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Theoretical, experimental and numerical methods for investigating the characteristics of laser radiation scattered in the integrated-optical waveguide with three-dimensional irregularities

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***Abstract*. We consider theoretical, experimental and numerical methods which make it possible to analyse the key characteristics of laser radiation scattered in the integrated-optical waveguide with three-dimensional irregularities. The main aspects of the three-dimensional vector electrodynamic problem of waveguide scattering are studied. The waveguide light scattering method is presented and its main advantages over the methods of single scattering of laser radiation are discussed. The experimental setup and results of measurements are described. Theoretical and experimental results confirming the validity of the vector theory of three-dimensional waveguide scattering of laser radiation developed by the author are compared for the first time.**

Keywords: *integrated optics, laser radiation, nanotechnology, integrated-optical sensor, waveguide modes, three-dimensional irregularity, three-dimensional vector electrodynamic scattering problem, numerical modelling, noise.*

1. Introduction

Improvement and active development of theoretical, experimental and numerical methods, as well as rapid technological progress determine the continuing interest in the fundamental problem of scattering of electromagnetic radiation in different waveguide structures (see, for example, [1 – 20]).

The solution of a three-dimensional electrodynamic problem is crucial for the development of nanotechnology in integrated optics and waveguide optoelectronics. Such a solution in the case of the electrodynamic problem of waveguide scattering of laser radiation makes it possible to accurately determine the damping factor, as well as to take into account the effect of three-dimensional irregularities of a waveguide structure on characteristics of scattered radiation and, in particular, on characteristics of optical integrated circuits and limiting characteristics of planar waveguide lasers (see, for example, [5, 6, 10 – 18]).

In recent years, various types of integrated-optical sensors have been actively developed, which is due to a number of their advantages: high sensitivity, fast response, simplicity of signal multiplexing and possibility of using integrated technologies in them [21 – 23]. It is important to emphasise that the scattering of laser light in the waveguide is one of the most important factors limiting the achievement of maximum sensitivity of integrated-optical chemical sensors [21 – 23]. This interest is manifested in the development of integrated-optical leaky-mode and radiation-mode sensors, as in this case there are opportunities to increase the sensitivity of sensors and to design fundamentally new types of sensors.

Investigation of scattering by three-dimensional irregularities of waveguides is also a priority for the development of waveguides (including channel waveguides) and devices based on them with low loss due to scattering of radiation, as well as for the development of compact integrated waveguide polarisers, filters, deflectors, prisms, lenses, etc. Such studies are important for the design and manufacture of advanced optimised devices, combining optical waveguide three-dimensional structures (filters, deflectors, prisms, lenses, multiplexers, etc.), for example, with metal-dielectric waveguides supporting surface plasmons (see, for example, [24 – 27]).

In this paper we examine the methods making it possible to analyse the basic characteristics of monochromatic electromagnetic radiation scattered in an integrated-optical waveguide with three-dimensional irregularities. The most important characteristics are amplitude and phase of the radiation field at a given point in space as well as the radiation pattern in different cross sections of the space.

2. Electrodynamic problem of waveguide scattering of electromagnetic waves and the method of its solution

Consider propagation and transformation of electromagnetic waves in an irregular dielectric (in particular, optical) waveguide with three-dimensional irregularities (Fig. 1). An irregular waveguide is a waveguide with a rough interface between the media forming it and/or with a nonuniform structure of these media.

Here are some examples of typical irregularities. Smooth 'irregularities': coupling devices that connect various elements of an integrated-optical processor, as well as, for example, such elements of optical integrated circuits as prisms and lenses (in particular, a generalised waveguide Luneburg lens). Statistical irregularities: roughness of the

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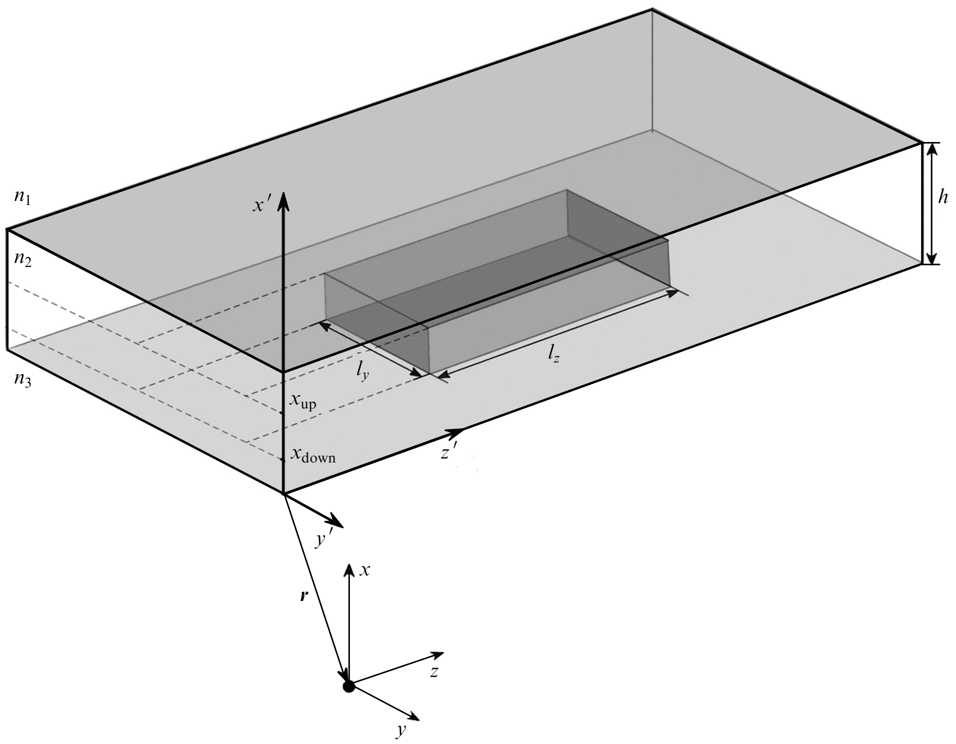

Figure 1. Irregular integrated-optical waveguide: n_1 is the refractive index of air; n_2 is the refractive index of the waveguide layer, n_3 is the refractive index of the substrate; h is the thickness of the waveguide layer; x, y, z and x', y', z' are the coordinates of the observation point and point where the three-dimensional irregularity of the waveguide layer is located; $\boldsymbol{r}$ is the radius vector of the observation point; $x_{\rm up}, x_{\rm down}$ and l_y, l_z specify the position and size of the inhomogeneous region.

interface between the media forming the waveguide and the inhomogeneity of the refractive indices between these media. Sharp irregularities: local (solitary, step-, groove- or insert-like) irregularities, such as the volume inhomogeneity of the refractive index of the waveguide layer and the surface roughness of the film or substrate in the form of steps, grooves or stripes.

Maxwell's equations for the electromagnetic field in the case of unabsorbed inhomogeneous linear isotropic medium (in the absence of currents and charges) in the SI system are reduced to the equations

$$\mathrm{rot}\boldsymbol{H} = \varepsilon\frac{\partial \boldsymbol{E}}{\partial t}, \quad \mathrm{rot}\boldsymbol{E} = -\mu\frac{\partial \boldsymbol{H}}{\partial t}, \tag{1}$$

where $\varepsilon = \varepsilon_{\rm r}\varepsilon_0$ is the permittivity of the medium; $\mu = \mu_{\rm r}\mu_0$ is the permeability of the medium; $\varepsilon_{\rm r}$ and $\mu_{\rm r}$ are relative permittivity and permeability, respectively (in a nonmagnetic medium $\mu_{\rm r} = 1$); ε_0 and μ_0 are dielectric and magnetic constants, respectively; $\omega\sqrt{\mu\varepsilon} = nk_0$; n is the refractive index (hereafter, layers of a multilayer integrated-optical structure under study); $k_0 = 2\pi/\lambda_0$; λ_0 is the wavelength; ω is the circular frequency of the electromagnetic field; $\boldsymbol{E}$ and $\boldsymbol{H}$ are the electric and magnetic field vectors.

In writing equations (1) we took into account that for a linear isotropic medium, the relations $\boldsymbol{D} = \varepsilon\boldsymbol{E}$, $\boldsymbol{B} = \mu\boldsymbol{H}$ are valid, where $\boldsymbol{D}$ is the electric induction vector, and $\boldsymbol{B}$ is the magnetic induction vector. From (1) we can derive an equation describing the field $\boldsymbol{E}(x, y, z) = \boldsymbol{E}(\boldsymbol{r})$ in an optical waveguide with arbitrary three-dimensional irregularities, which in Cartesian coordinates has the form:

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

where ∇ is the vector differential operator, which in Cartesian coordinates has the form $\nabla = (\partial/\partial x)\boldsymbol{x}_0 + (\partial/\partial y)\boldsymbol{y}_0 + (\partial/\partial z)\boldsymbol{z}_0$; $\boldsymbol{x}_0, \boldsymbol{y}_0, \boldsymbol{z}_0$ are the unit vectors; $\nabla^2 \equiv \Delta$ is a Laplacian.

Consider propagation of the first even (fundamental) TE_0 modes with components E_{0y}, H_{0x}, H_{0z} in the irregular integrated-optical planar waveguide along the z axis; below, the subscript 0 in the field components of the guided mode is omitted. Propagation of TM modes is investigated similarly. Note that propagation and scattering of (leaky) noneigen modes are also studied in a similar way, but has a number of important features and will be discussed in subsequent papers.

In the presence of small irregularities, guided modes experience perturbation in the domain of the irregularity, and a small portion of radiation of these modes can be re-emitted in the waveguide modes of other types (intermode conversion), and in the surrounding space. To find more information about the problems that arise when considering the initial electrodynamic problem, we recommend to consult papers [3, 5–7, 10–12, 19, 20] and references cited therein.

If we neglect the consideration of polarisation effects arising from the scattering, we can simplify the three-dimensional vector equation (2). For this we must require that the relative change in the dielectric constant at a distance of one wavelength was much smaller than unity. This condition is often fulfilled in optical media. In this case, the de-polarising term $\nabla(\boldsymbol{E}\nabla\varepsilon/\varepsilon)$ in equation (2) is much smaller than the other two (its ratio to any of them in the order of magnitude is equal to $\Delta\varepsilon/\varepsilon$, where $\Delta\varepsilon$ is the deviation of the dielectric constant from its average value). Consequently, when $\Delta\varepsilon/\varepsilon \ll 1$, the exact three-dimensional vector equation (2) can be replaced by an approximate wave vector equation

$$\Delta \boldsymbol{E} + n^2 k_0^2 \boldsymbol{E} = 0, \tag{3}$$

which is valid for each of the Cartesian components of the electric field vector. For the fundamental TE mode propagating along the z axis, if $\partial \boldsymbol{E}/\partial y = 0$, the vector wave equation (3) takes the well-known scalar form:

$$\frac{\partial^2 E_y}{\partial x^2} + \frac{\partial^2 E_y}{\partial z^2} + n^2 k_0^2 E_y = 0, \tag{4}$$

where $n^2(x,z) = n_m^2 + \Delta n_m^2(x,z)$; n_m^2 describes regular properties of the mth layer of the waveguide medium ($m = 1$ is the cover layer, $m = 2$ is the waveguide layer, $m = 3$ is the substrate) and the addition $\Delta n_m^2(x,z)$ describes the irregularities of the waveguide structure (both the rough interface between two media of the waveguide and the inhomogeneity of the refractive index of the mth layer of the waveguide). To use the perturbation theory, the addition $\Delta n_m^2(x,z)$ should not necessarily be the quantity of small order. It is sufficient that the region within which this addition is different from zero, was quite narrow.

If the conditions $\partial \boldsymbol{E}/\partial y = 0$ and $\partial \boldsymbol{H}/\partial y = 0$ are satisfied, i.e., we consider a two-dimensional solution of the original problem, we can write any arbitrary field distribution in a planar waveguide as a superposition of orthogonal TE and TM modes of an ideal straight waveguide.

Thus, any arbitrary field distribution, such as E_y for the TE_0 mode, of a planar integrated-optical waveguide is represented in the form of an expansion in the orthogonal set of (basis) functions [3, 5, 6, 12, 15]:

$$E_y = \sum_{v} c_v(z;\rho) E_{vy}(x,z;\rho) + \sum_{1}^{2} \int_0^{\infty} q(z;\rho) E_y(x,z;\rho) \mathrm{d}\rho, \tag{5}$$

where the first sum describes all even and odd TE modes, and the combination of the sum (in the general case, in even and odd modes of radiation) and the integral describes all the radiation modes; the variable v belongs to the set of natural numbers I and ranges from 0 to $+\infty$; c_v are the expansion coefficients of guided modes in E_{vy}; q is the effective scattering amplitude of the TE modes, defined as the coefficient of expansion of the field in all radiation modes E_y; $\rho^2 + \beta^2 = (k_0 n_m)^2$; ρ and β are the transverse and longitudinal components of the propagation constants of the radiation modes (along the axes x and z, respectively).

Similarly to (5) for TM modes we have an expression

$$H_y = \sum_{v} d_v H_{vy} + \sum_{1}^{2} \int_0^{\infty} p(\rho) H_y(\rho) \mathrm{d}\rho. \tag{6}$$

The expansion coefficients c_v, $q(\rho)$, d_v and $p(\rho)$ in expressions (5) and (6) are found from the known orthogonality relations.

In the case of three-dimensional irregularities, any* field distribution of an integrated-optical waveguide can be represented as an expansion in all possible modes of a planar waveguide [in the orthogonal set of (basis) functions $\boldsymbol{E}_{vy}$ and $\boldsymbol{E}_{\beta y}$] [12]:

$$\boldsymbol{E}(x,y,z) = \sum_{v} \int_{-\infty}^{+\infty} c_v(z;\beta_y) \boldsymbol{E}_{vy}(x,z;\beta) \exp(-\mathrm{i}\beta_y y) \mathrm{d}\beta_y + \int_{-\infty}^{+\infty} \mathrm{d}\beta_y \int_{-\infty}^{+\infty} q(\beta,\beta_y) \boldsymbol{E}_{\beta y}(x,z;\beta) \exp(-\mathrm{i}\beta_y y) \mathrm{d}\beta, \tag{7}$$

where c_v are the expansion coefficients of guided modes in E_{vy}; q is the effective scattering amplitude of the TE modes, defined as the coefficient of the field expansion in all radiation modes $E_{\beta y}$; the expansion coefficients c_v and q are found using the orthogonality relations; β_y is the longitudinal component of the propagation constant of radiation modes along the y axis.

The solution of the three-dimensional inhomogeneous equation (2) as (7) using the Fourier method of separation of variables and the Green's function method allows one to write an expression for the radiation field $\boldsymbol{E}_{\mathrm{s}}^{\mathrm{out}}$ outside the waveguide (see, for example, [12]):

$$\boldsymbol{E}_{\mathrm{s}}^{\mathrm{out}}(x,y,z) = \frac{\mathrm{i}k_0^2 n_m^2}{2} \int \mathrm{d}x' \int \mathrm{d}y' \int \mathrm{d}z' \int \mathrm{d}\beta \times \exp[-\mathrm{i}(\beta_y - \beta)y'] \boldsymbol{E}_{\beta y}^{*}(x',z') \beta^{-1} \boldsymbol{E}_{\beta y}(x,z) \times \Delta n_m^2(x',y',z') \boldsymbol{E}_y(x',z') \sin(\beta_y y)/(\beta_y y), \tag{8}$$

where x, y, z and x', y', z' are the coordinates of the observation point and the point, where the irregularity is located, for example, the waveguide layer; the function Δn_m sets the heterogeneity of the waveguide layer; the integration limits for primed variables are bounded in our case by the size of the region where the heterogeneity is located because only the contribution to the scattered light from a given local irregularities is taken into account. Note that expression (8) describes the radiation field at any distance from the waveguide.

For convenience of numerical calculations, the quadruple integral in (8) can be represented as a superposition of four nested functions depending on the integration interval and the values of the arguments of higher integrals [10].

3. Method of waveguide scattering

The method of waveguide scattering of electromagnetic radiation consists in registering the scattering diagram by a point photodetector in the near, intermediate or far field and the subsequent processing of digitised values of the scattered radiation intensity in a waveguide in accordance with the requirements of the experiment.

The used method of waveguide light scattering is based, in particular, on the works [8, 9, 12–17], where we gradually developed the vector theory of waveguide three-dimensional scattering of laser radiation and the theory of the inverse problem of waveguide scattering in the presence and absence of noise. Using the latter theory we can, for example, find an approximate correct solution of the inverse problem of waveguide scattering in statistically irregular waveguide that is robust to noise with a fairly high amplitude. As a result, we can reconstruct the statistical second-order properties (spectral density function and autocorrelation function of the irregularities), and define the parameters of irregularities (for example, the rms

*The case of leaky modes in such an approach requires a certain mathematical accuracy at each stage of both analytical and numerical solution of the formulated electrodynamic problem.

deviation of the mean value and the correlation radius) with high resolution even in the presence of noise [13, 15, 16].

The physical nature of the waveguide scattering is that the electromagnetic wave, coupled in the waveguide layer, propagates in it in the form of some excited mode, which is scattered in the interaction with the irregularities of the waveguide. In the optical-beam approximation, the wave propagates along the waveguide through multiple reflections from the interfaces between the media forming the waveguide [in the form of plane (Brillouin) waves, moving along zig-zag paths and experiencing frustrated total internal reflection at the boundaries of the waveguide].

It should be noted that an important advantage of this method is the use of waveguide scattering, which can improve measurement sensitivity by 100 – 1000 times compared with the methods of single scattering of light due to multiple in-phase scattering of light by a statistical ensemble of irregularities [13 – 17].

Another advantage is that the 'optical probe', which 'prescribes' the profile of surface roughness, is the waveguide mode itself. By controlling the properties of the 'probe', we can control contrast and other characteristics of scattered radiation, which forms an optical image of the irregularities. This is particularly important in studying smooth surfaces or low-contrast phase inhomogeneities.

An advantage of waveguide scattering is also the possibility of investigating irregularities in a wide range of lateral dimensions: from nano- to micrometers, including the size of the order of the wavelength of the probing radiation λ_0, as in the Mie scattering theory.

In addition, the waveguide scattering method is a perfect 'tool' of metrological control in integrated optics and waveguide optoelectronics, because the characteristics and parameters of the irregularities determined with its help characterise the waveguide as an integral structure rather than as a set of the individual media used to create it.

4. Experimental setup and results of measurements

The irregular integrated-optical waveguide under study is presented in Fig. 1. The scheme for registering the scattered laser light in the waveguide in the incidence plane xz and in the plane perpendicular to it is shown in Fig. 2. As a source of coherent radiation we used a 0.633-μm helium – neon laser with an output of 15 mW. The scattering diagram of the laser radiation was recorded with the help of a multimode fibre cable coupled to a PD-24 photodetector (the cable length is 485 mm; the ends of the cable, secured with a flexible plastic tube having a diameter of 6 mm, have metal cylindrical lugs; the diameters of the entrance and exit apertures of the cable are $\sim$ 2.5 mm). If it was necessary to increase the signal/noise ratio (in the experiments the recorded signal/noise ratio was at least 10), use was made of a photoelectronic multiplier. For convenience of the measurements, it is required to use an array of photodetectors followed by analogue-to-digital signal conversion and processing of measured data on the computer.

We studied experimentally the scattering of the fundamental TE mode in a polystyrene integrated-optical three-layer waveguide on a glass substrate where scattering on the rough surface of glass substrate dominates. The parameters of the waveguide are as follows: the refractive index of air, $n_1 = 1.000$; the refractive index of the waveguide layer (polystyrene film), $n_2 = 1.590$; the refractive index of the substrate, $n_3 = 1.515$; the thickness of the waveguide layer,

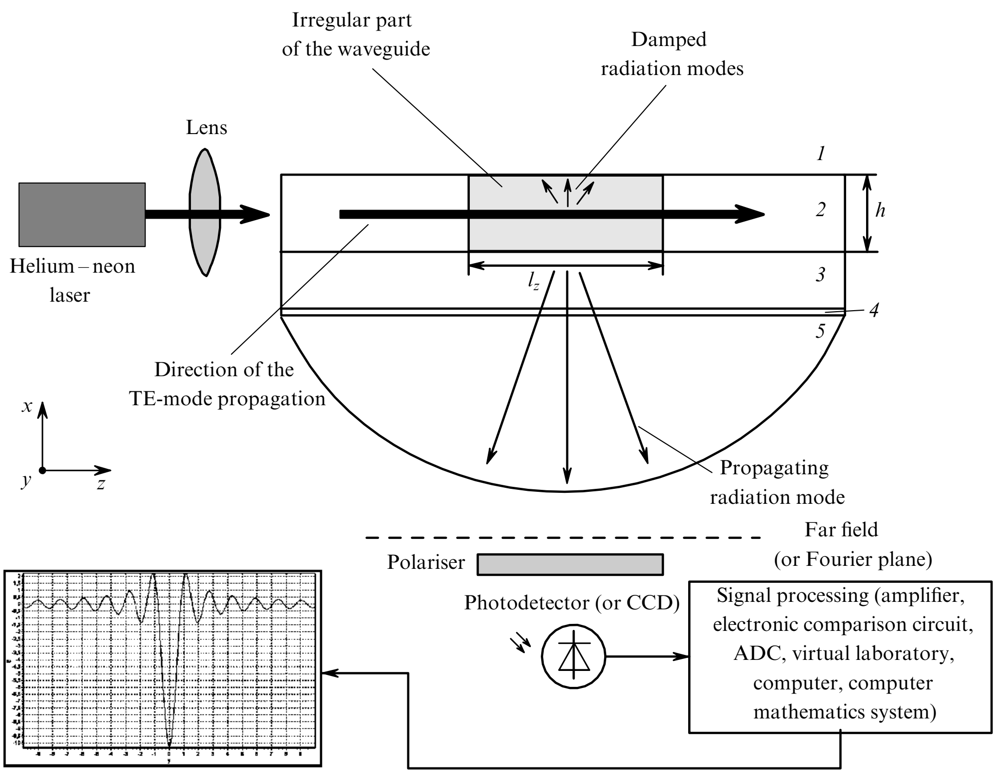

Figure 2. Scheme for detecting scattered laser radiation and an irregular integrated-optical waveguide: (*1*) cover layer (air); (*2*) waveguide layer (polystyrene film); (*3*) glass substrate; (*4*) thin layer of immersion; (*5*) quartz semi-circle (or hemisphere).

$h = 2.000$ μm; the coefficient of phase delay (or effective refractive index of the waveguide, showing how many times the speed of wave propagation in a vacuum is greater than the speed of wave propagation in the waveguide), $\gamma = 1.584$. The substrate had the roughness with the rms height of $\sigma \approx$ 250 Å. Note that in experiments we studied other types of waveguides.

We focused our attention in this article on the dependence of form $E(x, y, z) = E(a, y, b)$, where a, b are some fixed coordinates. Such a study can verify the compliance of our approximate three-dimensional theory of waveguide scattering of electromagnetic waves with the experimental results.

Experimental scattering diagrams were obtained through scanning by a fibre, coupled to a PD-24 photodetector, and by a photodetector with a point aperture (small area of the photosensitive region) along the y axis (in the xy plane) at a fixed distance x from the surface of the waveguide polystyrene film. Then, the diagrams were represented in the form of a discrete set of digital values of the intensity response in the required number of reference points for further data processing on the computer. Experimental scattering diagrams obtained in the form of dependencies $|\boldsymbol{E}(\vartheta)|^2$, where ϑ is the angle of deviation of the photodetector along the y axis from the plane of incidence. For further comparison of the theory with experiment, it was convenient to convert the angle ϑ in the propagation constant β_y.

Figure 3 shows one of the thus constructed smoothed experimental curves $|\boldsymbol{E}(\beta_y)|^2$. Note that the power of the scattered laser light in the centre of the diagram ($\beta_y = 0$) is approximately 10^{-7} W. The effect of the noise component was reduced by an effective smoothing of experimental data with the help of the 'Microcal Origin' graphical package.

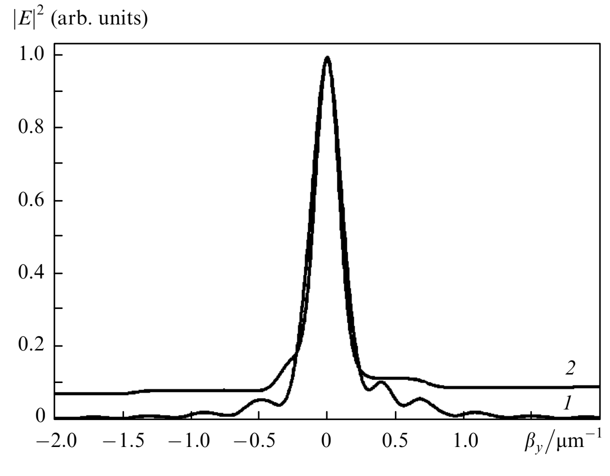

Figure 3. Smoothed theoretical (*1*) and experimental (*2*) scattering diagrams of the fundamental TE-mode radiation outside the waveguide layer of the investigated polystyrene integrated-optical waveguide.

5. Numerical simulation, comparison of theoretical and experimental results and their discussion

Calculations were performed for the parameters of the waveguide investigated experimentally. The roughness of the film – substrate interface was described by the model inhomogeneity of the refractive index, equivalent to roughness of the film – substrate interface in a given volume $V(x', y', z') = 0.025 \times 100 \times 200$ μm.

Figure 3 shows the smoothed calculated and experimental scattering diagrams $|\boldsymbol{E}(\beta_y)|^2$ of the TE_0-mode radiation on the substrate roughness of the investigated waveguide. The coordinates of the observation point are as follows: $x = 2$ μm, y, $z = 5$ μm. These diagrams describe the scattering of TE_0-mode radiation in the xy plane. The calculated scattering diagram was constructed in accordance with (8). It is seen that the calculated and experimental scattering diagrams are in good agreement.

We also investigated other dependences, in particular, $E(x, y, z) = E(x, c, b)$, $E(x, y, z) = E(a, c, z)$, where a, b, c are some fixed coordinates. These dependences illustrate, in particular, the influence of the coordinates of the observation point, the parameter γ, the position and size of the three-dimensional inhomogeneity on $E(x, y, z) = E(a, y, b)$.

Let us briefly describe the results obtained by numerical simulation. In the case of the fixed laser radiation parameters (wavelength, output power), fixed parameters of inhomogeneity (the size of the inhomogeneity, the amplitude of the equivalent inhomogeneity σ) and fixed coordinates of the observation point, we observed following dynamics with increasing γ from the minimum value ($\gamma_{\min} \approx 1.515$) to the maximum ($\gamma_{\max} \approx 1.589$) one. First, the amplitude of the 'negative' diagram $E(\beta_y)$ (inverted down with respect to the vertical axis by the central maximum) increases; then, the diagram turns from the lower half-plane to the upper half-plane and becomes 'positive'. Furthermore, its amplitude alternately decreases and increases, and then the diagram turns back from the upper half-plane to the lower half-plane, etc. Finally, at $\gamma_{\max} \approx 1.589$ the diagram $E(\beta_y)$ again turns from the upper half-plane of the lower half-plane, i.e., returns to its original state but the field amplitude in this case exceeds the original by about an order of magnitude.

Similar changes are observed upon variation of the parameters and type of inhomogeneity, as well as the coordinates of the observation point. A detailed analysis of scattering diagrams for this case will be given in our subsequent papers. Here we only point out that a slight change in the amplitude of the inhomogeneity, equivalent to the substrate roughness σ (from 0.025 to 0.026 μm, i.e. about 4 %), the maximum field amplitude $E(y)$ ranged from -5.787×10^{-7} to -5.694×10^{-7} (about 1.6 %) at the point with the same coordinates ($x = 2$ μm, y, $z = 5$ μm). This change in the field amplitude of scattered radiation can be detected in experiments using a photomultiplier in the recording path. Especially, if we use a scheme with the reference arm and registration of the signal after the resonance amplifier, such as a synchronous detector.

It is important to emphasise that the resulting view of the scattering diagram $|\boldsymbol{E}(\beta_y)|^2$ means that almost all the energy of scattered laser radiation is concentrated in the plane of incidence. This conclusion is also consistent with results of another approximate theory of waveguide three-dimensional scattering of light, constructed for specially selected conditions of scattering diagram measurements [9]. In paper [9] the portion of the dielectric constant dependent on y is replaced by the harmonic lattices with wave vector $\boldsymbol{K}_y$ and the spectrum $g(\boldsymbol{K}_y)$, which excite the light waves scattered at angles to the plane of incidence xz, i.e., to the plane containing an incident waveguide beam and perpendicular to the plane of the waveguide. The theory described in [9] is a special case (developed in [12, 15, 18]) of vector theory of waveguide three-dimensional scattering of electromagnetic waves by random irregularities in the presence of noise.

Thus, the numerical simulation results validated the use of well-known methods of calculation at all stages of the theoretical and numerical solution of the formulated electrodynamic problem. In this case, the reliability of the results is confirmed not only by comparison with experimental data but also by comparison of the conclusions of our study and an independent theory of waveguide three-dimensional monochromatic light scattering.

6. Conclusions

In this paper, we have considered theoretical, experimental and numerical methods for studying the key characteristics of laser radiation scattered in an integrated-optical waveguide with three-dimensional irregularities.

We have also described the experimental setup and measurement results. The main attention is paid to the scattering diagrams in the plane perpendicular to the plane of incidence. This study has shown very good agreement of the vector theory of waveguide three-dimensional scattering developed in our studies with experimental data.

We have studied numerically the influence of the coordinates of the observation points, coefficient of phase delay and size of the inhomogeneity of the waveguide layer on the amplitude and phase of the radiation field strength outside the waveguide.

The revealed dynamics of the scattering diagrams contains information that can be used to analyse the parameters of waveguide irregularities and to develop the physical basis of integrated-optical sensors, for example, OTDR-sensors.

The developed research methods are undoubtedly relevant and important for the design and development of optimised advanced devices connecting optical waveguide filters, deflectors, lenses, multiplexers, etc., such as metal-dielectric waveguides supporting surface plasmons.

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