$$
(32)

where m = N + 1 - n and N is the number of layers in the cell. Now we can start from $R_0 = \bar{R}_0 = 0$, $T_0 = \bar{T}_0 = 1$ and make use of (32) N times. As a result, we obtain $r = R_N$, $\bar{r} = \bar{R}_N$, $t = T_N$, $\bar{t} = \bar{T}_N$. The procedure of accurate calculation of the scattering matrix for one cell is not complicated for numerical calculations but very inconvenient for an analytical consideration.

That is why for further consideration we restrict ourselves to an approximation where we can neglect multiple reflections inside one cell. That does not mean the kinematical approximation at all but it demands the reflection by one boundary to be small. This is just so near the Bragg peaks but not so in the angular region of total external reflection. In this approximation it is easy to write the formulae for the elements of the scattering matrix for the cell containing N layers,

$$t = t_{1}t_{2} \dots t_{N-1}t_{N}, \qquad \bar{t} = \bar{t}_{N}\bar{t}_{N-1} \dots \bar{t}_{2}\bar{t}_{1},$$

$$r = r_{N} + \bar{t}_{N}t_{N}r_{N-1} + \dots + \bar{t}_{N} \dots \bar{t}_{2}t_{2} \dots t_{N}r_{1},$$

$$\bar{r} = \bar{r}_{1} + t_{1}\bar{t}_{1}\bar{r}_{2} + \dots + t_{1} \dots t_{N-1}\bar{t}_{N-1} \dots \bar{t}_{1}\bar{r}_{N}.$$
(33)



Fig. 2. Reflection and penetration in one cell

The physical sense of these formulae is illustrated in Fig. 2. Without multiple reflections the penetration rate through the cell is the simple product of penetration rates through all the boundaries in the cell, while the reflection rate is the sum of reflections by all boundaries with different weights which account for the penetration in the given layer and the penetration in the back direction.

Let us consider the particular case that all layers in the cell belong to two types of matter but can have different thicknesses. Under this condition the number of layers in the cell is always even. Taking into account (6) and that the (N + 1)-st layer is identical with the first layer we obtain

$$t = \bar{t} = c^{N} (C_{1} \dots C_{N})^{2},$$

$$r = bC_{1}^{2} [1 - c^{2}C_{N}^{4} + c^{4} (C_{N}C_{N-1})^{4} - \dots - c^{2N-2} (C_{N} \dots C_{2})^{4}],$$

$$\bar{r} = bC_{1}^{2} [1 - c^{2}C_{2}^{4} + c^{4} (C_{2}C_{3})^{4} - \dots - c^{2N-2} (C_{2} \dots C_{N})^{4}],$$
(34)

where

$$b = \frac{k_{z1} - k_{z2}}{k_{z1} + k_{z2}}, \qquad c = \frac{2\sqrt{k_{z1}k_{z2}}}{k_{z1} + k_{z2}}.$$
(35)

Formulae (34) are obtained in the linear approximation in parameter b and since $c = \sqrt{1 - b^2}$ we can put c = 1. Then it is easy to write the expression for the phase φ (see (20)) as

$$\varphi = 4\pi D \sin \theta / \lambda + \Delta \varphi, \qquad \Delta k_{zm} = K(|\sqrt{\sin^2 \theta + \chi_m} - \sin \theta),$$

$$\Delta \varphi = 2D[\Delta k_{z1}(d_1 + d_3 + \dots + d_{N-1}) + \Delta k_{z2}(d_2 + d_4 + \dots + d_N)],$$
(36)

where D is the thickness of the cell and d_m the relative thickness of the layer with number m inside the cell. It is clear that $\sum_{m} d_m = 1$.

As follows from (26) the Bragg peaks arise when $\varphi = 2\pi n$. This condition without taking into account $\Delta \varphi$ gives the Bragg condition $2D \sin \theta = n\lambda$. Taking into account $\Delta \varphi$ and the more accurate formula (21), leads to a slight displacement of the first Bragg peak position. Formula (34) is useful for the evaluation of the reflectivity by one cell r (structure factor) near the Bragg peaks. It is very important because the enhancement of the reflectivity is possible only for large values of r (see (26)). Let us consider, for example, a cell with N = 4 and $d_2 = d_4$ and omit Δk_{zm} for the sake of simplicity (they are small near the Bragg peaks). So we have

$$rC_1^{-2} = b[1 - \exp(i\varphi d_4)] [1 + \exp(i\varphi(d_3 + d_4))].$$
(37)

It is easy to see that if $d_3 + d_4 = 1/2$, then the odd-order Bragg peaks are absent. It is clear as the real period in this case equals D/2.

5. The Role of Defects

The real multilayer mirrors are far from being perfect. The defects may be divided in two sorts: defects inside and outside the cell. The defects of the first kind are represented by the roughness and absence of sharpness of the interface due to the technological production and the diffusion of atoms from one layer to another. These defects can be taken into account in the frame of an analytical solution by a modification of the cell scattering parameters. This can be made, for example, by introducing the Debye-Waller factor in the phase factors and by considering additional layers with intermediate density and composition.

Among the defects of the second kind long-wave changes of period and material of the layers, structure of the cell, etc. may be assumed. These defects cannot be accounted for accurately in the frame of the presented analytical formula. One of the ways to take them into account is taking the average value over the considered parameters. However, we want to note that these defects are the consequence of errors in the technological process which can be eliminated by means of accurate preparation of the sample.

6. Numerical Example

The main problem of using a multilayer mirror for soft X-rays is to decrease the effect of absorption. For X-rays with wavelength about 0.1 nm an additional problem arises, namely, a very small reflectivity by one boundary. That is why only small grazing angles of incidence may be used near the total reflection region. Let us consider an MLM which has a two-layer cell with layers of equal thickness $(d_1 = d_2)$. When $\theta \ge \theta_c$, we have the following formulae for the evaluation of n_{abs} and n_{ext} :

$$n_{\rm abs}^{(m)} = \frac{2\sin\theta_m}{(\mu_1 + \mu_2)D}, \qquad n_{\rm ext}^{(m)} = \frac{2\sin^2\theta_m}{|\chi_1' - \chi_2'|}; \qquad 2D\sin\theta_m = m\lambda.$$
(38)

The total Bragg reflection is possible only when the number of cells $n > n_{ext}^{(m)}$ and $n_{abs}^{(m)} \ge n_{ext}^{(m)}$. In the opposite case, for any $n > n_{abs}^{(m)}$ the maximum of reflectivity is $P_{\max} \approx (n_{abs}^{(m)}/n_{ext}^{(m)})^2$. It is clear from (38) that with increasing θ_m the reflectivity drops faster than the absorption and we obtain the last case.

For the sake of examination of the analytical approach presented above we elaborated computer programs using both the Parratt formula (9) and the analytical formula (21). Both methods give identical results in the whole angular region including the region of total external reflection but the computing time for large *n* is much smaller with the use of the analytical formula. Fig. 3 shows the results of calculation for the MLM: (Nb, Si) 1000/glass with $\lambda = 0.154$ nm (CuK_a), $d_1 = d_2 = 0.5$, and D = 3.85 nm. In this case only odd reflections exist and $\theta_m \approx 20m$ mrad, $n_{abs}^{(m)} \approx 70m$, $n_{ext}^{(m)} \approx 24m^2$. It is easy to see, the peaks become small and narrow with increasing *m* but the first Bragg peak is large enough.



Fig. 3. Reflectivity of CuK_a X-rays by the perfect (Nb, Si) 1000/glass multilayer mirror

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