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THEORY OF MULTILAYER X-RAY MIRRORS WITH SLOWLY VARYING PERIOD

A. V. Vinogradov and R. M. Feshchenko

P. N. Lebedev Physical Institute, Russian Academy of Sciences, Leninskii Pr. 53, Moscow 117924, Russia

Abstract

Broadening of multilayer-mirror reflection band is achieved by slow variation of its period. The paper is devoted to the theory of such optical elements based on a general theory of wave propagation through a quasi-periodic medium. The calculation results are presented for the reflection coefficient of broadband mirrors in the 1 to 50 Å range. A statement of the inverse problem is also considered, namely, creation of a multilayer structure possessing the prescribed reflection coefficient.

1. Introduction

Multilayer reflecting coatings are widely used for creating x-ray optical elements and systems. In the photon energy range from 30 keV to 30 eV [1], periodic coatings often consist of tens, hundred, or thousands of layers and possess high selectivity with respect to wavelength and sliding angle.

Obtaining wide reflection band of multilayer coatings is also a critical problem in x-ray optics. It is desirable in various physical applications: x-ray astronomy, monitoring of synchrotron emission, spectroscopy, and in material sciences, where integrals of the reflection coefficient are important with respect to the angle or energy rather than the maximum value of this coefficient.

It is obvious that the requirement for a maximum value of the reflection coefficient contradicts the broad band of reflection. Indeed, in the case of a periodic system optimized for maximum coefficient of reflection a substantial broadening of the reflection band is achieved by reducing the number of the layers. This inevitably reduces the maximum value of the reflection coefficient.

A theoretical study of reflection coefficients in periodic multilayer mirrors can be found in [2–4].

However, no serious analytical theory of aperiodic structures has been suggested yet. The existing theoretical models are too simplified or semi-empirical. We present a brief review of them.

The use of aperiodic multilayer mirrors in the x-ray range was discussed in [5]. A review of papers in this field is given in [6].

In [7], the reflection coefficient is approximated starting from simple speculations (in the kinematic approximation) about the radiation passing through a layered matter. On this basis, a calculation formula was derived for the inverse problem which makes it possible to determine the period $d(i)$ of the ith layer that provides a constant reflection coefficient in a wide wavelength range. This formula is written in the form

$$\mathrm{d}(i) = (m + i)^c, \quad c = 0.27, \quad m = 0.5.$$

This study was conducted for the hard x-ray range $E_\gamma > 30\,\mathrm{keV}$ for the structure W–C. One drawback of this approach is the absence of an analytical theory, which makes justification of the employed formulas difficult.

In [8], a numerical optimization is performed for the maximum reflection coefficient of the structure Mo–Si in the 130–190 Å range. The resulting reflection coefficient is 1.5 times greater compared to the corresponding periodic structure. The drawback is still the same, i.e., the absence of a theory prevents any justification of the numerical optimization used.

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In [9], the possibility of designing broad-band mirrors for astrophysical applications in the ranges 20–30 and 40–60 keV is investigated. The mirror is divided into a small number of groups comprising similar two-layer structures (conventionally four groups) and then the numerical matching parameters in the groups are found. In this way, mirrors with a broad reflection band in the mentioned ranges are obtained. This approach is easy due to the small number of parameters to be found. However, the coefficient of reflection exhibits noticeable variations in the spectral interval considered.

In the present paper, we study broadband x-ray optics on the basis of the wave propagation theory in multilayer structures with a slowly varying period.

2. Basic Equations

Let us note that actual x-ray coatings consist of a series of layers of different chemical compositions, which provides a jump-type character of dielectric susceptibility variation in the intermediate zone. In our analytical description of close-to-periodic coatings, we will use the following spatial distribution of dielectric susceptibility:

$$\epsilon(z) = \tilde{\mu_0} + 4\tilde{B} f(t), \quad t = \int_0^z q(z')\,dz', \tag{1}$$

where

$$\tilde{\mu_0} = \frac{\epsilon_1 + \epsilon_2}{2}, \quad \tilde{B} = \frac{\epsilon_1 - \epsilon_2}{8},$$

ϵ_1 and ϵ_2 are dielectric susceptibilities of corresponding components of the multilayer structure, z is the distance from the structure surface, and $f(t)$ is a stepwise function of the period 2π shown in Fig. 1. The origin of coordinates is taken so that the function $f(t)$ is even. It has no effect on the results because the Fresnel reflection from the structure surface is negligible and we are interested in resonance interaction of the wave with a great number of layers.

Let us take a Fourier series expansion of the function $f(t)$:

$$\epsilon(z) = \mu_0 + 4B_1 \cos\left[2\int_0^z q(z')\,dz'\right] + 4\sum_{n=2}^{\infty} B_n \cos\left[2n\int_0^z q(z')\,dz'\right], \tag{2}$$

where

$$\mu_0 = \beta\epsilon_1 + (1-\beta)\epsilon_2, \quad B_n = \frac{\epsilon_1 - \epsilon_2}{2n\pi}\sin \pi n\beta, \quad \beta = \frac{d_1}{d_1 + d_2}.$$

The corresponding equation for the field $E(z)$ of the x-ray wave falling on the structure surface at the angle θ has the form

$$E'' + k^2\left\{\mu_0 - \cos^2\theta + 4B * \cos\left[2\int_0^z q(z')\,dz'\right]\right\}E = 0, \quad B = B_1, \tag{3}$$

where, according to [1, 2], we keep in expression (2) for ϵ(z) only one varying term, which corresponds to consideration of the first Bragg resonance of the reflection coefficient. The relationship between the structure described by (2) and a real multilayer structure will be considered below.

Now we present E in the form

$$E(z) = \sqrt{\frac{q(0)}{q(z)}}\left(b_+(z)\exp\left\{i\int_0^z q(z')\,dz'\right\} + b_-(z)\exp\left\{-i\int_0^z q(z')\,dz'\right\}\right), \tag{4}$$

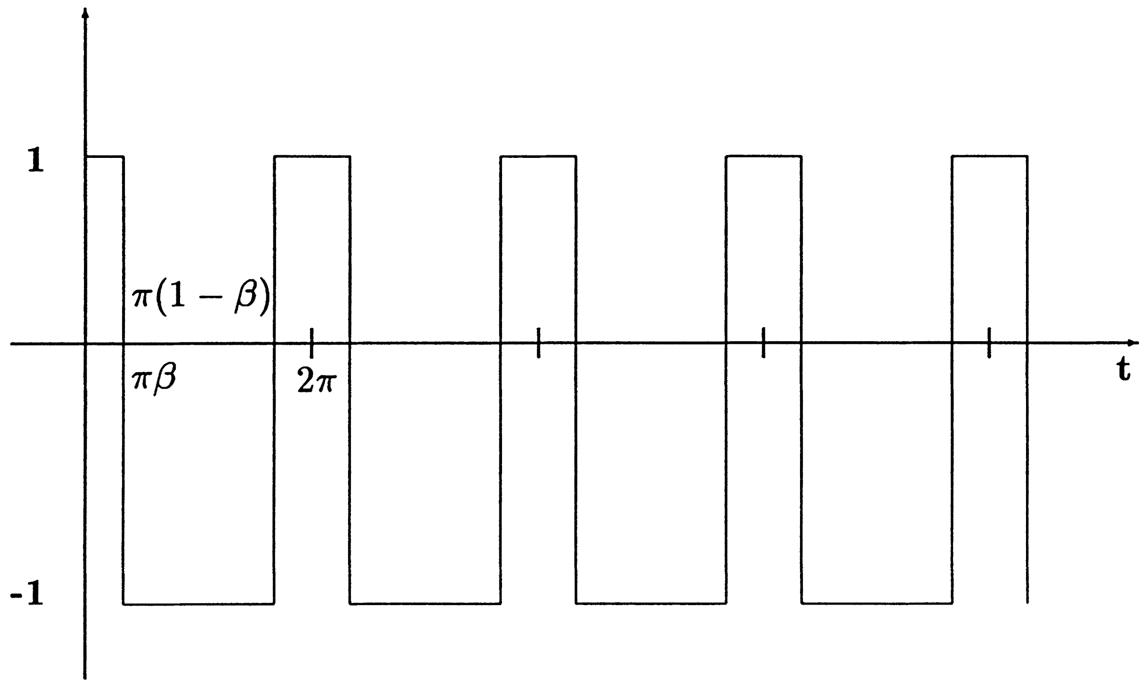

Fig. 1. Spatial dependence of dielectric susceptibility of almost periodical structure [see formula (1)]. The parameter $\beta = d_1/(d_1 + d_2)$ is a fraction of the period occupied by the first component; d_1 and d_2 are the widths of the layers 1 and 2, respectively.

where b_+ and b_- are slowly varying amplitudes of the falling and reflecting waves, respectively.

By substituting the expression for E into (3) we arrive at a system of two equations with boundary conditions. Here we neglect the exponents with double period and the second derivatives b_+ and b_- (slowly varying amplitudes (see [2],p. 79). Finally, we obtain the following system of equations:

$$\begin{aligned} b'_+ &= i\frac{k^2}{2q(z)}\left(\mu - \frac{q^2(z)}{k^2}\right) * b_+ + i\frac{k^2 B}{q(z)} * b_-, \qquad \mu = \mu_0 - \cos^2\theta, \\ b'_- &= -i\frac{k^2 B}{q(z)} * b_+ - i\frac{k^2}{2q(z)}\left(\mu - \frac{q^2(z)}{k^2}\right) * b_-, \end{aligned} \tag{5}$$

with the boundary conditions

$$\begin{aligned} b_+(0) &= 1, \\ b_-(z_N) &= 0, \qquad z_N \to +\infty, \end{aligned} \tag{6}$$

where the reflection coefficient is determined by the formulas

$$\mathrm{r} = b_-(0), \qquad \mathrm{R} = |b_-(0)|^2. \tag{7}$$

The boundary conditions here are determined by the absence of the reflected wave outside the structure, whereas the falling wave has a unit amplitude on the structure's surface. These conditions define the solutions and the reflection coefficient in a unique manner.

Let us formulate the energy conservation law for the system (5). We assume no initial absorption; then the coefficients of the system (5) are imaginary. Hence, if

$$\begin{pmatrix} b_+ \\ b_- \end{pmatrix}$$

is a solution of (5), then, taking the complex conjugate, we come to the conclusion that

$$\begin{pmatrix} b_-^* \\ b_+^* \end{pmatrix}$$

is the solution as well. Calculating the Wronskian for these two solutions ($\mathbf{b_1}$ and $\mathbf{b_2}$) we obtain

$$\begin{vmatrix} b_+ & b_-^* \\ b_- & b_+^* \end{vmatrix} = |b_+|^2 - |b_-|^2 = \text{const.} \tag{8}$$

The Wronskian is a constant because the spur of the matrix (5) is zero. Note that

$$b_-(\infty) = 0 \qquad \text{and} \qquad |b_+(\infty)|^2 = \mathrm{T},$$

where T is the coefficient of transmission.

From the energy conservation law, it follows that

$$|b_+(\mathrm{z})|^2 - |b_-(\mathrm{z})|^2 = \mathrm{T}. \tag{9}$$

Note also that

$$b_+(0) = 1 \qquad \text{and} \qquad b_-(0) = \mathrm{r};$$

then, in view of (9),

$$\mathrm{R} + \mathrm{T} = 1.$$

If we also take absorption into account, then we can write

$$\mathrm{R} + \mathrm{T} + \mathrm{Q} = 1 \to \mathrm{R} + \mathrm{T} < 1,$$

where Q is the fraction of energy absorbed by the medium. Thus, the system (5) satisfies the energy conservation law.

By excluding $b_+(z)$ from the system (5), we can reduce it to the single second-order equation

$$b'' + \frac{q'}{q}b' + \left[-iq' - \frac{k^2}{2}\mu + \frac{k^4}{4}\frac{(\mu^2 - 4B^2)}{q^2} + \frac{q^2}{4}\right] b = 0, \qquad b = b_-(z), \tag{10}$$

with the boundary conditions

$$b\,(+\infty) = 0, \qquad b'(0) + i\frac{\mathrm{k}^2}{2\mathrm{q}}\left(\mu - \frac{\mathrm{q}^2}{\mathrm{k}^2}\right) b(0) = -i\,\frac{\mathrm{k}^2\mathrm{B}}{\mathrm{q}}. \tag{11}$$

Expression (6) for the reflection coefficient can be reduced to the form

$$r = i\,\frac{k^2}{q(0)}\,B\,\frac{1}{i\,\dfrac{k^2}{q(0)}\left[\dfrac{q^2(0)}{k^2} - \mu\right] - \dfrac{b'(0)}{b(0)}}. \tag{12}$$

One can see that the reflection coefficient is expressed in terms of a logarithmic derivative of the solution (10) at zero point, which tends to zero at $z \to +\infty$.

3. WKB Asymptotics in a Solution of the Equation for Slowly Varying Amplitudes

Let us reduce (10) to the standard form in order to apply the WKB[1] approximation. First, we introduce the function y(z):

$$b(z) = \frac{y(z)}{\sqrt{q}},$$

and make a substitution

$$z = tp, \qquad p \to 0, \qquad \text{and} \qquad \frac{\dot{q}(t)}{q(t)} \sim 1.$$

Making substitutions in (10) we arrive at

$$\ddot{y} + \left[\frac{f_0}{p^2} + \frac{f_1}{p} + f_2\right] y = 0, \tag{13}$$

where

$$\begin{aligned} f_0 &= \frac{q^2}{4} + \frac{k^4}{4}\frac{(\mu^2 - 4B^2)}{q^2} - \frac{k^2}{2}\mu, \\ f_1 &= -i\dot{q}, \\ f_2 &= \frac{1}{4}\left(\frac{\dot{q}}{q}\right)^2 - \frac{1}{2}\frac{\ddot{q}}{q}. \end{aligned}$$

Then we construct the formal expansion for the solutions (13). We present the function $y(z)$ in the following form:

$$y = e^S,$$

where S is a new function. By substituting y into (13) we obtain the Riccati equation for S:

$$S'' + (S')^2 = -F(z), \qquad F(z) = \frac{f_0}{p^2} + \frac{f_1}{p} + f_2. \tag{14}$$

Expanding S in a power series of p

$$S = \frac{1}{p}\sum_{k=0}^{\infty} S_k p^k, \tag{15}$$

substituting the obtained expansion into (14), and comparing factors corresponding to equal powers, we can determine the functions S_k. The formal expansion is valid only far from singular points that are determined by the condition

$$\gamma(z_i) = \sqrt{-f_0(z)} = 0. \tag{16}$$

Restricting our consideration to the first power terms in (15) we obtain

$$b(z) = \frac{1}{\sqrt{q\gamma}}\left(C_1\left[i(q^2 + 2\beta) + 2q\gamma\right]^{1/2}\exp\left\{\int^z \gamma(z')\,dz'\right\} + C_2\left[i(q^2 + 2\beta) + 2q\gamma\right]^{-1/2}\exp\left\{-\int^z \gamma(z')\,dz'\right\}\right), \tag{17}$$

[1]The Wentzel–Kramers–Brillouin approximation

where

$$\beta = -\frac{k^2}{2}\mu.$$

Integration should be performed from singular points along the contour in the complex space.

In the general case of monotonic function $q(z)$, there are two roots for Eq. (16), which are singular (turning) points of Eq. (13). It can be shown that there are several domains in the plane of the complex coordinate z, where the solutions of (13) have asymptotics in the form (17) but with different factors C_1 and C_2. The solutions should fall at $z \to +\infty$ and we must join the asymptotics of various domains passing the turning points.

First, let us neglect absorption of the reflecting structure material. In this case, the solutions of (16)

$$q = k\sqrt{\mu \pm 2B} \tag{18}$$

are arranged on the real axis. For a given wavelength (and the parameters θ, μ_0, and B), there can be one, two, or no singular points depending on the interval of $q(z)$ variation across the considered quasi-periodic structure. We assume here that the period $d(z) = \pi/q(z)$ monotonically varies across the structure.

The case of two singular points is most interesting from the viewpoint of broadening the reflection band. In terms of x-ray crystal optics, one can say that in this case the multilayer comprises both edges of the total reflection bands [11].

In the case of a weak absorption (only a weak absorption can provide band broadening without a noticeable reduction of the reflection coefficient), according to (18) the singular points are shifted up from the real axis (if $q(z)$ increases) or down (if $q(z)$ falls). Generally, the asymptotics will be the same. Let us assume that the asymptotics increase. We will determine these asymptotics for various domains.

Assume that a singular point z_1 is to the left from a singular point z_2. Then, in the domain to the right of z_1 the WKB asymptotics of a solution to Eq. (13) has the form

$$b(z) = \frac{C}{\sqrt{q\gamma'}} \frac{\exp\left\{-i\int\limits_{z_1}^{z} \gamma'(z')\,dz'\right\}}{\left[A + \sqrt{A^2 - 1}\right]^{1/2}}, \quad z > z_1, \tag{19}$$

where

$$A = \frac{1}{2B}\left(\mu - \frac{q^2(z)}{k^2}\right), \quad \gamma' = \sqrt{f_0}.$$

Here, $b(z)$ falls at $+\infty$ (see the boundary conditions in Sec. 2).

In the domain between singular points,

$$b(z) = \frac{C}{\sqrt{q\gamma}}\left\{\frac{M}{\left[A - i\sqrt{1 - A^2}\right]^{1/2}} e^{\psi_1} + i\left(\frac{1}{M} - M\right)\left[A - i\sqrt{1 - A^2}\right]^{1/2} e^{-\psi_1}\right\}, \tag{20}$$

where

$$z_2 < z < z_1, \qquad \psi_1 = \int\limits_{z_2}^{z} \gamma(z')\,dz', \qquad M = \exp\left\{-\int\limits_{z_2}^{z_1} \gamma(z')\,dz'\right\}.$$

In the domain to the left from z_2,

$$b(z) = \frac{C}{\sqrt{q\gamma'}}\left\{\frac{\left[A - \sqrt{A^2 - 1}\right]^{1/2}}{M} e^{-i\psi} + i\left(\frac{1}{M} - M\right)\frac{1}{\left[A - \sqrt{A^2 - 1}\right]^{1/2}} e^{i\psi}\right\}, \tag{21}$$

where

$$z < z_2, \qquad \psi = -\int_{z_2}^{z} \gamma'(z')\, dz'.$$

Finally, we have obtained the asymptotics of the solution (13) on the total complex space. According to (12), the reflection coefficient is expressed in terms of logarithmic derivative of asymptotics (19)–(21) at the zero point. The considered case of two singular points z_1, z_2 inside the quasi-periodic structure is most important in the hard spectrum range. This is the case where the x-ray wavelength is within the limits

$$\frac{2\pi\sqrt{\mu}}{q_{\max}} < \lambda < \frac{2\pi\sqrt{\mu}}{q_{\min}}, \tag{22}$$

which correspond to the resonance part of the reflection band.

In view of (21) and the general expression (12), the reflection coefficient can be presented within the band (22) by the formula

$$\mathrm{r} = \frac{1 + i\omega \dfrac{e^{2i\psi}}{\mathrm{A} - \sqrt{\mathrm{A}^2 - 1}}}{\mathrm{A} + \sqrt{\mathrm{A}^2 - 1} + i\omega e^{2i\psi}}, \tag{23}$$

where

$$\psi = \int_{0}^{z_2} \gamma'(z')\, dz', \qquad \omega = 1 - e^{-2\epsilon},$$

$$\epsilon = \int_{z_2}^{z_1} \gamma(z')\, dz', \qquad \mathrm{A} = \frac{1}{2\mathrm{B}}\left(\mu - \frac{\mathrm{q}^2(0)}{\mathrm{k}^2}\right).$$

The parameter A is small if the radiation takes place in resonance with periods of the multilayer structure near the surface. However, the range of the resonance is not large, so we can take $|A| \gg 1$. Then expression (23) can be reduced to the form

$$\mathrm{r} = \frac{1}{2\mathrm{A}} + i\omega e^{2i\psi}. \tag{24}$$

The first term in (24) is much less than the second one and we arrive at

$$\mathrm{R} = |r|^2 = -\mathrm{Im}\left(\frac{1}{\mathrm{A}}\omega e^{2i\psi}\right) + |\omega|^2 e^{-4\psi''}, \tag{25}$$

where

$$\psi'' = \mathrm{Im}\,(\psi).$$

The first summand in (25) describes oscillations of the reflection coefficient. The second summand is the mean of the latter. Taking the average with respect to oscillations we obtain

$$\mathrm{R} = \left|1 - e^{-2\epsilon}\right|^2 e^{-4\psi''}. \tag{26}$$

In the assumption of a wide reflection band and weak absorption, we can estimate the parameters ϵ and ψ'',

$$\epsilon = \pi \mathrm{k}^2 \frac{\mathrm{B}^2}{\mathrm{Re}\,(\mu)} \left(\frac{dq}{dz}(z^*)\right)^{-1}, \tag{27}$$

$$\psi'' = \gamma \frac{\mathrm{k}^2}{\mathrm{q}_0 + \mathrm{k}\sqrt{\mathrm{Re}\,(\mu)}} z^*, \qquad \gamma = \mathrm{Im}\,(\mu), \tag{28}$$

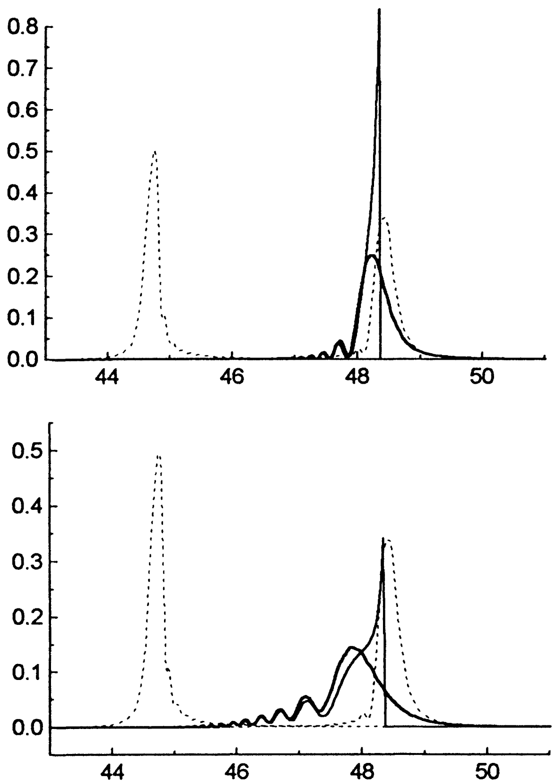

Fig. 2. Reflection coefficient calculated by the approximate formula (23) (thin curve) and by recurrent sequences approach (bold curve). The structure Cr–C is considered, $q = q_0 \tanh(pz + \rho)$, $q_0 = 1.4 \cdot 10^{-1}$ Å^{-1}, $\rho = 1.58$, $\beta = 0.4$, $\vartheta = 90°$. Dashed lines show the limiting periodic curves for $p = 0$ and $p \to \infty$.

where z^* is a solution of the equation

$$q(z) = k\sqrt{\mu}.$$

It is seen from (26)–(28) that R tends to zero at the boundaries of the reflection band (22) and has a maximum inside it. The integral reflection coefficient can be obtained by integrating (26) with respect to k or λ within the limits of the band (22).

Notice that at $\epsilon \to 0$ (i.e., at rapid variation of the period) expression (26) reduces to the formula

$$\mathrm{R} = 4|\epsilon|^2 e^{-4\psi''}. \tag{29}$$

If we assume that the effective number of layers reflecting the wave with a given k is

$$N = \frac{q}{\pi} k \frac{2B}{\sqrt{\mathrm{Re}\,(\mu)}} \left(\frac{dq}{dz}(z^*)\right)^{-1}, \tag{30}$$

then formula (29), in turn, reduces to the expression given in [7] for the reflection coefficient and obtained in the kinematic approximation.

It is interesting to compare the solution to Eq. (13) and that of the reflection problem with a potential prescribed by the function f_0. There is a correspondence between the two solutions if the turning points

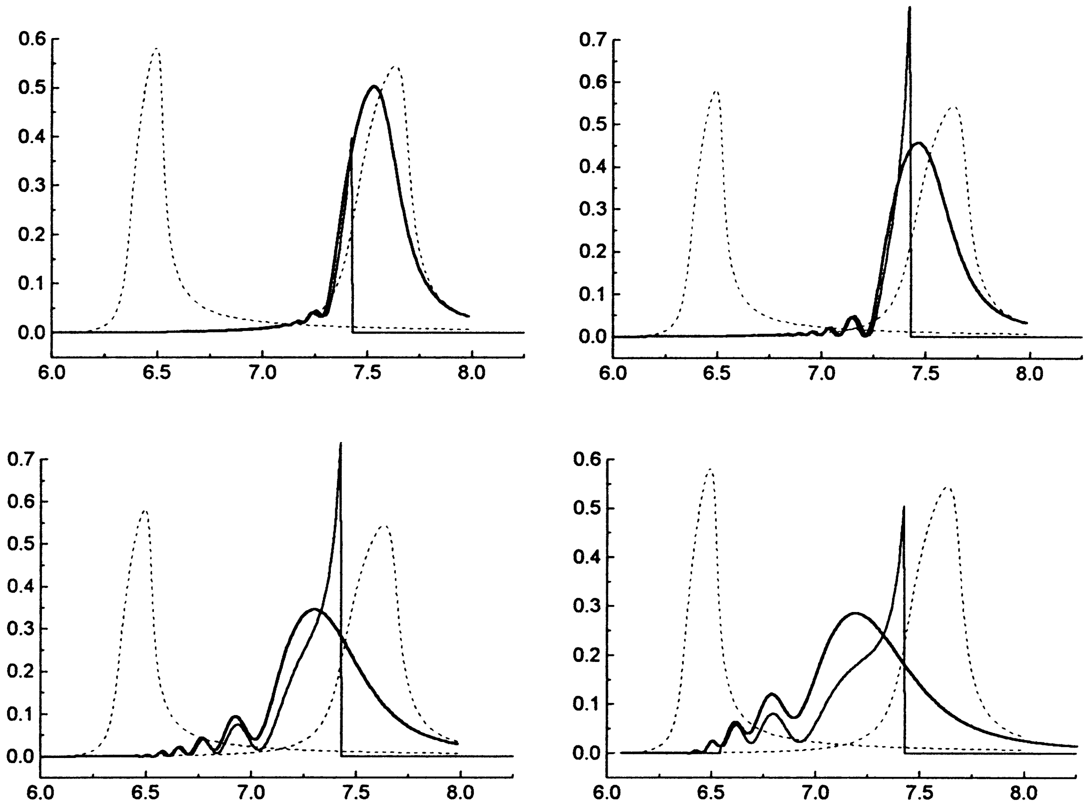

Fig. 3. Reflection coefficient calculated by the approximate formula (23) (thin curve) and by recurrent sequences approach (bold curve). The structure Mo–B_4C is considered, $q = q_0 \tanh(pz + \rho)$, $q_0 = 8.2 \cdot 10^{-2}$ Å^{-1}, $\rho = 1.21$, $\beta = 0.5$, $\vartheta = 5°$. Dashed lines show the limiting periodic curves for $p = 0$ and $p \to \infty$.

(zeroes of the function f_0) are far below the structure surface. In particular, formula (26) is similar to that for the case of reflection from a barrier. However, if the turning points are close to the surface, then the problem is quite different, because in the case of the reflection coefficient we need the value of the logarithmic derivative at the zero point, whereas in the scattering problem this value at $z \to -\infty$ is required.

Thus, the solution of Eq. (13) has much in common with the scattering problem from a barrier, however; it cannot be reduced to the latter.

Let us compare now the results of calculations by approximate formulas obtained in this section with those obtained from recurrent sequences [2]. Let us consider the function $q(z)$ and calculate the reflection coefficients by (23) and then determine this coefficient by the method of recurrent sequences (MRS) [2]. In the MRS approach, we have to construct a discrete multilayer structure on the basis of $q(z)$. This construction will be performed in the following way.

Function $q(z)$ is defined by formula (2). It is the starting point for determining the function $d(i)$. Assume that the zeroes of $\cos\left[2\int_0^z q(z')\,dz'\right]$ coincide with the layer boundaries of the multilayer structure. In view of the fact that each period corresponds to two layers, we obtain the equation for the coordinates z_n of the period boundaries

$$\int\limits_0^{z_n} \mathrm{q}(z')\,dz' = \pi n.$$

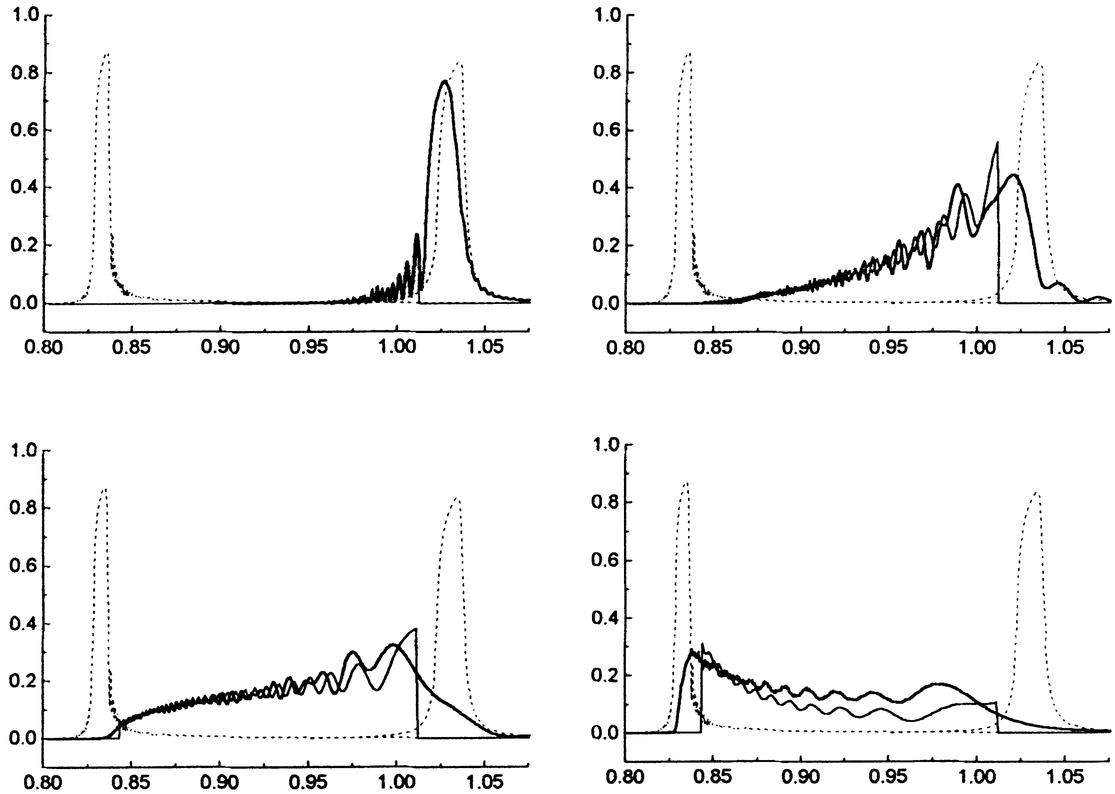

Fig. 4. Reflection coefficient calculated by the approximate formula (23) (thin curve) and by recurrent sequences approach (bold curve). The structure Cr–C is considered, $q = q_0 \tanh(pz + \rho)$, $q_0 = 1.3 \cdot 10^{-1}$ Å^{-1}, $\rho = 1.1$, $\beta = 0.5$, $\vartheta = 1°$. Dashed lines show the limiting periodic curves for $p = 0$ and $p \to \infty$.

Hence, the dependence $d(i)$ has the form

$$d(i) = z_i - z_{i-1}.$$

Finally, we find a quasi-periodic multilayer structure with the prescribed $d(i)$, β, and sufficiently large number of layers. The reflection coefficient for such a structure is calculated by means of MRS.

In Figs. 2–4, the results of calculations are presented. The function $q_0\tanh(pz + \rho)$ was taken, because an analytical solution of Eq. (10) is known for this case. In Table 1, integral (with respect to wavelength) reflection coefficients are presented corresponding to Figs. 2–4 (including the limiting case of periodic structures).

It is seen that the approximate formulas describe well the reflection coefficient in the domain where two turning points are inside the structure. Oscillations of the reflection coefficient are also described. In the domain where singular points are close to the surface, we obtain a considerable discrepancy. This discrepancy is not surprising, because formula (23) cannot be applied to this domain. Table 1 shows that a substantial increase in the reflection coefficient can be observed only for hard x-ray radiation where the absorption is low.

TABLE 1. Integral (with Respect to the Wavelength) Reflection Coefficients Corresponding to the Curves in Fig. 2–4, Obtained by Recurrent Sequences.

Figure number	0	3×10^{-5}	5×10^{-5}	6×10^{-5}	10^{-4}	3×10^{-4}	5×10^{-4}	∞
2	0.155	0.158	—	0.164	0.169	0.177	—	0.167
3	0.173	—	0.171	—	0.171	0.183	0.195	0.128
4	0.0153	—	0.0176	—	0.0315	0.0349	0.0298	0.0096

Columns correspond to various values of the parameter p [Å^{-1}]. Integral reflection coefficients are presented in [Å^{-1}].

4. Conclusion

The paper presents the results of a theoretical study of multilayer x-ray mirrors with a slowly varying period. An analytical theory based on the method of slow varying amplitudes (SVA) and the WKB approximation is the result of this investigation.

By means of the SVA method we obtained a system of equations comprising only slowly varying functions, the solutions of which are approximately written in terms of WKB asymptotics. In this way, we obtain formulas for the reflection coefficient, which approximate this coefficient in the most important range. The formulas obtained for the reflection coefficient are simple, namely, the coefficient is expressed via a function responsible for the structure period variations and its derivative. This approach can be a starting point for the solution of the reverse problem, i.e., creation of multilayer structures with a prescribed dependence of the reflection coefficient on the wavelength or the sliding angle. In addition, the formulas obtained can be used in the optimization of the integral reflection coefficient, which is important in various applications.

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