

INTEGRATED-OPTICAL WAVEGUIDES

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Theoretical and numerical analysis of propagation and scattering of eigen- and non-eigenmodes of an irregular integrated-optical waveguide

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Abstract. **We consider theoretical and numerical methods for studying propagation and scattering of laser radiation of eigenmodes and non-eigenmodes in an irregular integrated-optical waveguide. Scattering of non-eigenmodes in an irregular integrated-optical waveguide is investigated for the first time. We present the calculated dispersion curves for TE and TM eigenmodes and TE non-eigenmodes. For the leaky TE_0 modes we plot the dependence of the complex dispersion relation and show the vertical complex profile of the field. The dependence of the scattered laser radiation field on the effective refractive index is obtained for the given parameters of the waveguide. We compare for the first time the calculated complex scattering diagram of laser radiation outside the waveguide layer in the plane, perpendicular to the plane of incidence, for the leaky and guided TE_0 modes.**

Keywords: *eigen- and non-eigenmodes, dispersion relation, three-dimensional irregularity, vector three-dimensional problem of scattering, linear and nonlinear media, second-harmonic generation.*

1. Introduction

One of the urgent problems of integrated optics is the development of new methods for studying propagation, conversion, and scattering of electromagnetic waves in an integrated-optical waveguide with three-dimensional (3D) irregularities [1–21]. Moreover, the solution of these problems is crucial for the design and development of advanced nanotechnologies in integrated optics and waveguide optoelectronics [7–15, 19–24], since the waveguide is a basic element of various optical integrated circuits, including high-density integrated circuits for advanced telecommunication optical systems [9]. Such a solution, in particular, allows one: to find the attenuation coefficient with high accuracy, to consider the influence of 3D irregularities on the characteristics of scattered radiation (for example, optical integrated circuits), to take into account the effect of scattering of light on detecting capabilities of integrated-optical sensors, etc. (see, for example, [1–21] and references therein). These studies are also important for the design of advanced optimised devices that combine optical waveguide devices (filters, lenses, etc.) with metallodielectric waveguides that support surface plasmons.

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The solution to these urgent problems of integrated optics is hampered by lack of comprehensive theoretical methods that make it possible to study propagation, conversion and scattering of eigen- and non-eigenwaves in an integrated-optical waveguide with 3D-irregularities within a unified approach. In this case, analytical and numerical solutions should ensure a possibility of studying both integral and differential characteristics of scattered radiation at an arbitrary distance from the waveguide, as well as when changing the radius of correlation of statistical irregularities in a wide range of variation of their transverse dimensions, including the size of the order of the wavelength of probe radiation as in the Mie scattering theory [1, 5, 11–14].

In this paper, we report theoretical and numerical analysis of waveguide propagation and scattering of laser radiation of eigen- and non-eigenmodes in an irregular integrated-optical waveguide within a unified approach, based on perturbation theory, the coupled mode method, the Green's function method and the method of Fourier separation of variables [1, 3–5, 11–19]. Scattering of non-eigenmodes is investigated for the first time. The calculated dispersion curves are presented for the case of propagation of TE and TM eigenmodes and TE non-eigenmodes in the waveguides under study. The dependences of the field of scattered laser radiation on the effective refractive index are obtained for the given parameters of the waveguide. Complex profiles of the field of fast and slow leaky modes and some other dependences are calculated.

2. Electrodynamic problem of waveguide light scattering and methods of its solving

2.1. Linear media

The problem of waveguide scattering of electromagnetic radiation in an irregular integrated-optical waveguide (Fig. 1) with 3D-irregularities is solved by the coupled-mode method and perturbation theory [1–5, 11–15, 18, 19].

Maxwell's equations for the electromagnetic field in the case of a nonabsorbing linear isotropic medium (in the absence of charges and currents) in SI units are reduced to equations [1]

$$\mathrm{rot}\boldsymbol{H} = \varepsilon\partial\boldsymbol{E}/\partial t, \quad \mathrm{rot}\boldsymbol{E} = -\mu\partial\boldsymbol{H}/\partial t, \qquad (1)$$

where ε, μ are the dielectric and magnetic permeabilities of the medium, respectively; $\omega\sqrt{\varepsilon\mu} = nk_0$ (n is the refractive index, $k_0 = 2\pi/\lambda_0$, λ_0 is the wavelength of electromagnetic radiation in vacuum, $\omega = 2\pi f$, f is the frequency of the electromagnetic

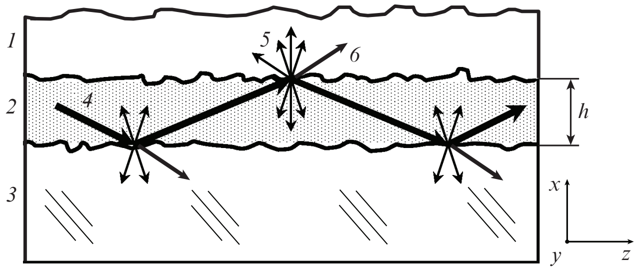

Figure 1. Irregular integrated-optical waveguide: (*1*) cladding layer (air); (*2*) waveguide layer; (*3*) substrate; (*4*) optical beam; (*5*) scattered radiation; (*6*) leaky waves; h is the thickness of the waveguide layer.

field); $\boldsymbol{E}$, $\boldsymbol{H}$ is the vector of the electric and magnetic field strengths.

Equations (1) yield the equation

$$\nabla^2 \boldsymbol{E} + \nabla(\boldsymbol{E}\nabla\varepsilon/\varepsilon) + \omega^2\mu\varepsilon\boldsymbol{E} = 0, \tag{2}$$

describing the electromagnetic field in an irregular optical 3D waveguide.

We consider propagation of a guided {eigenmode, i.e., a solution to the problem on eigenfunctions (fields) and eigenvalues (propagation constants) [1 – 5]} TE_0 mode in a waveguide along the z axis. Similarly, we perform an analysis for the guided TM modes. Figure 1 illustrates the process of propagation and scattering of guided modes in the ray-optics approximation.

2.1.1. Real propagation constants. Sewing the fields at interfaces of the waveguide, we finally obtain the dispersion relation, for example, in the trigonometric form [1 – 5, 20]:

$$\rho_{\mathrm{f}} h = \arctan(\rho_{\mathrm{c}}/\rho_{\mathrm{f}}) + \arctan(\rho_{\mathrm{s}}/\rho_{\mathrm{f}}) + \begin{cases} (p-1)\pi \\ p\pi \end{cases}, \tag{3}$$

which allows one to find the propagation constants (eigenvalues) of the corresponding guided modes (subscripts 'c, f, s' denote media 1, 2 and 3, respectively; Fig. 1). Here, h is the thickness of the waveguide layer; ρ is the transverse component of the propagation constants of guided modes (along the x axis); $\rho^2 + \beta^2 = (k_0 n_m)^2$, where β is the longitudinal component of the propagation constants of radiation modes (along the z axis), n_m is the index refractive index of the corresponding layer of a multilayer optical waveguide; the mode number is $p = 1, 2, \dots$ in the first case and $p = 0, 1, 2, \dots$ in the second case.

Figure 2 shows the dispersion curves $\gamma = \gamma(h)$ [plotted in accordance with formula (3)] for the first five TE and TM modes of a regular three-layer planar polystyrene waveguide (γ is the coefficient of the phase delay). The integrated-optical waveguide parameters (for the wavelength of a helium – neon laser $\lambda_0 = 0.633$ μm) are as follows: the refractive indices of air, $n_{\mathrm{c}} = 1.000$; of the waveguide layer (polystyrene film), $n_{\mathrm{f}} = 1.590$; and of the substrate, $n_{\mathrm{s}} = 1.515$. The dispersion curves allow one to find (for the given γ) the corresponding value of h and vice versa for the selected mode.

We will represent any arbitrary distribution of the field components (e.g., E_y for the TE_0 mode of a planar integrated-

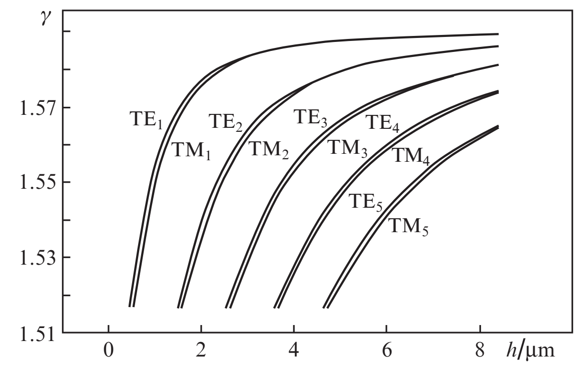

Figure 2. Dispersion curves $\gamma = \gamma(h)$ for the first five guided (eigen) TE modes of a polystyrene waveguide.

optical waveguide) in the form of expansion (in the series and integral) in an orthogonal set of basis eigenfunctions [1 – 5, 11 – 15, 19]:

$$E_y = \sum_{\nu} c_\nu(z;\rho) E_{\nu y}(x,z;\rho) + \sum_{1}^{2}\int_0^\infty q(z;\rho) E_y(x,z;\rho)\mathrm{d}\rho, \tag{4}$$

where the first sum describes all even and odd TE modes, and the combination of the sum (in general, for even and odd modes of radiation, symbolically denoted by 1 and 2) and integration – all the modes of radiation. In expression (4) the variable ν varies from 0 to $+\infty$; c_ν are the expansion coefficients of guided modes $E_{\nu y}$; q is the effective scattering amplitude of TE modes, defined as the coefficient of expansion of the field over all the modes of radiation E_y. Let us make some physical remarks on the radiation modes of, for example, a substrate [2, 19]. The field of the radiation mode of the substrate can be treated as if this mode is excited by a plane wave incident from the substrate under the condition $\rho_{\mathrm{s}} = k_0 n_{\mathrm{s}} \times \cos\theta_{\mathrm{s}}$ (θ_{s} is the angle of incidence of a plane wave from the substrate at the substrate – film interface). The plane wave incident from the substrate is refracted and partially reflected at the interface with the film and undergoes total internal reflection (TIR) at the film – air interface. As a result of interference between incident and reflected plane waves there arises a standing wave with a characteristic sinusoidal field distribution in the substrate and film.

In the case of 3D-irregularities we represent the field distribution in the form of expansion over all possible eigenmodes of a plane regular waveguide [1 – 5, 11 – 15]:

$$\boldsymbol{E}(x,y,z) = \sum \int c_\nu(z;\beta_y) \boldsymbol{E}_{\nu y}(x,z;\beta) \mathrm{e}^{-\mathrm{i}\beta_y y} \mathrm{d}\beta_y$$

$$+ \int \mathrm{d}\beta_y \int q(\beta,\beta_y) \boldsymbol{E}_{\beta y}(x,z;\beta) \mathrm{e}^{-\mathrm{i}\beta_y y} \mathrm{d}\beta. \tag{5}$$

Here, q is the effective scattering amplitude, defined as the coefficient of expansion of the field over all modes of radiation $\boldsymbol{E}_{\beta y}$; β_y is the longitudinal component along the y axis of the radiation mode propagation constant. The expansion coefficients in (4) and (5) are found using the known orthogonality relations.

The solution of the inhomogeneous three-dimensional equation (2) in form (5) using the Fourier method of separation of variables and the Green's function method allows one to write the corresponding expression for the radiation field E_s^{out} outside the waveguide [11–15, 18, 19]:

$$\boldsymbol{E}_s^{out}(x,y,z;\beta_y) = i0.5k_0^2\bar{n}_m^2$$

$$\times \int dx' \int dy' \int dz' \int d\beta e^{-i(\beta_{0y}-\beta)y'} \boldsymbol{E}_{\beta y}^*(x',z')\beta^{-1}$$

$$\times \boldsymbol{E}_{\beta y}(x,z)\Delta n_m^2(x',y',z')\boldsymbol{E}_y(x',z')\sin(\beta_y y)/(\beta_y y), \quad (6)$$

where x, y, z and x', y', z' are the coordinates of the observation point and the coordinates of the point, where the irregularity (for example, the waveguide layer) is located; the function Δn_m sets the inhomogeneity of the waveguide layer; $\bar{n}_m^2$ is the average refractive index of the waveguide layer; β_{0y} is the modulus of the longitudinal component of the vector of propagation $\boldsymbol{k}_y n_2$ of the guided TE_0 mode along the y axis; $\boldsymbol{E}_{\beta y}$ is the field strength of the guided TE mode of the substrate; $\boldsymbol{E}_y$ is the field strength of the guided TE mode of the waveguide. In expression (6) integration over the primed variables is limited by the size of the volume where the inhomogeneity is concentrated. The nonlinear scattering integral (6) describes the radiation field at any distance from the waveguide.

2.1.2. Complex propagation constants. If the waveguide media are absorbing, the propagation constant of the modes of even a regular waveguide will be complex. Consider guided modes, which exist at the waveguide thickness below the critical one h_{cr} (Fig. 3). These modes are called leaky modes. In terms of ray-optics representation the leaky waves propagate due to the effect of the frustrated TIR at interfaces between the media forming a waveguide; therefore, some power of the guided modes radiates ('leaks') into the space surrounding the waveguide. In leaky modes the amplitude increases with distance from the waveguide along the vertical x axis (at a fixed longitudinal distance z and in the absence of losses in the waveguide), but while propagating along the z axis, these modes decay due to the continuous transfer of energy from the waveguide layer to the surrounding medium. Functionally, the fields of leaky modes (see Fig. 4a) are identical to the fields of conventional guided modes.

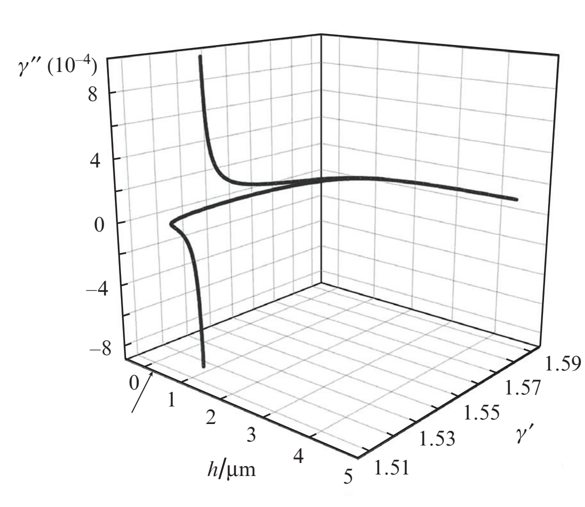

Figure 3. Dispersion curves for the leaky (non-eigen) TE_0 mode of a polystyrene waveguide ($\gamma = \gamma' + i\gamma''$); $h_{cr} = 0.24$ μm (shown by an arrow).

In the case of TE modes the equations for the amplitudes $E_y(x)$ in the substrate, film and cladding layer of a planar waveguide (assuming that $\partial/\partial y \equiv 0$) are of the form [1–5, 20]:

$$\frac{d^2E_y^s}{dx^2} - (n^2k_0^2 - \beta_s^2)E_y^s = \frac{d^2E_y^s}{dx^2} - \rho_s^2E_y^s = 0,$$

$$\frac{d^2E_y^f}{dx^2} + (n^2k_0^2 - \beta_f^2)E_y^f = \frac{d^2E_y^f}{dx^2} + \rho_f^2E_y^f = 0, \quad (7)$$

$$\frac{d^2E_y^c}{dx^2} - (n^2k_0^2 - \beta_c^2)E_y^c = \frac{d^2E_y^c}{dx^2} - \rho_c^2E_y^c = 0.$$

The expressions for other field components are found in accordance with the formulas

$$H_x = \frac{-i}{\omega\mu}\frac{\partial E_y}{\partial z} \equiv \frac{-\beta}{\omega\mu}E_y, \qquad H_z = \frac{i}{\omega\mu}\frac{\partial E_y}{\partial x}.$$

In the case of TM modes the equations for the amplitudes of the fields in the substrate, film and cladding layer of the waveguide are analogous to (7) (see, for example, [1–5]).

We assume that in the waveguide under study, the waveguide layer absorbs, i.e., refractive index of this layer is complex: $n_2 = n_2' + in_2''$. Using the expressions for the fields, we write the tangential boundary conditions, from which after some elementary mathematical transformations, we obtain the complex dispersion relation for the case of propagation of leaky (non-eigen) modes in the waveguide [5, 18, 20, 21]:

$$(\rho_f' + i\rho_f'')h = \arctan\frac{\rho_c' + i\rho_c''}{\rho_f' + i\rho_f''}$$

$$+\arctan\frac{\rho_s' + i\rho_s''}{\rho_f' + i\rho_f''} + p\pi. \quad (8)$$

Here, $\rho_m(\gamma',\gamma'') = \rho_m'(\gamma',\gamma'') + i\rho_m''(\gamma',\gamma'')$; $\gamma = \gamma' + i\gamma''$ is a complex coefficient of the phase delay; $p = 0, 1, 2, \dots$

Determination of complex roots of dispersion equations is of fundamental importance in the electrodynamic theory of optical waveguides. Despite its long history, the problem has not been yet satisfactorily studied. This explains the presence of a number of alternative computational methods of its solution [2, 5, 16–18, 21–24]. Below, we consider three well-known methods for solving dispersion equations, which are nonlinear equations.

The method of the segment bisection (bisection method) is a numerical method for solving nonlinear equations of form $f(x) = 0$. This method assumes only the continuity of the function $f(x)$. The zero-search (root) algorithm x_0 of the function is based on the assumption that at the endpoints of the segment, $f(x)$ has different signs, whereas in the middle of this segment there is a point x_0, where $f(x_0) = 0$.

Newton's method (method of tangents) is an iterative numerical method for finding the root of the given function $f(x)$. The algorithm for finding the numerical solution of the equation $f(x) = 0$ reduces to the iterative procedure of calculation: $x_{n+1} = x_n - f(x)/f'(x)$, where $f'(x)$ is the first derivative of the function. We give a geometric interpretation of Newton's method. First, we set the initial approximation near the expected root, and then construct the tangent to the function in question at a point of approximation for which intersection with the abscissa is found. This point is taken as the next

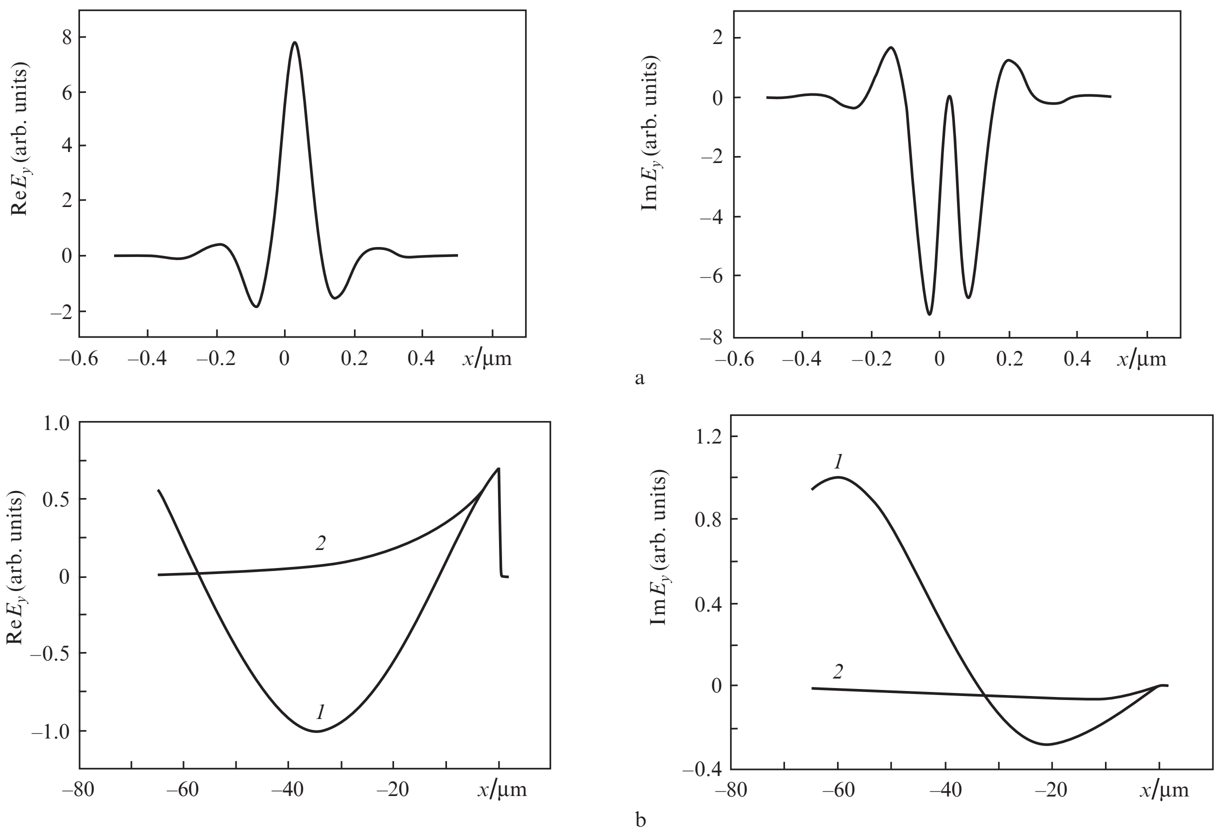

Figure 4. Real and imaginary components of a complex vertical profile of the field of a fast leaky TE_0 mode (mode of fast leakage, $\gamma''/\gamma' \geqslant 1$) (a) and comparison of real and imaginary components of the vertical profiles of radiation (*1*) and leaky (*2*) modes at a distance $x = -65$ μm from the polystyrene film – substrate interface (b). The waveguide parameters for the modes of gradual leakage ($\gamma''/\gamma' \ll 1$) are as follows: $\gamma = 1.5150 - i2.464\times10^{-6}$, $n_f = 1.5900 + i0.0001$, $h = h_{cr} \approx 0.3$ μm.

approximation. And so on, until the required accuracy is reached.

In generalising Newton's method to the functions of a complex argument, the algorithm in the case of real variables remains unchanged. Here, the function may have several zeros, and the solution may converge to different values. This problem was solved only in the 1970s with the advent of computer technology. It turned out that at the intersections of domains of attraction, so-called fractals – infinite self-similar geometric figures (Newton fractals) – are formed. The solution of the dispersion relation is sought in the complex plane of the propagation constants (non-eigenvalues). As a zero approximation use is often made of the values of the roots of the dispersion relation for a metal waveguide (see, for example, [21]) with perfectly conducting walls, whose imaginary part of the transverse propagation constant is $\rho'' \to \infty$ (reflection from the boundary layers reduces).

The Nelder – Mead method (flexible polyhedron method) is a method for unconstrained optimisation of functions of several variables $f(x_1, x_2, x_3,...)$, which does not use a derivative (gradient) function and is applicable to nonsmooth and/or noisy functions. The method consists in the successive displacement and deformation of a simplex* around the point of extremum. It is assumed that severe restrictions on the domain of the function do not exist, i.e., the function is defined at all points. A detailed description of the Nelder – Mead algorithm is given, for example, in [25].

Figure 3 shows an example of a solution to equation (8) for the leaky TE_0 mode of the waveguide using the bisection method [16–18] (solutions were investigated by the other two methods). The waveguide parameters are the same as in Fig. 2, but the refractive index of the waveguide layer (a film with an absorbing impurity) is $n_f = 1.5900 + i0.0001$. In the numerical solution we selected the branch of the two-valued function of the square root, where $\rho'_s > 0, \rho'_f > 0, \rho'_c > 0$. The signs of the imaginary parts of ρ''_c, ρ''_s will set the direction of propagation of leaky modes along the x axis. The sign of ρ''_f determines the increase/decrease in the amplitude of the standing wave along the x axis.

Figure 4a presents a complex profile of a fast leaky (non-eigenwave with a high decay coefficient) TE_0 mode. Polystyrene waveguide parameters are as follows: $\gamma = 1.527 - i2.489$, $h = 0.055$ μm (the critical thickness of the waveguide for a guided TE_0 mode is $h_{cr} = 0.24$ μm). As can be seen from the figure, the profile of this mode is similar to the known profile of guided modes in the case of real ρ.

Figure 4b compares the real and imaginary components of the vertical profiles of radiation and leaky modes. Research has shown that this type of dependence of the fields takes place in a wide range of parameters of the waveguides and the wavelength of electromagnetic radiation.

In most publications on the leaky modes there are no numerically calculated graphs of the fields of different types of leaky modes. However, the authors of several publications

* A simplex or an n-dimensional tetrahedron is a geometric figure, which is an n-dimensional generalisation of the triangle. By definition, a 0-simplex is a point, a 1-simplex is a linear segment, and a 2-simplex is a triangle, etc.

(e.g., [22]) suggest replacing the leaky modes by radiation modes in limited domains. Our research has shown that such a replacement may lead, first, to a large error in calculating losses and, secondly, to an inaccurate calculation of field profiles of leaky modes at distances greater than several wavelengths ($\geqslant 2\lambda_0$).

Note that the number of leaky modes with gradual leakage is limited, unlike the continuum of radiation modes. At the same time, leaky waves with gradual leakage form a discrete spectrum and are plane inhomogeneous waves, while the radiation modes form a continuum (with a continuous spectrum) and are plane homogeneous waves. The replacement of some waves by other waves that is sometimes used [22] requires a serious analysis in each case. As a consequence, there is an urgent need to develop new algorithms for the calculation of the fields of radiation and leaky modes, which surpass standard methods in the calculation rate (e.g., FDTD method) and are not inferior to them in terms of accuracy.

We believe that the solution of the inhomogeneous three-dimensional equation (2) in the form of the scattering integral (6), describing the radiation field $\boldsymbol{E}_{\mathrm{s}}^{\mathrm{out}}$ outside the waveguide, holds true in the case of guided eigenmodes (propagating in the waveguide at $h < h_{\mathrm{cr}}$). In our opinion, the better it describes the scattering of leaky modes (e.g., in the xy plane), the better their vertical profile (along the x axis) corresponds to the vertical profile of radiation modes. However, we emphasize that in the world literature the problem of orthogonality (quasi-orthogonality) and the completeness of the set of the fields (basis functions) used in this case still remain unsolved [2, 5, 11, 15, 26].

2.2. Nonlinear media. Nonlinear effects in optical waveguides

Nonlinear optical phenomena are observed upon interaction of light fields with matter, which has a nonlinear response of the polarisation vector $\boldsymbol{P}$ on the vector of the electric field strength $\boldsymbol{E}$ of the light wave. In most materials nonlinearity is only observed at very high intensities of laser radiation. In a optical waveguide this nonlinearity can be obtained at a low intensity of radiation. Second harmonic generation (SHG) is the simplest nonlinear effect described by nonlinear susceptibility $\chi^{(2)}$.

2.2.1. Advantages of optical waveguides for nonlinear transformations. Let us enumerate main advantages of optical waveguides which make it possible to effectively implement a nonlinear transformation. The natural dispersion of the material is replaced by the dispersion of waveguide modes (depending on the structure of the waveguide). Nonlinear interactions can occur in any component of the waveguide structure (for example, in our case, the cladding layer, waveguide film or substrate). The weak dispersion and strong double refraction of the material are not necessary conditions for phase matching. Laser radiation with a high power density can easily propagate through a long waveguide, whereas its propagation in a bulk medium is limited by diffraction effects.

2.2.2. Propagation of waveguide TE modes in a nonlinear medium. The equation for the TE modes at the second harmonic frequency 2ω has the form [27]

$$\nabla\times\nabla\times\boldsymbol{E}^{(2\omega)} - 4(\omega/c)^2\varepsilon^{(2\omega)}\boldsymbol{E}^{(2\omega)} = 16\pi(\omega/c)^2\boldsymbol{P}^{(2\omega)} \qquad (9)$$

(we consider the nonmagnetic media without absorption, i.e., the case of real propagation constants).

The nonlinear frequency conversion is efficient if the value of the overlap integral for the fundamental frequency

$$I = \int E^{(\omega)}P^{(\omega)}\mathrm{d}x\mathrm{d}y \qquad (10)$$

is large. Integration in (10) is performed over the cross section of the waveguide. To ensure the fulfilment of the condition $I\to\max$ in (10) it is required that the spatial overlap of the field of the TE mode in question and nonlinear polarisation in the transverse plane be maximal. One can see that I is better to optimise for weakly oscillating profiles (as in the lower modes) of the transverse distribution of the field energy. In addition, to ensure efficient mode coupling on the entire length of interaction it is required to fulfill phase-matching condition, i.e., equality of the wave vectors of nonlinear polarisation and the pump mode in (9): $\beta_{\mathrm{p}}^{(2\omega)}(h) = 2\beta_m^{(\omega)}(h)$.

It is important to note that in optical waveguides due to the presence of modes with different polarisations (TE and TM) with respect to the given plane, even in an isotropic medium there already exists ‘splitting’ of the curve $\beta(h)$ [or $\gamma(h)$] for the given frequency ω or of the curve $\beta(\omega)$ for the given h. But it is not possible to achieve phase matching for TE_0 and TM_0 modes, when the overlap integral is maximum because their dispersion curves do not intersect.

In passing from an isotropic material of the film to the anisotropic one, the dispersion curves of the TE modes are split into three dispersion curves, and the dispersion curves of TM modes are split into six dispersion curves. In an anisotropic waveguide phase matching of fundamental modes is possible. In this case, the birefringence is sufficient to compensate for the dispersion of the modes of the same order at the fundamental frequency and second harmonic frequency.

An important advantage of the wave interactions in the case of SHG in waveguide structures in comparison with the classical bulk nonlinear media is the possibility of a substantial (up to several orders of magnitude) increase in the efficiency of frequency conversion, which in the case of volume interaction can be written as [27]

$$\eta_{\mathrm{bk}} \approx 2K\lambda_0^{-1}d^2LP^{(\omega)}\left[\frac{\sin(\Delta kL/2)}{\Delta kL/2}\right]^2, \qquad (11)$$

where $K = 2\omega^2n^{-3}(\mu_0\varepsilon_0)^{3/2}$; n is the refractive index; d is the effective nonlinear coefficient; $P^{(\omega)}$ is the total power of radiation at the fundamental frequency; L is the length of interaction of electromagnetic waves; $\Delta k = k^{(2\omega)} - 2k^{(\omega)}$ is the phase mismatch.

In formula (11), the function sinc(x) reflects the contribution of the phase mismatch Δk between the wave vectors at the fundamental frequency and second harmonic frequency. The length L is limited by the cross section of the Gaussian laser beam, within which the power density remains approximately constant.

The efficiency of frequency conversion in a planar waveguide can be written as [27]

$$\eta_{\mathrm{wg}} = Kd^2L^2P^{(\omega)}Ih^{-1}\left[\frac{\sin(\Delta kL/2)}{\Delta kL/2}\right]^2, \qquad (12)$$

where I is the overlap integral between the transverse distribution of nonlinear polarisation and the second harmonic field (in the section of the waveguide). It is assumed that $I_{\max} = h^{-1}$.

From expressions (11) and (12) we obtain the estimates for η in both cases:

$$\eta_{\rm bk} \approx \lambda_0^{-1} L P^{(\omega)}, \quad \eta_{\rm wg} \approx L^2 (P^{(\omega)}/h^2). \quad (13)$$

This implies that the efficiency of the bulk SHG depends directly proportionally on $P^{(\omega)}$ and L, whereas the efficiency of the waveguide SHG – on the power density $P^{(\omega)}/h^2$ and L^2. Assuming that $h \approx \lambda_0$, we have

$$\eta = \eta_{\rm wg}/\eta_{\rm bk} \approx L/\lambda_0. \quad (14)$$

Let us make a simple estimate in accordance with (14). At L = 5 cm (a typical integrated-optical waveguide) and λ_0 = 1.3 μm (near-IR range), we have $\eta \approx 4\times10^4$ – this is a theoretical gain in efficiency in going from the bulk SHG to the waveguide SHG. Note that in reality, the gain (at a constant pump power and interaction length) is about two orders of magnitude smaller.

The main advantage of the waveguide as compared with bulk materials is the possibility of conservation of power of laser radiation injected into the waveguide at a theoretically infinite length of an ideal (without irregularities and absorption) waveguide with transverse dimensions of the order of λ_0. This property plays an important role in nonlinear waveguide phenomena. Undoubtedly, the study of the SHG phenomena in optical waveguides with uneven (rough) interfaces between the media forming the waveguide is very promising, including both nonlinear bulk and surface phenomena taken into account.

3. Numerical study of light scattering in an integrated-optical waveguide

Main objectives of the numerical study in the general case are formulated in [15, 16, 19]. They include development of new algorithms and software packages for calculating the fields of radiation and leaky modes, which surpass the standard methods (e.g., FDTD [28]) in the calculation rate and are not inferior to them in terms of accuracy; calculation and plotting of the dispersion curves of TE and TM modes for the selected types of waveguides, a series of calculations of the nonlinear scattering integral (6) for different sets of input parameters of the problem; construction of 3D-field profiles (1D- and 2D-diagrams), in particular, $E_s(x)$, $E_s(y)$, $E_s(z)$, and $E_s(\gamma)$.

For example, we considered the scattering of the fundamental TE mode on an extended bulk inhomogeneity (insert type) of a nonabsorbing or absorbing waveguide layer, which is easily implemented in practice by a polystyrene waveguide. A three-layer waveguide was formed by a thin layer of polystyrene deposited on a glass substrate. Its parameters (all for the given λ_0) were as follows: the refractive index of air, n_c = 1.000; the refractive index of the waveguide layer, n_f = 1.590; the refractive index of the substrate, n_s = 1.515. In the numerical simulation we used the parameters of a helium–neon laser (wavelength, λ_0 = 0.633 μm; normalised output power, P_0 = 1).

3.1. Light scattering in an integrated-optical waveguide with linear media

3.1.1. Real propagation constants. To simplify the numerical calculations we assume that the 3D inhomogeneity of the refractive index has a quasi-periodic distribution of the inhomogeneity of the refractive index of unit density. Type of irregularity can be modified by changing the form of the function $\Delta n_{\rm m}^2(x', y', z')$ of the position of the irregularity in the waveguide as well as by changing the size of the region within which integration in expression (6) is carried out.

For the fluctuations of the refractive index inhomogeneity we used the following values: $\sqrt{n_f^2 - n_s^2}/n_s$ = 0.32 (relative to the substrate) and $\sqrt{n_f^2 - n_c^2}/n_c$ = 1.24 (relative to air).

As an example, Fig. 5a shows the dependence of the field E_s on γ for the guided mode for the given parameters of the waveguide. The maximum of the field scattering diagram is located near $\gamma \approx \gamma_{\rm opt}$, close to the inflection point on the dispersion curve [20]. In calculations we found the expected nonlinear dependence of E_s on the parameters of the inhomogeneity (at other fixed parameters of the problem) [19].

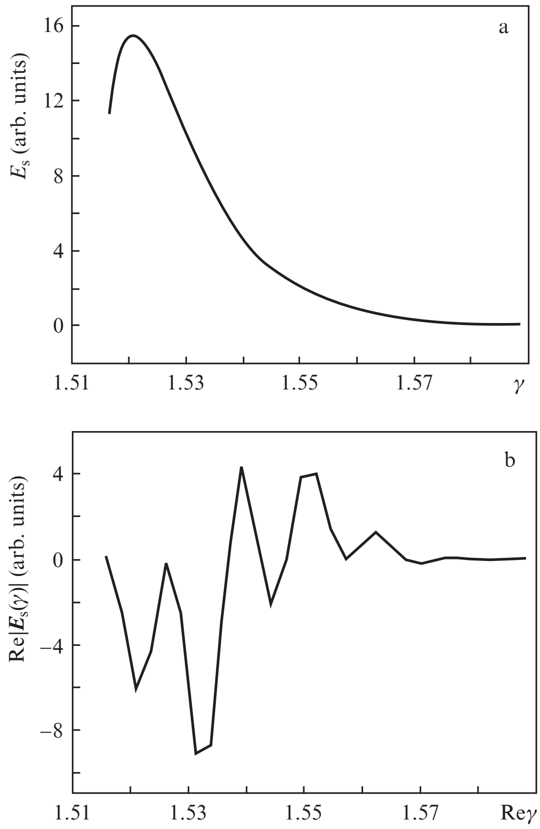

Figure 5. Dependences of the vertical profiles of the fields on γ in the case of scattering of a guided mode (waveguide parameters are: $\gamma = \gamma'$ = 1.5238, h = 0.3416 μm) (a) and in the case of scattering of a leaky mode (waveguide parameters are: γ = 1.5238 – i0.0007, h = 2.544×10^{-7}) (b). The dimensions of the irregularity are $x'\times y'\times z'$ = 4×200×400 μm, the coordinates of the observation point are x, y, z = 6, 0, 0 μm.

It should also be noted that expression (6) for the radiation field outside the waveguide is an integral expression, in which the contribution of scattered radiation from the various harmonic components of the inhomogeneity is averaged and is poorly visible against the background of the central peak of the dependences $E_s(y)$. By physical nature expression (6) reflects the nonlocal relation between the parameters of the medium (irregularity) under study and the guided TE mode field.

The validity of our results is confirmed both by comparison with experimental data, and by comparison of the conclusions that follow from the results of our study with the conclusions arising from the independent theory of waveguide 3D scattering of monochromatic optical radiation [15].

3.1.2. Complex propagation constants. Figure 6 presents two field diagrams of scattering on the same irregularity of the waveguide for the slow leaky (non-eigenwave with small attenuation) TE_0 mode and guided (eigen) TE_0 mode. The amplitudes of the fields are normalised to unity.

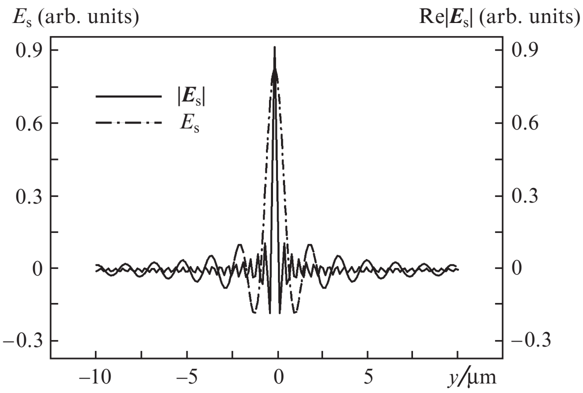

Figure 6. Dependences $|E_s(y)|$ in the case of scattering of a slow leaky TE_0 mode and $E_s(y)$ in the case of scattering of a guided TE_0 mode by the irregularity of the waveguide. The dimensions of the irregularity are $x' \times y' \times z'$ = 4×200×400 μm, the coordinates of the observation point are x, y, z = 2, 0, 0 μm, γ = 1.515 – i0.02.

As can be seen from the figure, the period of oscillations of sidelobes on the diagram of scattering of the guided mode in the transverse xy plane is about three times higher than in the diagram of scattering of the leaky modes, the first minima of the scattering diagrams being located in the vicinity of ±1 μm (guided mode) and about ±0.3 μm (leaky mode).

3.2. Light scattering in an integrated-optical waveguide with nonlinear media

A detailed study of light scattering in an optical waveguide with nonlinear media is beyond the scope of this paper. Here, we only estimate the degree of increase in scattering losses in a waveguide with a nonlinear film upon generation of second and third harmonics without taking into account the coefficient of the conversion of the fundamental-frequency mode power into the harmonic-frequency mode power.

We assume for simplicity that the scattering losses in the waveguide film obey the Rayleigh law, i.e., the intensity of the scattering losses is $I_s \propto \lambda_0^{-4}$. Let the wavelength of fundamental radiation (pump radiation) be λ_0 = 3 μm, and the power losses for this radiation in an integrated-optical processor, such as thin-film waveguide generalised Luneburg lens of radius 1 cm be 1 dB [the attenuation coefficient is $\alpha^{(\omega)} \approx$ 0.2 cm^{-1}]. Then at the second harmonic frequency, these losses will amount to ~16 dB [$\alpha^{(2\omega)}$ = 4 cm^{-1}], and the third harmonic losses will reach 81 dB [$\alpha^{(3\omega)}$ = 20 cm^{-1}]. These estimates show, on the one hand, the complexity of the experimental measurements of such losses in nonlinear waveguides, and, on the other hand, considerable promise of using nonlinear optical phenomena for the study and diagnostics of various irregularities in multilayer waveguide structures.

4. Conclusions

We have analysed theoretical and numerically waveguide propagation and scattering of laser radiation of eigen- and non-eigenmodes in an integrated-optical waveguide with 3D-irregularities. The analysis is performed within a unified approach, based on the perturbation theory, the coupled-mode method, the Green's function method and the method of Fourier separation of variables. We have studied for the first time scattering of leaky (non-eigen) modes. We have briefly considered the fundamentals of waveguide nonlinear optics. The numerical study of the characteristics of laser radiation scattered in a waveguide with 3D inhomogeneity has made it possible to find a significant effect of the coefficient of the phase delay of the waveguide, the size and position of three-dimensional inhomogeneity of the waveguide layer, as well as coordinates of points of observation on the amplitude and phase of the field strength of radiation of eigen- and non-eigenmodes outside the waveguide. We have discovered a complex process of transformation of the radiation field of eigen- and non-eigenmodes as they propagate in the waveguide and from the irregularity in the case of the output of radiation into the surrounding medium. The method for calculating the radiation field, presented in this paper, has an advantage over the standard FDTD method.

The developed methods can be useful for the theoretical and numerical studies of optical waveguides that support eigen- and non-eigenmodes, as well as the characteristics of laser radiation of the corresponding modes, scattered in optical waveguides with three-dimensional irregularities.

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