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Nanooptics of gradient dielectric films

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Abstract*. The propagation of light through subwave photonic barriers formed by dielectric nanofilms with the refractive indices changing across the films according to the specified law $n(z)$ is considered. Generalised Fresnel formulae depending on the gradient and profile curvature of the refractive index and describing reflection and transmission of such inhomogeneous films are found. For the specified material and thickness, the optical properties of such nanofilms can change from total transmission to total reflection by producing a technologically controlled profile $n(z)$. The obtained results are based on exact analytic solutions of Maxwell's equations for new multiparametric models of inhomogeneous dielectric media. The possibility of producing new subwave dispersion elements, whose action is based on the dependence of the reflection and transmission spectra of gradient photonic barriers on their local dispersion determined by the shape and geometrical parameters of the profile $n(z)$, is shown. The schemes are considered for producing such spectra in the visible and IR regions with the help of periodic nanostructures containing subwave photonic barriers with the normal and anomalous nonlocal dispersion.

Keywords: *dielectric films, nanooptics, subwave dispersion elements.*

1. Introduction. Nonlocal dispersion of gradient photonic barriers

The development of nanotechnology has lead to the creation of materials with unique optical properties, which do not exist in nature. These materials have been attracting attention for the last two decades due to their possible application for controlling electromagnetic radiation at subwave distances. A number of such problems are solved in optics by using thin dielectric films whose refractive index changes across the film (the so-called gradient photonic barriers). In this case, special attention is paid to the processes of reflection and transmission of the waves by thin layers of inhomogeneous materials, whose layer dimensions and the scales of inhomogeneities are comparable to the wavelength. These processes are caused by a special mechanism of wave dispersion in inhomogeneous dielectrics. It is necessary to emphasise the fundamental difference of this mechanism both from material dispersion determined by the parameter $\partial^2 n/\partial\omega^2$ (n is the medium index) and from spatial dispersion of homogeneous media, which leads, as is known from crystal optics and plasma physics [1], to small corrections to the refractive index of the order $a/\lambda \ll 1$ (a is a crystal lattice period or the mean free path of particles in the medium and λ is the wavelength). Away from the resonance frequencies of the medium such effects are slowly accumulated as the waves propagate over distances greatly exceeding the wavelength. Unlike this, the gradient media are characterised by the inverse relation between the inhomogeneity scale d and the wavelength: $\lambda \leqslant d$ [2, 3]. To fabricate gradient dielectric nanofilms with a technologically controlled distribution of the refractive index, a number of methods have been developed, including etching and photolithography [4], ionic implantation [5], molecular epitaxy [6], and special deposition regimes [7].

The aim of this paper is to study reflection and transmission of gradient photonic barriers as functions of their thickness and refractive index profile. These properties are considered below by a simple example of an isotropic unabsorbing dielectric layer, whose refractive index smoothly changes in one direction.

By assuming that the direction, along which the refractive index changes, coincides with the z axis, we can represent the medium permittivity in the form

$$\varepsilon(z) = n_0^2 U^2(z), \quad U(0) = 1. \tag{1}$$

Here, n_0 is the refractive index at the medium interface $z = 0$; U is some dimensional function determining the spatial profile of the refractive index; the material dispersion of the medium $n_0(\omega)$ and its absorption are neglected. Considering the propagation of an electromagnetic wave incident from vacuum perpendicular to the interface $z = 0$ in the direction $z > 0$, we can express the wave field components E_x and E_y via the auxiliary function Ψ:

$$E_x = -\frac{1}{c}\frac{\Psi}{\partial t}, \quad H_y = \frac{\partial\Psi}{\partial z}. \tag{2}$$

The function Ψ is determined by the wave equation, which results from Maxwell's equations:

$$\frac{\partial^2\Psi}{\partial z^2} = \frac{n_0^2 U^2(z)}{c^2}\frac{\partial^2\Psi}{\partial t^2} = 0. \tag{3}$$

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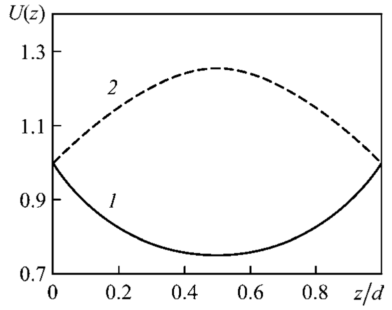

Figure 1. Concave (*1*) and convex (*2*) profiles $U(z)$ of type (4); z/d is the normalised coordinate.

The reflection and transmission of electromagnetic waves in a gradient dielectric barrier with the finite thickness d are found by using a flexible model $U(z)$, which allows an exact solution of (3) without any assumptions about the smallness or slowness of changes in the fields and medium parameters. Below we consider a model describing a nonmonotonic profile $U(z)$ [3]:

$$U(z) = \left(1 + \frac{s_1 z}{L_1} + \frac{s_2 z^2}{L_2^2}\right)^{-1}, \quad s_1 = 0, \pm 1, \quad s_2 = 0, \pm 1. \quad (4)$$

Model (4) contains two free parameters, which denote characteristic lengths L_1 and L_2. The case $s_1 = -1$, $s_2 = +1$ correspond to a convex profile, while at $s_1 = +1$, $s_2 = -1$, expression (4) describes a concave profile (Fig. 1). Note that the Rayleigh profile often used in electrodynamics of inhomogeneous media [1] is a particular case of (4) corresponding to $s_2 = 0$. The lengths L_1 and L_2 are related to the layer thickness d and the extreme values of the function $U_{\rm m}$ as:

$$U_{\rm m} = (1 + s_1 y^2)^{-1}, \quad y = L_2/2L_1, \quad L_2 = d(2y)^{-1},$$

$$y^2 < 1, \quad U(0) = U(d) = 1. \quad (5)$$

Model (4) makes it possible to represent the field inside the barrier in a simple form by solving exactly inhomoheneous wave equation (3) for a monochromatic wave; this solution can be written as a sum of forward and backward waves

$$\Psi = \frac{[\exp({\rm i}q\eta) + Q\exp(-{\rm i}q\eta)]\exp(-{\rm i}\omega t)}{\sqrt{U(z)}}. \quad (6)$$

Here, the variable

$$\eta = \int_0^z U(z_1)dz_1$$

is the phase path length;

$$Q = -\exp(2{\rm i}\delta)\frac{1 - {\rm i}s_1\gamma/2 - n_{\rm e}}{1 - {\rm i}s_1\gamma/2 + n_{\rm e}} = Q_0 \quad (7)$$

is the dimensionless quantity, which is determined from the continuity condition of the fields at the back boundary of the barrier $z = d$ [2] and corresponds to the contribution of the backward wave to the field inside the barrier; $\delta = q\eta_0$; $n_{\rm e} = n_0 N$.

The quantity q in (6) can be treated as a wave number of the wave propagating in the phase space $\eta(z)$:

$$q = \frac{\omega}{c} n_0 N, \quad (8)$$

where $N^2 = 1 - p^2c^2/\omega^2$; $p^2 = (y^2 - s_2)/(n_0^2 L_2^2)$.

The parameter N is related to the nonlocal film dispersion determined by the characteristic lengths L_1 and L_2. Its analysis allows one to reveal the fundamental difference between the convex and concave photonic barriers (Fig. 1). For the convex barrier, $p_2 < 0$, while the parameter N and the wave number q can be expressed via some characteristic frequency Ω_1:

$$N = \sqrt{1 + \frac{\Omega_1^2}{\omega^2}}, \quad \Omega_1 = pc = \frac{2cy\sqrt{1 - y^2}}{n_0 d}. \quad (9)$$

One can see from (9) that the wave number q remains real at any frequencies ω.

For the concave barrier, the parameter N and the characteristic frequency Ω_2 are given by the expressions:

$$N = \sqrt{1 - \frac{\Omega_2^2}{\omega^2}}, \quad \Omega_2 = \frac{2cy\sqrt{1 + y^2}}{n_0 d}. \quad (10)$$

This frequency dependence $q(\omega)$ resembles the normal dispersion of a waveguide or a plasma-like medium with the cutoff frequency Ω_2: for low frequencies ($\omega < \Omega_2$) the wave number q becomes imaginary.

The appearance of the characteristic frequencies Ω_1 and Ω_2 is caused by the nonlocal dispersion of the inhomogeneous medium; as the scales of inhomogeneities L_1 and L_2 are increased, these frequencies decrease ($\Omega \to 0$, $\Omega_2 \to 0$).

2. Reflection from gradient photonic barriers (generalised Fresnel formulae)

The classical Fresnel formulae describe the reflection of light from the interface of homogeneous media with different refractive indices. Unlike this case, the gradient optics considers the reflection of light from the interface of the media with continuous changes in the profiles $n(z)$. The complex reflectance $R(\omega)$ of the wave with the frequency ω incident from the vacuum perpendicular to the interface $z = 0$ in the direction $z > 0$ can be found by using the continuity condition of the wave field components E_x and H_y at the film interfaces $z = 0$ and $z = d$. Let us assume that at the interface $z = d$, the film is fixed on the surface of a homogeneous substrate, whose thickness is significantly larger than the pulse 'length' and the refractive index is equal to n; by using these continuity conditions, we will find the reflectance $R(\omega)$ for the convex profile $n(z)$ of type (4):

$$R(\omega) = \left[\left(n + \frac{\gamma^2}{4} - n_{\rm e}^2\right)t + n_{\rm e}\gamma - {\rm i}(n-1)\left(n_{\rm e} - \frac{t\gamma}{2}\right)\right]$$

$$\times\left[\left(n - \frac{\gamma^2}{4} + n_{\rm e}^2\right)t - n_{\rm e}\gamma + {\rm i}(n-1)\left(n_{\rm e} - \frac{t\gamma}{2}\right)\right]^{-1}, \quad (11)$$

where

$$n_{\rm e} = n_0\sqrt{1 + u^2}; \quad u = \frac{\Omega_1}{\omega}; \quad \gamma = \frac{2n_0 uy}{\sqrt{1 - y^2}}; \quad t = \tan\delta;$$

$$\delta = l\sqrt{1 + \frac{1}{u^2}}; \quad l = \arctan\left(\frac{2y\sqrt{1 - y^2}}{1 - 2y^2}\right). \quad (12)$$

Similarly, we will find the reflectance for the concave profile $n(z)$:

$$R(\omega) = \left[\left(n + \frac{\gamma^2}{4} - n_e^2\right)t - n_e\gamma - i(n-1)\left(n_e - \frac{t\gamma}{2}\right)\right]$$

$$\times\left[\left(n - \frac{\gamma^2}{4} + n_e^2\right)t + n_e\gamma + i(n+1)\left(n_e - \frac{t\gamma}{2}\right)\right]^{-1}. \quad (13)$$

Unlike (11), the quantities n_e, γ, and t in (13) are determined by the expressions

$$n_e = n_0\sqrt{1-u^2}, \ \gamma = \frac{2n_0uy}{\sqrt{1+y^2}}, \ t = \tan\delta, \quad (14)$$

where

$$u = \frac{\Omega_2}{\omega} < 1; \ \delta = l\sqrt{\frac{1}{u^2} - 1}; \ l = \ln\left(\frac{y_+}{y_-}\right);$$

$$y_\pm = \sqrt{1+y^2} \pm y.$$

Expressions (10) and (12) determine the reflectance of the gradient film deposited on a homogeneous substrate with the refractive index n. By placing m homogeneous transparent layers between the film and the substrate, we can select their thicknesses and refractive indices so that for some frequency all this structure (m layers and a substrate) will not affect the reflection from the gradient film [4]; this structure is optically equivalent to a medium with $n = 1$. We will reveal the properties of the reflection spectra inherent in the gradient films themselves by considering expressions (11) and (13) with $n = 1$.

(i) The power reflectances $|R(\omega)|^2$ in the visible and near-IR regions for photonic barriers consisting of one gradient film are shown in Fig. 2 for concave and convex films. At equal barrier thicknesses d, equal refractive indices n_0 of the initial materials, and equal characteristic lengths L_1 and L_2, the difference in the nonlocal dispersion of the films studied leads to the difference in their reflection spectra.

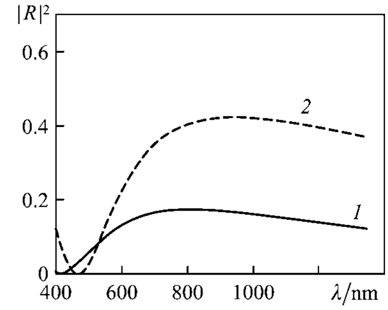

Figure 2. Reflection spectra of single gradient photonic barriers ($n_0 = 1.8$, $y = 0.45$, $d = 120$ nm) in the visible and near-IR region; curves (*1*) and (*2*) correspond to concave and convex profiles of type (4).

(ii) The gradient nanofilms with the profile $n(z)$ of type (4) are characterised by two free parameters L_1 and L_2. At fixed L_1 and L_2, we can produce structures with new reflection spectra by using periodic nanostructures comprising m similar nanofilms. By using successively expressions (11) and (13) to calculate the reflectance between adjacent nanofilms, we can easily show that reflection of such a periodic nanostructure is also described by expressions (11)–(14), when the quantity δ is replaced by $m\delta$. The reflection spectra of such nanostructures depend, at constant n_0 for all films, on the gradient jumps and the profile curvatures $n(z)$ at the interfaces of adjacent films.

Consider first reflection from simple structures consisting of pairs of equal concave (Fig. 3a) or convex (Fig. 3b) gradient photonic barriers in which the values of d, n_0, and U_m (5) are equal. Reflection from the interface of adjacent barriers is caused by the break of the gradient $U(z)$. Thus, for concave profiles $U(z)$, the values of grad$U$ expressed in normalised coordinates $x = z/d$ experience a jump at the interface $x = 1$ from $dU/dx|_{1-0} = 4y^2$ to $dU/dx|_{1+0} = -4y^2$. In this case, the curvature of both profiles retains a constant value: $K_1 = K_2 = 8y^2(4y^2+1)(1+16y^4)^{-3/2}$. Figure 4a presents the difference in radiation reflection from the pair ($m = 2$) of analogues barriers (concave and convex). The double-hump reflection spectrum of the pair of concave barriers (Fig. 3a) describes the reflectionless transmission $[|R(\omega)|^2 = 0]$ in the frequency range where reflection from the pair of convex photonic barriers (Fig. 3b) is maximal.

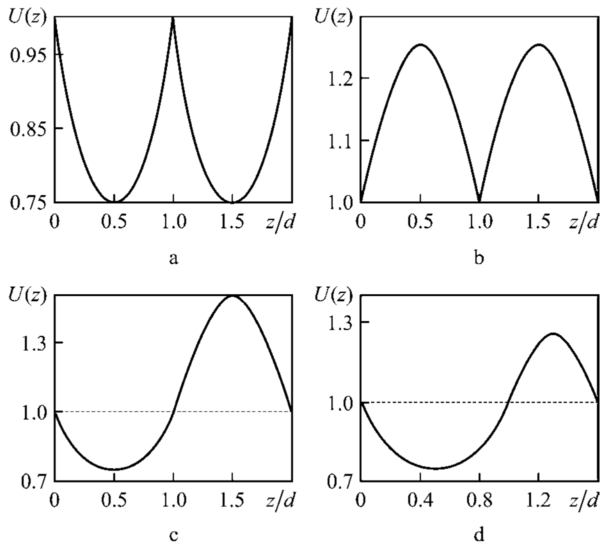

Figure 3. Systems of adjacent photonic barriers of type (4) with a continuous change in the refractive index $U(z)$ and breaks of the gradients and curvatures of the profile $U(z)$ at the interface between the barriers z/d; $U(d) = 1$. Shown are the break of the gradient for a concave ($y^2 = 1/3$) (a) and convex ($y^2 = 1/5$) (b) profiles $U(z)$ as well as profiles with a continuous value of grad U ($y_1^2 = y_2^2 = 1/3$, $d_1 = d_2$) (c) and a break in the curvature values at the interface between the barriers [$y_1^2 = 1/3$, $y_2^2 = 0.2025$, $d_2 = (y_2/y_1)^2 d_1$] (d).

(iii) Unlike identical barriers (Figs 3a, b), a periodic nanostructure can be produced by pairs of alternating gradient barriers with convex and concave profiles $U(z)$, which have similar thicknesses and the values of n_0 (Fig. 3c). To provide under these conditions a smooth contact of the profiles at the interface $U = 1$, their characteristic lengths L_1 should be equal; in this case, the deviation of the maximum (U_{max}) and minimum (U_{min}) of these profiles from the interface value $U = 1$ are different: $U_{max} - 1 \neq 1 - U_{min}$. The values of the parameter y for both profiles coincide and the maximum and minimum of the profile $U(z)$ are related by the expression

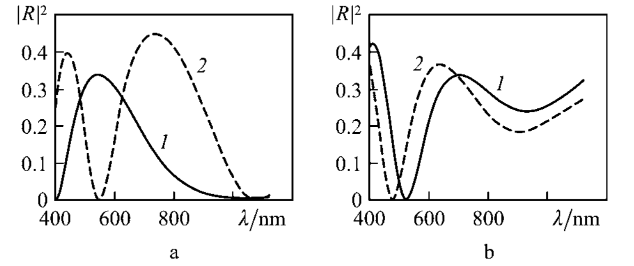

Figure 4. Reflectances with respect to power $|R|^2$ from adjacent gradient photonic barriers ($n_0 = 2$) presented in Fig. 3: reflection from the point corresponding to the break of the gradient $U(z)$, spectra (*1*) and (*2*) correspond to profiles in Figs 3a and b (a), and reflection from the point corresponding to the break in the curvature values $U(z)$, spectra (*1*) and (*2*) correspond to profiles in Figs 3c and d (b).

$$\frac{U_{\max}}{U_{\min}} = \left(\frac{1+y^2}{1-y^2}\right)^{1/2}. \qquad (15)$$

Unlike the structure shown in Figs 3a and b, the gradients of the convex and concave profiles at the interface $x = 1$ are continuous (grad U_1 = grad $U_2 = 4y^2$) and the reflection at this interface appears because of the break in the values of the curvatures of concave (K_1) and convex (K_2) profiles: $K_{1,2} = 8y^2(4y^2 \pm 1)(1+16y^4)^{-3/2}$.

A periodic structure can be produced by another pair of films containing concave [curve (*1*)] and convex [convex (*2*)] profiles, which are characterised by equal deviations $1 - U_{\min} = U_{\max} - 1$ (Fig. 3d). In this case, the film thicknesses d_1 and d_2 and the parameters y_1 and y_2 are related by the condition of smooth contact of the profiles $U(z)$ at the interface $z = d$:

$$\frac{d_2}{d_1} = \left(\frac{y_2}{y_1}\right)^2. \qquad (16)$$

Figure 4b illustrates the reflection spectra of such gradient nanostructures in the visible and IR regions caused by the difference in curvatures of refractive index profiles at the barrier interface. The minima and maxima of the spectral dependences $|R(\omega)|^2$ for the structures shown in Fig. 3a are displaced with respect to analogous points for the structure in Fig. 3b; the maxima $|R(\omega)|^2$ are different in height. Note that the mentioned difference in the reflection appears at smooth profiles $n(z)$ characterised by a continuous change in n and grad n at the contact point.

3. Resonance tunnelling of light through dielectric nanofilms

In analysing gradient photonic barriers with a normal dispersion of the waves, we pointed out a peculiarity inherent in such barriers – appearance of the cutoff frequency Ω_2 determined by the nonlocal dispersion of the dielectric nanofilm. At low frequencies ($\omega < \Omega_2$), the field inside the barrier is determined instead of (6) by the function $\Psi_{\rm t}$ and the imaginary wave number $q = {\rm i}p$:

$$\Psi_{\rm t} = \frac{[\exp(-p\eta) + Q_0 \exp(p\eta)]\exp(-{\rm i}\omega t)}{\sqrt{U(z)}}, \qquad (17)$$

where

$$p = \frac{\omega}{c} N_-; \;\; N_- = \sqrt{u^2 - 1}\,; \;\; u = \frac{\Omega_2}{\omega} \geqslant 1.$$

By replacing $q = {\rm i}p$ in the expression for $R(\omega)$ (13), we will find the complex reflectance for low frequencies:

$$R = \frac{(n + \gamma^2/4 + n_{\rm e}^2)t - \gamma n_{\rm e} - {\rm i}(n-1)(n_{\rm e} - \gamma t/2)}{(n - \gamma^2/4 - n_{\rm e}^2)t + \gamma n_{\rm e} + {\rm i}(n+1)(n_{\rm e} - \gamma t/2)}, \qquad (18)$$

where

$$t = \tanh\delta; \;\; \delta = l\sqrt{1 - \frac{1}{u^2}}; \;\; n_{\rm e}^2 = n_0^2(u^2 - 1). \qquad (19)$$

The quantity l in expression (19) was determined in (14). By using the expression for R (18), we can calculate the barrier transmittance with respect to power $|T|^2$:

$$|T|^2 = 1 - |R|^2. \qquad (20)$$

As is known, transmission of a homogeneous rectangular photonic barrier for the wave with the frequency smaller than the cutoff frequency (for example, transmission of a homogeneous plasma layer for the transverse wave whose frequency is smaller than the plasma frequency) decreases exponentially with the barrier width [1]; in this case, the reflectivity $|R|$ approaches unity. However, an opposite situation is possible for some gradient photonic barriers, when the interference of the forward and backward waves inside the barrier results in disappearance of reflection ($R = 0$) and total transmission of the energy flow of the tunnelling wave ($|T| = 1$). This situation appears for a system of m gradient barriers with a concave profile of the refractive index. The condition for the appearance of the resonance reflectionless tunnelling regime can be found by equating the expression for R (18) to zero and assuming $n = 1$ there for simplicity:

$$\tanh(mp\eta_0) = \frac{\gamma n_{\rm e}}{1 + \gamma^2/4 + n_{\rm e}^2}. \qquad (21)$$

The reflectionless tunnelling emission spectra (Fig. 5) show that depending on the barrier parameters the total transmission regime ($T = 1$) can appear both in the resonance region near the cutoff frequency (Fig. 5a, $u = 1.02$) and outside this region (Fig. 5c, $u = 1.46$).

The concept of resonance light tunnelling through thin films of nanostructured metamaterials with free carriers was considered in papers [8–11] in connection with tunnelling of narrow-band radiation through a metal foil near the plasma frequency of metal. Unlike this, the mechanism of wave

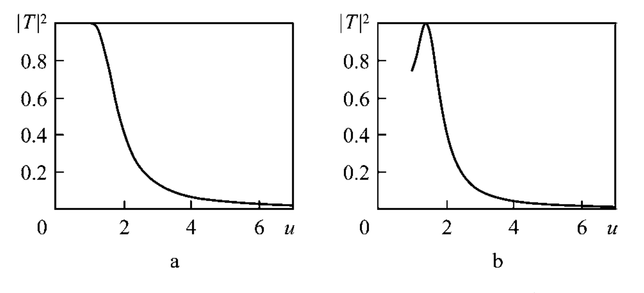

Figure 5. Transmission spectra with respect to power $|T|^2$ in the case of reflectionless tunnelling through gradient photonic barriers with the parameters $y = 0.577$, $m = 3$ at $n_0 = 2.216$ (a) and $n_0 = 3.529$ (b); the dimensionless variable u is determined in (12).

tunnelling based on nonlocal dispersion in a dielectric has a number of peculiarities.

(i) Tunnelling of waves in a single-dimensional inhomogeneous structure with the refractive index $n(z)$ is possible not only in the frequency region, where $n^2 < 0$, but also in the region, where $n^2 > 0$ but $\mathrm{d}n^2/\mathrm{d}z < 0$.

(ii) Tunnelling of light through gradient dielectric films does not result from the presence of free carriers, which broadens the range of materials promising for gradient nanooptics.

(iii) Reflectionless tunnelling of waves through gradient films is possible in a broad spectral region determined by technologically controlled parameters of the films.

4. Conclusions

The control of light fluxes with the help of gradient photonic barriers is of interest in designing dispersion elements – photonic crystals. Synthesis of such elements opens up new opportunities for optimising processes of energy transfer by the waves of different spectral regions.

(i) The dispersion of waves in a gradient layer depends not only on the spatial scale of the inhomogeneity but also on the gradient and curvature of the spatial profile n. The effects of this nonlocal dispersion, which accumulate at a distance of the order of wavelength, can completely change the reflection and transmission spectra of the layer, leading, for example, to the appearance of the cutoff frequency Ω in the layer of the weakly dispersive material (the cutoff frequency is controlled by the inhomogeneity parameters) and to the appearance of the tunnelling regime for the frequencies $\omega < \Omega$.

(ii) It is possible to select such a material and profile $n(z)$ for the given spectral range that the effect of nonlocal dispersion will be concentrated in the frequency band that is away from the absorption band of the material. The dynamics of the waves in such media is described by exact analytic solutions of Maxwell's equations constructed without any assumptions about the smallness or slowness of changes in the parameters of the medium or the field [12].

(iii) Reflection from the system of gradient dielectric films is caused not only by the contrast of the refractive index $n(z)$ between adjacent films but also by the contrast of gradients and the curvature $n(z)$ at the interfaces. The combined action of these effects allows one to change substantially reflection and transmission of gradient photonic barriers even in the case of their subwave thickness.

We have considered in this paper nonmagnetic media ($\mu = 1$). The combined change in distributions $\varepsilon(z)$ and $\mu(z)$ caused by the transition of these distributions through a zero can result in a resonance amplification of the electric field [13].

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