THE AMPLITUDE-PHASE RELATION FOR THE REFLECTION COEFFICIENT OF A LAYERED MEDIUM

A. V. Tikhonravov and I. V. Zuev

Applicability of the Kramers–Kronig relations to the problem of unambiguous reproduction of the amplitude reflection coefficient from the energy reflection coefficient for a layered medium is considered. Examples of nonuniqueness of the solution are given. The conditions necessary for the existence of a one-to-one correspondence between the amplitude and phase of the amplitude reflection coefficient (the conditions for unambiguous reproduction of the amplitude reflection coefficient from the energy one) are determined.

INTRODUCTION

The frequency (wavelength) dependence of the incident light reflection coefficient is an important physical characteristic of surfaces, thin films, and coatings. Many techniques for determining and studying the parameters of these objects are based on measuring this dependence. Generally, the amplitude reflection coefficient $r(\omega)$ carries more information about the object under study than the energy reflection coefficient $R(\omega)$. However, it is the latter quantity that is measured in the experiment.

The amplitude and energy reflection coefficients are related as

$$r(\omega) = (R(\omega))^{1/2} \cdot \exp\{i\varphi(\omega)\},$$

where $\varphi(\omega)$ is the phase shift in reflection, which will, for shortness, be called the phase of the reflection coefficient in what follows. Sometimes there is an unambiguous relation between $R(\omega)$ and $\varphi(\omega)$. The corresponding equations are usually called Kramers-Kronig equations. They are extensively used in studying surfaces and thin films [1–5], because they make it possible to reproduce the $r(\omega)$ function from measurements on $R(\omega)$ and thus determine the sought parameters of the objects of study.

In the simplest situation of a medium homogeneous across its depth, the conditions ensuring the unambiguity are well known [6–7]. Of great practical importance is the determination of the conditions for the existence of a one-to-one correspondence between $R(\omega)$ and $\varphi(\omega)$ in more complex objects, such as thin films and layered coatings. The frequency dependence of the reflection coefficients is then determined not only by the dispersion properties of the optical parameters but also by interference effects. It is known that, generally, there is no unambiguous relation between $R(\omega)$ and $\varphi(\omega)$ for a layered medium. It has been shown in [8] that the existence of such relation is closely associated with the arrangement of the zeros of the amplitude reflection coefficient of a layered medium in the complex plane of frequencies. The prime objective of this work is to determine the conditions that should be imposed on layered medium parameters to ensure a regular arrangement of these zeros, so that $R(\omega)$ and $\varphi(\omega)$ be related unambiguously. We do not take account of the dispersion of layered medium optical parameters and assume the frequency dependence of the reflection coefficient to be fully determined by interference effects.

1. TRANSFORMATIONS OF LAYERED MEDIUM PARAMETERS INVARIANT WITH RESPECT TO THE ENERGY REFLECTION COEFFICIENT

Consider normal incidence of a plane electromagnetic wave on a layered medium with a refractive index $n(z)$ (the OZ axis coincides with the direction of medium stratification). Let 0 and z_a be the coordinates of the boundaries between the layered medium and the substrate and external medium, respectively. The refractive indices of the substrate and external medium are constant and equal n_0 and n_a, respectively, and the magnetic permeability μ is 1. Maxwell's equations then take the form

$$dE/dz = ikH, \qquad dH/dz = ik(n(z))^2 E, \tag{1}$$

where E and H are the complex amplitudes of the electric and magnetic fields, respectively, and $k = \omega/c$ is the wave number in vacuum. Introducing the substitutions

$$x(z) = \int_0^z n(z)\,dz, \qquad y_1(x, k) = E(x, k), \qquad y_2(x, k) = n_0 H(x, k) \tag{2}$$

for the variable and functions transforms set (1) into

$$dy_1/dx = ik\rho(x)y_2, \qquad dy_2/dx = ikx_1/\rho(x), \tag{3}$$

where $\rho(x) = n_0/n(x)$ is the wave resistance of the layered medium.

Let $y_{1,2}(x, k)$ be a solution to set (3) with the initial conditions

$$y_1(0, k) = 1, \qquad y_2(0, k) = 1. \tag{4}$$

The amplitude reflection coefficient is then given by [9]:

$$r(k) = \frac{y_1(x_a, k) - \rho_0 y_2(x_a, k)}{y_1(x_a, k) + \rho_0 y_2(x_a, k)}, \tag{5}$$

where $x_a = \int_0^{z_a} n(z)\,dz$ is the optical thickness of the layered medium, and $\rho_0 = n_0/n_a$.

Studying the properties of the amplitude reflection coefficient requires a transition from real wave numbers k to the complex plane of wave numbers $\nu = k + i\sigma$. Let $r(\nu)$ be the analytic continuation of the $r(k)$ function into this complex plane. Set (3) will further, where necessary, also be considered to involve complex wave number ν values in place of real k ones.

The analytic properties of the $r(\nu)$ function were studied in detail in [9]. The results necessary for our purposes are as follows:

1) $r(\nu)$ is a meromorphic function;

2) $r^*(\nu) = r(-\nu^*)$, the zeros and poles of the amplitude reflection coefficient are symmetric with respect to the imaginary axis of wave numbers;

3) In the $\mathrm{Im}\,\nu \leqslant 0$ region, the $r(\nu)$ function has no poles.

The amplitude reflection coefficient on the real axis of wave numbers will be written

$$r(k) = |r(k)|\exp\{i\varphi(k)\}.$$

As mentioned above, in the general case, there is no unambiguous relation between $|r(k)|$ and $\varphi(k)$. Amplitude reflection coefficient transformations invariant with respect to the modulus of this coefficient on the real axis of frequencies were studied in [8], where formulas describing the corresponding variations in the wave resistance of a layered medium (the refractive index) were also obtained. The principal result that will be used below is as follows.

Theorem 1. *Let $r(\nu)$ be the amplitude reflection coefficient of a layered medium with the wave resistance $\rho(x)$, and let ν_0 and ν_0^* be a pair of zeros of $r(\nu)$ in the upper half-plane of wave numbers. The function*

$$\tilde{r}(\nu) = \frac{(\nu + \nu_0)(\nu - \nu_0^*)}{(\nu - \nu_0)(\nu + \nu_0^*)} r(\nu) \tag{6}$$

is then the amplitude reflection coefficient of the layered medium with the wave resistance $\tilde{\rho}(x) = \rho(x)\mu^2(x)$, where $\mu(x)$ written in terms of solutions to set (3) has the form

$$\mu(x) = \mathrm{Re}[\nu_0 y_1^*(x, \nu_0) y_2(x, \nu_0)] / \mathrm{Re}[\nu_0 y_1(x, \nu_0) y_2^*(x, \nu_0)]. \tag{7}$$

It is easy to see that transformation (6) is invariant with respect to the modulus of the amplitude reflection coefficient on the real axis of wave numbers. Note also that this transformation transfers the pair of zeros of the amplitude reflection coefficient into the symmetrically related points on the lower half-plane.

To demonstrate the nonuniqueness of the relation between $|r(k)|$ and $\varphi(k)$, consider a monolayer coating with a constant refractive index, $n(z) = \text{const}$. Then

$$r(\nu) = \frac{(n_a - n_0)\cos(\nu n z_a) - i(n_0 n_a/n - n)\sin(\nu n z_a)}{(n_a + n_0)\cos(\nu n z_a) - i(n_0 n_a/n + n)\sin(\nu n z_a)}.$$

The zeros of the amplitude reflection coefficient in the complex plane of wave numbers are the points

$$\nu_m = \pi(1 + 2m)/(2nz_a) + i\ln[(n_0 - n)(n + n_a)]/[(n - n_a)(n_0 + n)]/(2nz_a),$$

where $m = 0, \pm 1, \pm 2, \ldots$.

Thus, the zeros of the amplitude reflection coefficient are situated on an axis parallel to the real axis k, symmetrically with respect to the imaginary axis, and with a constant spacing of (π/nz_a).

Note that the zeros of the $r(\nu)$ function occur in the upper half-plane of the wave number ν (Fig. 1) if

(a) $n_a n_0 > n^2$, $n > n_0$, and (b) $n_a n_0 < n^2$, $n < n_0$,

and they occur in the lower half-plane if

(c) $n_a n_0 > n^2$, $n < n_0$, and (d) $n_a n_0 < n^2$, $n > n_0$.

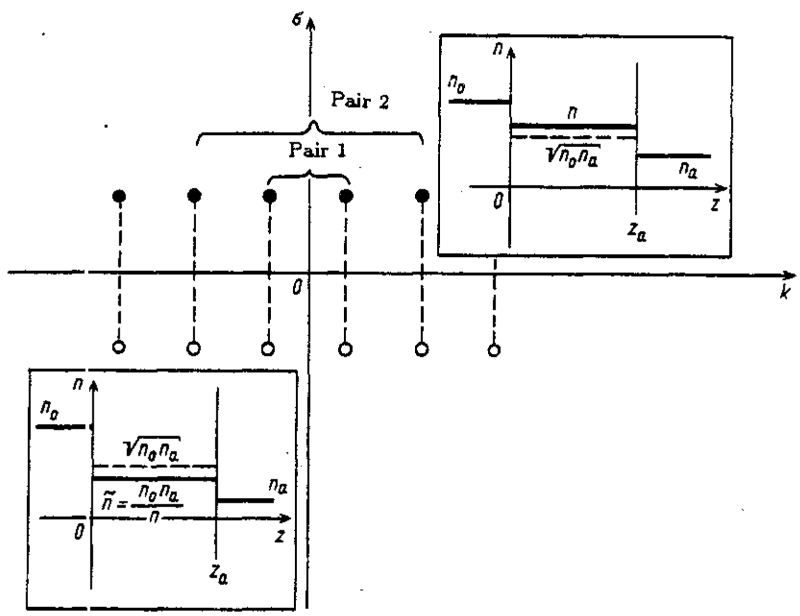

Fig. 1

Inequalities (b) and (c) correspond to situations most interesting practically, because the refractive index of the substrate is usually larger than that of the external medium.

Consider two monolayer coatings with the refractive indices $n_1 > (n_0 n_a)^{1/2}$ and $n_2 = n_0 n_a/n_1$ (clearly, $n_2 < (n_a n_0)^{1/2}$). Let the layers have the same optical thicknesses. It is easy to see that the zeros of the amplitude reflection coefficient corresponding to the first coating are then symmetric with respect to the zeros of the reflection coefficient of the second coating (see Fig. 1), the moduli of the two amplitude reflection coefficients are equal to each other, and the phases are different. This simplest example clearly demonstrates the nonuniqueness of the relation between $|r(k)|$ and $\varphi(k)$.

As follows from the theorem given above and the example just considered, there is no one-to-one correspondence between $r(k)|$ and $\varphi(k)$, because the zeros of the amplitude reflection coefficient can be situated in both the upper and the lower complex half-planes of wave numbers.

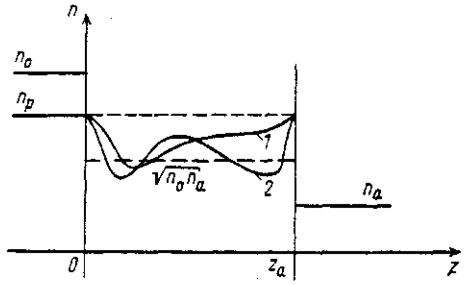

Fig. 2

To determine the conditions ensuring a certain regularity in the arrangement of the zeros of $r(\nu)$ (specifically, the absence of zeros in the upper or lower half-plane), consider the effect produced on layered medium parameters by transfer of one or more pairs of reflection coefficient zeros from the upper half-plane to the lower one.

Figure 2 demonstrates variations in the refractive index of a monolayer coating with $n_0 > n_p > (n_0 n_a)^{1/2}$ caused by transfer of the first (curve 1) and second (curve 2) pairs of zeros marked in Fig. 1 into the lower half-plane. The calculations were made according to Eq. (7) and the generalization of this equation to the case of transfer of several pairs of zeros. Figure 2 shows that transfer of only the first pair of zeros immediately breaks the condition $n(z) > (n_0 n_a)^{1/2}$. It is therefore only reasonable to suggest that meeting this condition is one of the principal requirements ensuring regularity in the arrangement of $r(\nu)$ zeros.

For elucidating in more detail the relation between the arrangement of $r(\nu)$ zeros and the restrictions on the optical parameters of the layered medium, it is expedient to consider separate classes of layered structures.

2. ANALYSIS OF THE ARRANGEMENT OF REFLECTION COEFFICIENT ZEROS IN THE COMPLEX PLANE OF WAVE NUMBERS FOR VARIOUS CLASSES OF LAYERED STRUCTURES

We begin our analysis of possible arrangements of $r(\nu)$ zeros with layered systems characterized by a piecewise constant distribution of parameters. This can conveniently be done by considering the so-called admittance phase plane. Let us introduce the $A(z,\nu) = n_0 y_1(x,\nu)/y_2(x,\nu)$ admittance, where $y_1(x,\nu)$ and $y_2(x,\nu)$ are solutions to set (3). It follows from Eq. (5) that the amplitude reflection coefficient expressed via the admittance has the form

$$r(\nu) = \frac{n_a - A(z_a,\, \nu)}{n_a + A(z_a,\, \nu)}. \tag{8}$$

Using set (3) and initial conditions (4) readily yields the admittance of any layered structure with an arbitrary dependence $n(z)$ in the form

$$dA/dz = i\nu(n^2(z) - A^2(z,\, \nu)) \tag{9}$$

with the initial condition

$$A(0,\, \nu) = n_0. \tag{10}$$

Here, we are considering a piecewise constant $n(z)$ function, which successively takes on the values $n_1, n_2, \ldots$.

A solution to differential equation (9) with initial condition (10) gives a curve in the complex admittance plane. This curve is conventionally called the admittance phase trajectory. It is easy to check that solution (9) for an arbitrary homogeneous layer with a constant refractive index n and the initial condition $A(\hat{z},\nu) = \hat{A}$ in the interval $z \in [\hat{z}, z]$ is

$$A(z,\, \nu) = \frac{in\sin(\nu n(z-\hat{z})) + \hat{A}\cos(\nu n(z-\hat{z}))}{\cos(\nu n(z-\hat{z})) + i\hat{A}\sin(\nu n(z-\hat{z}))/n}.$$

The portion of the phase curve, with a real wave number $k(\nu = k)$, described by this equation can be shown to occur on a circle of radius R, the center of which ξ is situated on the real axis in the complex admittance plane:

$$\xi = \frac{|\widehat{A}|^2 + n^2}{2\mathrm{Re}\,\widehat{A}} \quad \text{and} \quad R = \frac{|\widehat{A}^2 - n^2|}{2\mathrm{Re}\,\widehat{A}}.$$

For example, for a two-layer system we obtain a phase trajectory formed by arcs of two circles corresponding to the n_1 and n_2 values (Fig. 3).

For a two-layer system to have a zero reflection coefficient at a given $k = k_0$ value, it is necessary and sufficient that $A(z_a, k_0)$ be equal to n_a (see Fig. 3). This means that with $k = k_0$, the admittance phase trajectory starts at the point n_0 and ends at the point n_a. The problem of obtaining a zero amplitude reflection coefficient at a given value of the wave number ν using two-layer systems was studied in detail (see, e.g., [10]). It is known that there is a wide range of n_1 and n_2 values within which the two-layer systems with layers of certain thicknesses are translucent, that is, have a zero reflection coefficient.

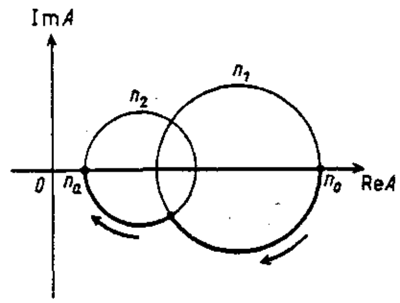

Fig. 3

It appears that if for some layered system the zero of the amplitude coefficient is situated on the real axis of frequencies, small variations in the thickness of the layers can shift this zero to either the lower or the upper wave-number half-plane. According to the results described in the preceding section, this means that such classes of multilayer systems can by no means satisfy the conditions ensuring a one-to-one correspondence between $R(\omega)$ and $\varphi(\omega)$. This property of the arrangement of zeros is established by the following theorem.

Theorem 2. *Let a layered system with a piecewise constant $n(z)$ function have a zero of the amplitude reflection coefficient on the real wave number axis at point k_0, and let at least one of the layers have an optical thickness not multiple of $(\pi/2k_0)$. Then for all $\sigma \in (-\sigma_0, \sigma_0)$, where σ_0 is a fairly small real number, there exists a layered system with the same refractive indices of the layers as those in the initial system, and the amplitude reflection coefficient of this new system has a zero at $k_0 + i\sigma$.*

The proof (not given here) is based on the well-known Poincaré theorem on a continuous dependence of the solution to a differential equation on the parameter.

The formulated theorem enables us to substantially narrow the range of layered systems among which we should search for classes satisfying the condition that ensures the existence of an unambiguous phase-amplitude relation for $r(k)$. Thus, numerous layered structures with nonmonotonic refractive indices $n(z)$ certainly do not satisfy this condition. Indeed, it has been shown [11] that a layered system with any amplitude reflection coefficient value, including zero, can be composed of layers with only two refractive indices (n_1 and n_2). This means that in a class of systems with refractive indices $n(z)$ taking on two values, n_1 and n_2 (no other condition need be imposed), there certainly exist layered systems whose amplitude reflection coefficient has zeros both on the real axis and in any of the two half-planes.

3. LAYERED STRUCTURES SATISFYING THE NECESSARY CONDITIONS FOR ONE-TO-ONE CORRESPONDENCE BETWEEN THE MODULUS AND PHASE OF THE AMPLITUDE REFLECTION COEFFICIENT

It follows from the results described above that it is advisable to search for layered media satisfying the conditions of unambiguity of phase-amplitude relations in a class of systems with monotonic refractive indices not exceeding the $(n_0 \cdot n_a)^{1/2}$ value. According to the theorem formulated above, the arrangement of zeros of the amplitude reflection coefficient then exhibits regularity sufficient for the relation to be unambiguous.

Theorem 3. *Let the refractive index of a layered medium be a piecewise smooth function of one of the following four classes:*

(a) $n(z)$ *is a monotonically nonincreasing function, and* $n_0 \geqslant n(z) \geqslant n^* > (n_0 \cdot n_a)^{1/2} > n_a$;

(b) $n(z)$ *is a monotonically nondecreasing function, and* $n_0 < (n_0 \cdot n_a)^{1/2} < n^* \leqslant n(z) < n_a$;

(c) $n(z)$ *is a monotonically nondecreasing function, and* $n_0 \leqslant n(z) < n^* \leqslant (n_0 \cdot n_a)^{1/2} < n_a$;

(d) $n(z)$ *is a monotonically nonincreasing function, and* $n_0 > (n_0 \cdot n_a)^{1/2} > n^* \geqslant n(z) \geqslant n_a$.

Then for the functions (b) *and* (d) *the amplitude reflection coefficient* $r(\nu)$ *has no zeros in the lower half-plane of the complex wave number* ν, *and for the functions* (a) *and* (c) *there is no zeros in the upper half-plane.*

The proof of this theorem is rather lengthy and is not given here.

Let us now show that for layered structures possessing the specified regularity in the arrangement of zeros, the Kramers–Kronig relations are valid. We will only consider functions of class (a).

To use some of the results obtained in [9], let us assume in addition that $n(z)$ is a smooth function with zero derivatives at the points 0 and z_a satisfying the condition $n(0) = n_0$ (the refractive index of the layered medium is smoothly joined with the refractive index of the substrate). All the $r(\nu)$ zeros are then situated in the upper half-plane.

Let $\tilde{r}(\nu)$ be the amplitude reflection coefficient of a layered medium with the index of refraction $n(z)$, and let the external medium be homogeneous and have the $n(z_a)$ refractive index. As has been shown in [12], it follows from the general properties of layered systems that there exists a one-to-one correspondence between the amplitude reflection coefficients $r(\nu)$ and $\tilde{r}(\nu)$. We have

$$r(\nu) = \frac{\tilde{r}(\nu) + r_0}{1 + r_0\tilde{r}(\nu)},$$

where r_0 is the amplitude coefficient of reflection from the boundary between the homogeneous media with the refractive indices $n(z_a)$ and n_a:

$$r_0 = [n(z_a) - n_a]/[n(z_a) + n_a].$$

As has been shown in [9], the properties of the $n(z)$ function specified above ensure the asymptotic behavior $\tilde{r}(\nu) = O(1/\nu^2)$ of the $\tilde{r}(\nu)$ function in the lower half-plane. Therefore $r(\nu) = r_0 + O(1/\nu^2)$ if $\nu \geqslant 0$. Consider the $\ln(r(\nu))$ function in the upper half-plane. Because of the absence of $r(\nu)$ zeros, this function is regular if $\operatorname{Im}\nu \geqslant 0$. When $\nu \to \infty$ and $\operatorname{Im}\nu \geqslant 0$,

$$\ln(r(\nu)) = \ln(r_0) + O(1/\nu^2).$$

Consider the $\oint\limits_C \ln(r(\nu)/r_0)(\nu - \xi)\,d\nu$ integral about closed path C shown in Fig. 4. By virtue of regularity of the integrand within the region enclosed by C, we have

$$\left(\int\limits_{C_R} + \int\limits_{-R}^{\xi-R} + \int\limits_{\xi+R}^{R} + \int\limits_{C_\rho}\right) \ln(r(\nu)/r_0)/(\nu - \xi)\,d\nu = 0.$$

The meaning of the symbols ξ, ρ, and R is clear from Fig. 4.

Passing to the $\rho \to 0$, $R \to \infty$ limit and taking the asymptotic behavior of $r(\nu)$ into account, we obtain

$$\mathrm{V.p.}\int\limits_{-\infty}^{\infty} (\ln(|r(k)|/r_0) + i\varphi(k))/(k - \xi)\,dk - i\pi \ln|r(\xi)| + \pi\varphi(\xi) = 0.$$

Separating the real and imaginary parts of this equality yields

$$|r(\xi)| = \exp\Big\{(1/\pi)\cdot \mathrm{V.p.}\int\limits_{-\infty}^{\infty} \varphi(k)/(k - \xi)\,dk\Big\},$$

$$\varphi(\xi) = -(1/\pi)\cdot \mathrm{V.p.}\int\limits_{-\infty}^{\infty} \ln(|r(k)|/r_0)/(k - \xi)\,dk.$$

Or, by virtue of the $|r(-k)| = |r(k)|$ symmetry property on the real axis,

$$|r(\xi)| = \exp\Big\{ 2(\xi/\pi)\cdot \text{V.p.}\int_0^\infty \varphi(k)/(k^2-\xi^2)\,dk \Big\},$$

$$\varphi(\xi) = -2(\xi/\pi)\cdot \text{V.p.}\int_0^\infty \ln(|r(k)|/r_0)/(k^2-\xi^2)\,dk.$$

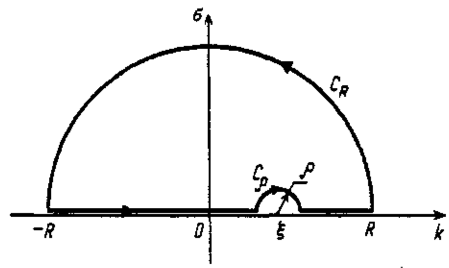

Fig. 4

The derivation of the Kramers–Kronig relation for all other regular arrangements of $r(\nu)$ function zeros is trivial.

Some final remarks should be made. As follows from Sections 1 and 2, the classes of structures that have been considered in Section 3 and for which the Kramers–Kronig relations can be obtained can hardly be extended considerably. The condition of smoothness of the $n(z)$ function is significant for obtaining the equations given above. Any refractive index breaks will affect the asymptotic behavior of the amplitude reflection coefficient and, accordingly, cause changes of the Kramers–Kronig relations derived in this work.

REFERENCES

1. T. G. Arkatova, N. M. Gopshtein, E. G. Makarova, and B. A. Mikhailov, *Opt.-Mekh. Prom.*, no. 9, p. 44, 1981.
2. L. N. Didrikul', *Zh. Prikl. Spektrosk.*, vol. 23, no. 5, p. 920, 1975.
3. G. Lévêque and Y. Villachon-Renard, *Appl. Opt.*, vol. 29, no. 22, p. 3207, 1990.
4. P. Grosse and V. Offerman, *J. Appl. Phys.*, vol. A52, p. 138, 1991.
5. B. Harbeke, *J. Appl. Phys.*, vol. A40, p. 151, 1986.
6. L. D. Landau and E. M. Lifshits, *Electrodynamics of Continuous Media* (in Russian), p. 386, Moscow, 1982.
7. H. Nussenzveig, *Causality and Dispersion Relations*, Academic Press, New York, 1972.
8. A. V. Tikhonravov, *Zh. Vych. Mat. Mat. Fiz.*, vol. 25, no. 3, p. 442, 1983.
9. A. V. Tikhonravov, *Zh. Vych. Mat. Mat. Fiz.*, vol. 22, no. 6, p. 1421, 1982.
10. G. V. Rozenberg, *Optics of Thin-Layer Coatings* (in Russian), Moscow, 1958.
11. A. V. Tikhonravov, in: *Computer Optics. Collected Papers MTsNTI* (in Russian), no. 7, p. 33, Moscow, 1990.
12. P. G. Kard, *Analysis and Synthesis of Multilayer Interference Films* (in Russian), Tallin, 1971.

15 June 1992

Department of Mathematics