

Theory of Gaussian Beam Diffraction by a Transmission Dielectric Grating

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Abstract—An advanced 2D mode theory of plane electromagnetic wave diffraction by a transmission dielectric grating (rectangular relief or planar sinusoidal one) is considered. On the bases of this theory, a new model of diffraction of a spatially inhomogeneous light field (a Gaussian beam) by a transmission grating with arbitrary thickness is developed. It provides the opportunity to compute the transverse spatial structure of radiation diffraction orders and to estimate character of their distortions in comparison with the initial Gaussian beam structure. It is shown that such distortions appear under abrupt variations of intensity of all orders and can be caused by transformation of a certain diffraction order from the radiation regime of propagation into the waveguide regime and inversely (Wood's anomalies), and also it can be induced by a set of additional reflections on the boundaries of a thick substrate.

1. INTRODUCTION

The problem of electromagnetic diffraction by gratings, i.e., structures with periodic change of physical properties in space, is of increasing interest among researchers. Such structures are widely used in modern science and engineering, and provide the opportunity to realize effective spatial transformation of light fields with high selectivity of temporal and spatial frequencies [1–5]. Recently, the field of application of grating structures has expanded substantially owing to using of new artificially created nano- and metamaterials [6, 7]. As a consequence, one should expect that the theory of diffraction by periodic structures [1–4] up to now constitutes a fully established physical theory, describing all fundamental behaviors of this phenomenon.

Unfortunately, this is wrong in spite of that the number of published works on this topic does not decrease from year to year. Probably, one of the reasons is nontrivial and even has paradoxical nature of the phenomenon of light diffraction by a grating, when small effects of a field change in the microscale, being amplified many times in a resonant manner, manifest themselves at the macrolevel. And last but not least, the difficulties of the theory are explained by cumbersomeness of its mathematical apparatus, which has to be constantly complicated and supplemented in order to cover the versatile properties of this phenomenon.

Usually, in theoretical consideration of diffraction by periodic structures [1–4], researchers restrict themselves to a plane-wave model of a light beam, and there are still few works where the spatial inhomogeneity of diffraction beams is taken into account in the framework of more complex models (see, for example, [8, 9]). These are works devoted to the consideration of a rather specific case of Gaussian beam diffraction by volume thick gratings. Meanwhile, the effects of transverse spatial inhomogeneity of the initial light beams, which are usually insignificant, begin to play an important role under conditions when the field or part of it (one of the diffraction orders, for example) undergoes transition from the free propagation regime to the regime of total internal reflection at the boundaries of dielectric media,

Received 1 September 2021, Accepted 22 October 2021, Scheduled 3 November 2021

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and inversely [10] (see also [11, 12]). In this case, abrupt variations in intensities of all diffraction orders are observed in metallic and dielectric gratings (so-called Wood's anomalies) [1, 13].

It is still unclear how, under these conditions, the spatial inhomogeneity of the diffracting beam affects the intensities of fields of different diffraction orders, and inversely, how such changes affect their spatial structure. In this work, we have advanced and improved the mode formulation of the plane-wave model of diffraction by a dielectric grating in order to use it as the basis for a more general theory of inhomogeneous light field diffraction. Such a diffraction model for a Gaussian beam is constructed using the Fourier-mode method [8–10] for the case when the beam width is much greater than the wavelength. This model allows for calculation of the beam field structure for each radiation diffraction order at any distances from a grating. We restrict ourselves to considering a two-dimensional model of relief and planar dielectric gratings with periodic modulation of physical parameters (surface or bulk dielectric permittivity) in one direction — parallel to the grating boundaries. Such gratings operate mainly for transmission (the intensity of the reflected field is much less than that of the transmitted field), and therefore are usually called transmission gratings, although it would be wrong to reduce the diffraction effects for them only to excitation of the transmission radiation.

2. MODE DESCRIPTION OF PLANE WAVE DIFFRACTION BY A GRATING

Diffraction grating, operating for transmission, is usually characterized by periodic change of dielectric permittivity along the boundaries. For relief gratings, such periodicity is provided by the presence of grooves, which are cut on a plane substrate and replicated periodically at displacement along the boundary on the distance, multiple of the grating period, which we denote by Λ . The elemental shape of a relief grating is a simple binary grating with one rectangular ruling per period (Fig. 1). Besides, an additional type of gratings is planar (slab) ones, with periodic modulation of dielectric parameters in the bulk of the material of itself, for example, of the index of refraction or of absorption. These can be holographic gratings [14] or liquid crystals [15].

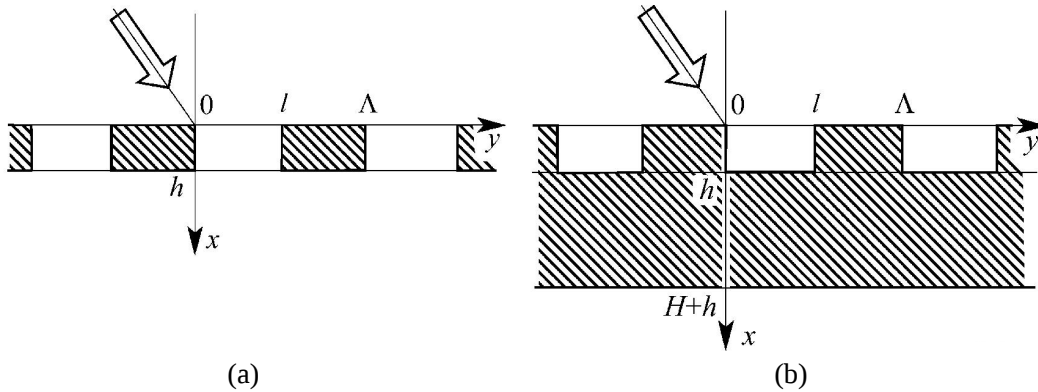


Figure 1. Simple binary relief grating (a) without and (b) with a substrate. h is the thickness of a grating, Λ is its spatial period, l is the length of an air groove between two neighbour rulings, H is the thickness of a substrate.

We set the physical properties of grating being change along only one tangential coordinate y : $\varepsilon_g = \varepsilon_g(y)$ (Fig. 1), i.e., its dielectric permittivity ε_g does not depend on the normal coordinate x . We consider the two-dimensional problem of monochromatic fields diffraction, when electromagnetic field is represented in terms of a superposition of two independent polarizations, TE and TM [16], with each being determined by a scalar field function $u(x, y)$, i.e., when

$$E_z = u; \quad H_x = -\frac{i}{k} \frac{\partial u}{\partial y}; \quad H_y = \frac{i}{k} \frac{\partial u}{\partial x}; \quad (1a)$$

for the TE polarization, or

$$E_x = \frac{i}{k} \varepsilon_g^{-1} \frac{\partial(\varepsilon_g u)}{\partial y}; \quad E_y = -\frac{i}{k} \frac{\partial u}{\partial x}; \quad H_z = \varepsilon_g u \quad (1b)$$

for the TM polarization, where $i = \sqrt{-1}$ is the imaginary unit, $k = \omega/c = 2\pi/\lambda$ the wave number, and λ the radiation wavelength. The temporal multiplier $\exp(-i\omega t)$ is omitted everywhere. At that, the field function should satisfy the wave Helmholtz equation [16]

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + k^2 \varepsilon_g u = 0 \quad (2a)$$

for the TE polarization, and

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial}{\partial y} \left(\varepsilon_g^{-1} \frac{\partial(\varepsilon_g u)}{\partial y} \right) + k^2 \varepsilon_g u = 0 \quad (2b)$$

for the TM polarization.

We consider a simple planar grating, which is the only sinusoidal grating in the dielectric permittivity

$$\varepsilon_g(y) = \varepsilon + \mu \cos(Ky) \quad (3)$$

where ε is the mean value of the dielectric permittivity of a grating, which is a constant value, $K = 2\pi/\Lambda$; Λ is the spatial period of a grating along the y axis; μ is the amplitude of permittivity modulation.

The simple rectangular relief grating, which will also be considered below, is characterized by the following function of dielectric permittivity (Fig. 1)

$$\varepsilon_g(y) = \begin{cases} 1, & \text{for } n\Lambda \leq y \leq n\Lambda + l \\ \varepsilon, & \text{for } n\Lambda + l \leq y \leq (n+1)\Lambda \end{cases} \quad (4)$$

where n is an integer, ε the dielectric permittivity of grating rectangular ruling (constant value), and l the length of air groove between two neighbour rulings.

A periodic function (4) can be expanded in an infinite Fourier series

$$\varepsilon_g(y) = \sum_{n=-\infty}^{+\infty} G_n e^{inKy} \quad (5a)$$

where the constant coefficients of this series are

$$G_0 = 1 + (1 - l/\Lambda)(\varepsilon - 1); \quad G_n = i(\varepsilon - 1)[1 - \exp(-inKl)]/2\pi n \quad (6a)$$

Dielectric permittivity of a simple sinusoidal grating in Eq. (3) can be considered as an expansion in the Fourier series in Eq. (5a) with coefficients

$$G_0 = \varepsilon; \quad G_{-1} = G_{+1} = \mu/2; \quad G_n = 0 \quad \text{for } |n| > 1 \quad (7a)$$

The value ε_g^{-1} , which is inversely proportional to inhomogeneous dielectric permittivity, can also be expanded in the Fourier series

$$\varepsilon_g^{-1}(y) = \sum_{n=-\infty}^{+\infty} \bar{G}_n e^{inKy} \quad (5b)$$

Its coefficients are

$$\bar{G}_0 = 1 - (1 - 1/\varepsilon)(l/\Lambda); \quad \bar{G}_n = -G_n/\varepsilon \quad (6b)$$

for the rectangular relief grating in Eq. (4), and

$$\bar{G}_n = \frac{1}{\sqrt{\varepsilon^2 - \mu^2}} \left(\frac{\sqrt{\varepsilon^2 - \mu^2} - \varepsilon}{\mu} \right)^{|n|} \quad (7b)$$

for the sinusoidal planar grating in Eq. (3).

By this way, we have uniformly defined the properties of planar and relief gratings in terms of the infinite Fourier series in Eq. (5). A relief grating is described as a periodically inhomogeneous dielectric layer with two plane boundaries and specifically determined coefficients of a Fourier expansion for the given inhomogeneity in terms of plane waves. Such a model of a relief grating seems to be a crude approximate one and incapable of true results. However, application of more rigorous theoretical

model [17] of a rectangular grating, which takes into account reflection and refraction on its vertical rectangular rulings explicitly, yields results very close to those of the given model of continuous grating medium. From here, a great merit of a selected model is obvious, which is found sufficiently universal and is suitable to a wide class of various diffraction gratings.

Let a grating be illuminated by a uniform plane wave of the TE or TM polarization

$$u_0 = \exp(ik[\alpha_0 x + \beta_0 y]) \quad (8)$$

where $\alpha_0 = (1 - \beta_0^2)^{1/2} = \cos \vartheta$ and $\beta_0 = \sin \vartheta$ are the parameters of normal and tangential propagation of a wave in the x and y coordinates in air before a grating, and ϑ is the angle of incidence. Since the incident field in Eq. (8) and dielectric permittivity of a medium are periodic functions of the y coordinate, the field function u in the interior of a grating should be represented as a superposition of the exponential functions [1, 3] (the Floquet theorem)

$$u(x, y) = \sum_{n=-\infty}^{+\infty} \sum_{m=-\infty}^{+\infty} B_{mn} [A_m^+ \exp(ik\sigma_m x) + A_m^- \exp(-ik\sigma_m(h - x))] \exp(ik\beta_n y) \quad (9)$$

where

$$\beta_n = \beta_0 + nK/k = \beta_0 + n\lambda/\Lambda \quad (10)$$

$A_m^\pm$ are arbitrary amplitude multipliers to be determined under solution of the general boundary problem. B_{mn} and σ_m^2 are the eigenvectors and eigenvalues of the matrix problem

$$\sum_{m=-\infty}^{+\infty} \left(G_{n-l} - \beta_n \sum_{p=-\infty}^{+\infty} \beta_p W_{nlp} \right) B_{ml} = \sigma_m^2 B_{mn} \quad (11)$$

where the index m numbers various eigenvalues and eigenvectors, but the index n numbers various components of one eigenvector,

$$W_{nlp} = \begin{cases} \delta_{np} \delta_{nl} & \text{for TE polarization} \\ G_{p-l} \bar{G}_{n-p} & \text{for TM polarization} \end{cases}$$

δ_{nl} are the Kroneker symbols ($\delta_{nl} = 1$ for $l = n$ and $\delta_{nl} = 0$ for $l \neq n$).

Figure 2 shows the real eigenvalues σ_m^2 of the matrix in Eq. (11), computed for planar and relief gratings in the cases of TE polarization, as functions of the tangential propagation parameter β_0 of an incident wave (for the TM polarization, the given dependences appear similarly). The eigenvalues σ_m^2 from Fig. 2 are thus seen as positive as negative ones, which corresponds to a sinusoidally propagating or exponentially decaying character of the modes field in Eq. (9) changing on the depth of a grating. Fig. 2 also shows that the curves depicting various eigenvalues can pass very close to each other or intersect entirely, which signifies the coincidence of two various matrix eigenvalues in isolated points.

The field representation in the form of Eq. (9) is consistent with the mode or dynamic theory of electromagnetic waves diffraction by periodic structures [1–4]. In the given theory, the field is considered as a superposition of the set of individual grating modes, defined by the index m , which is characterized by constant wave amplitudes $A_m^\pm B_{mn}$ inside a grating, by the wavevectors $\mathbf{k}_{nm}^\pm = k(\pm\sigma_m \mathbf{e}_x + \beta_n \mathbf{e}_y)$ and by the values of effective dielectric permittivity ($\beta_n^2 + \sigma_m^2$). Hence, it appears that various grating modes, numbered by the index m , are recognized in the normal component $k\sigma_m$ of a wavevector, but their tangential components $k\beta_n$ can be identical. However, out of a grating, various diffraction modes are characterized by the index n .

The fields in all media obey the condition of spatial periodicity. Hence it follows that in air above a grating, the field should have the form of a periodic Fourier series

$$u(x, z) = \exp[ik(\alpha_0 x + \beta_0 y)] + \sum_{n=-\infty}^{+\infty} R_n \exp[ik(-\alpha_n x + \beta_n y)] \quad (12)$$

where the augend corresponds to an incident wave (8) of the unit amplitude, and R_n is the complex amplitudes of the waves of diffraction orders, reflected from a grating. Their parameters of tangential

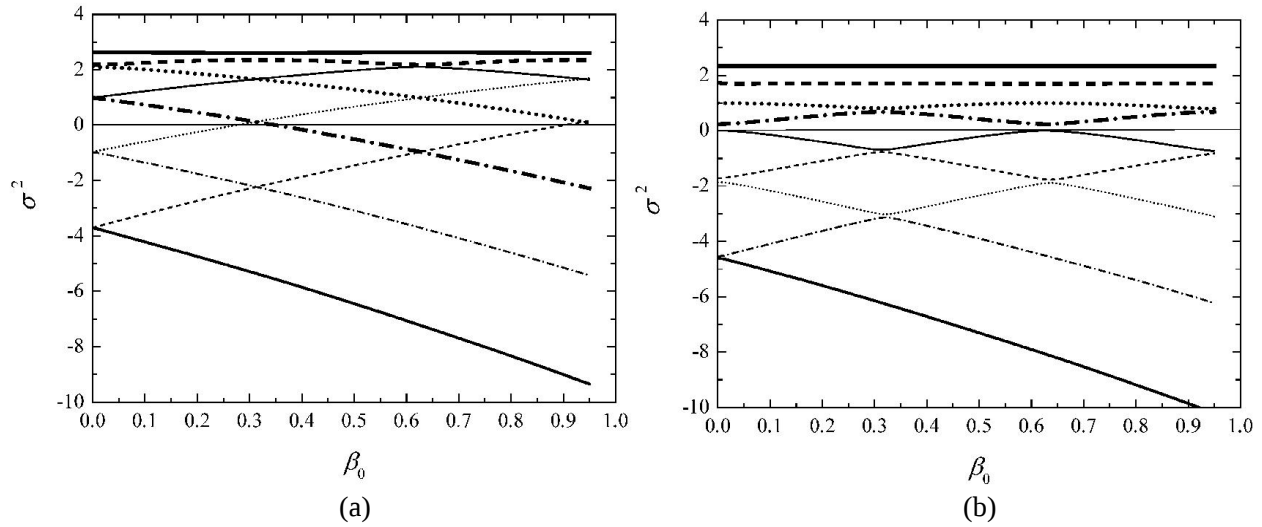


Figure 2. Dependence of eigenvalues of the matrix (11) on the parameter of tangential propagation of incident TE wave for (a) a planar sinusoidal and (b) a rectangular relief grating with the thickness $h = 1.25\lambda$, the spatial period $\Lambda = 1.6\lambda$ and the index of refraction of a dielectric $n_g = 1.6$.

propagation β_n are determined by the same expression (10) as for waves inside a grating, and the parameters of normal propagation are

$$\alpha_n = \sqrt{1 - \beta_n^2} \quad (13)$$

with the branch of root having nonnegative imaginary part, because the reflected field in Eq. (12) should remain bounded in magnitude on infinity.

Squared absolute values of R_n can be interpreted as energetic reflection coefficients for the waves of corresponding diffraction orders (diffraction efficiencies of every order). Indeed, in a two-dimensional case for a plane electromagnetic wave as for a beam with narrow angular spectrum, the local energy density, or the light field intensity [18], determined via the Poynting vector [16] using the representation in Eq. (1), appears proportional to the squared absolute value of the field function u , corresponding to the given wave or beam.

In a similar manner, the fields in another homogeneous media outside a grating are constructed in the form of a superposition of plane waves with the parameters of tangential propagation (10). Note that in a substrate, bounded from the top and bottom by two plane boundaries ($h \leq x \leq h + H$), one should take into account the possibility of wave propagation in two opposite directions of the x normal:

$$u(x, y) = \sum_{n=-\infty}^{+\infty} [S_n^+ \exp(ik\gamma_n[x - h]) + S_n^- \exp(ik\gamma_n[h + H - x])] \exp(ik\beta_n y) \quad (14)$$

but in the region behind the substrate ($x \geq h + H$) waves can propagate only in one direction along the normal

$$u(x, y) = \sum_{n=-\infty}^{+\infty} T_n \exp(ik[\alpha_n(x - h - H) + \beta_n y]) \quad (15)$$

In Eqs. (14), (15), the coefficients $S_n^\pm$ and T_n represent unknown constant wave amplitudes, and the values T_n can be considered as amplitude complex transmission coefficients (diffraction efficiencies) for the waves of various diffraction orders,

$$\gamma_n = \sqrt{\varepsilon_s - \beta_n^2} \quad (16)$$

is the parameter of normal propagation of waves in a substrate; ε_s is the dielectric permittivity of the last; and the parameters of normal propagation α_n in air is determined by the same expression (13), as before a grating. In the case of absence of a substrate, one should set $H = 0$.

The choice of parameters of normal modes propagation in the form of Eqs. (13) and (16) provides at once satisfaction of Equation (2) for the fields before a grating, in a substrate and behind that, without the appearance of additional parameters of phase mismatch in amplitude equations.

The unknown field amplitudes of Eqs. (12), (14), (15) in various regions are determined using the continuity conditions for tangential electric and magnetic field components E_y , E_z and H_y , H_z on both sides of every boundary. From these conditions, the amplitudes of all waves out of a grating are expressed in terms of the grating mode amplitudes:

$$R_n = \sum_{m=-\infty}^{+\infty} \left(A_m^+ + A_m^- e^{ik\sigma_m h} \right) \bar{B}_{mn} - \delta_{0n} \quad (17)$$

$$T_n = \varepsilon_s^\nu \left(S_n^+ e^{ik\gamma_n h} + S_n^- \right) \quad (18a)$$

$$S_n^+ = \frac{1}{\varepsilon_s^\nu [1 + P_n \exp(2ik\gamma_n H)]} \sum_{m=-\infty}^{+\infty} \left(A_m^+ e^{ik\sigma_m h} + A_m^- \right) \bar{B}_{mn}; \quad S_n^- = P_n S_n^+ e^{ik\gamma_n H} \quad (19)$$

$$P_n = \frac{\gamma_n - \varepsilon_s^\nu \alpha_n}{\gamma_n + \varepsilon_s^\nu \alpha_n}$$

For the field of TE polarization $\nu = 0$ and $\bar{B}_{mn} = B_{mn}$, and for the field of TM polarization $\nu = 1$ and the value $\bar{B}_{mn}$ is determined by the expression

$$\bar{B}_{mn} = \sum_{l=-\infty}^{+\infty} G_{n-l} B_{ml}$$

In doing so, for the amplitudes of waves inside a grating $A_m^\pm$, one obtains the system of linear algebraic equations

$$\sum_{m=-\infty}^{+\infty} \left\{ (\alpha_n \bar{B}_{mn} + \sigma_m B_{mn}) A_m^+ + (\alpha_n \bar{B}_{mn} - \sigma_m B_{mn}) e^{ik\sigma_m h} A_m^- \right\} = 2\alpha_0 \delta_{0n} \quad (20a)$$

$$\sum_{m=-\infty}^{+\infty} \left\{ (V_n \bar{B}_{mn} - \sigma_m B_{mn}) e^{ik\sigma_m h} A_m^+ + (V_n \bar{B}_{mn} + \sigma_m B_{mn}) A_m^- \right\} = 0 \quad (20b)$$

where n runs over integer numbers from $-\infty$ to $+\infty$ in each of these two equations,

$$V_n = \frac{\gamma_n}{\varepsilon_s^\nu} \frac{1 - P_n \exp(2ik\gamma_n H)}{1 + P_n \exp(2ik\gamma_n H)}$$

In the absence of a substrate $V_n = \alpha_n$, and for the transmission coefficients, instead of Eq. (18a), we have

$$T_n = \sum_{m=-\infty}^{+\infty} \left(A_m^+ e^{ik\sigma_m h} + A_m^- \right) \bar{B}_{mn} \quad (18b)$$

The number of Equation (20), as the number of unknown mode amplitudes $A_m^\pm$, is infinite. However, we should note that for great diffraction orders n , the propagation parameters α_n in Eq. (13) and β_n in Eq. (10) become great in absolute value, which provides sufficiently great values of eigenvalues σ_m^2 of the matrix in the left hand side of Eq. (11). It causes noticeable decrease in the values of the mode amplitudes $A_m^\pm$ in a grating as solutions of Equation (20) and, correspondingly, decrease in the mode amplitudes in Eqs. (17), (18) outside of it. Besides, with the growth of the value n , the amplitudes of corresponding Fourier-components of a grating in Eqs. (6), (7) also decrease. The pointed circumstances lead to that, at the output of a grating, amplitudes of limited number of diffraction orders differ noticeably from zero, being in the order close to an incident wave.

One should also take into consideration that not all diffraction orders can propagate outside a grating. If the parameter of tangential propagation β_n of Eq. (10) in magnitude exceeds unity due to

great value of n , the parameter of normal propagation α_n in Eq. (13), which characterizes propagation of the given mode in the x axis (in air), becomes imaginary, and waves of this mode will decay exponentially. In this case, diffraction orders undergo total internal reflection on the boundaries of a grating. By analogy of modes of plane dielectric films [19], it would be natural to call such modes waveguide, or trapped ones, in contrast to radiation, or free modes of a grating, which generate freely propagating reflected and transmitted diffraction orders, visible in outer space. Strictly speaking, waveguide modes are also propagating, but only inside a grating in the direction, parallel to its boundaries. From here one can define the condition of a radiation (freely observed) diffraction order with positive or negative number n :

$$-1 < \beta_n = \beta_0 + n\lambda/\Lambda < +1 \quad (21)$$

Therefore, the stated problem can be reduced to consideration of finite number diffraction orders out of a grating (let their number be N) and inside that. It is expedient to take into account all observed diffraction orders, whose parameters of tangential propagation satisfy the condition (21), and still further two-three additional trapped orders in plus and minus of n . Then, we shall have matrices in Eq. (11) with dimension $N \times N$, $2N$ equations (20), N nonzero solutions for mode amplitudes A_m^+ and N for A_m^- , and so many nonzero amplitudes R_n and T_n for waves out of a grating.

In specific computations, the eigenvalue problem in Eq. (11), for a complex nonsymmetrical matrix with the dimension $N \times N$, has been solved using the iteration Jakobi method of rotations [20]. After that, eigenvectors have been determined in terms of solution of corresponding homogeneous systems of linear algebraic equations [20] by the method of separation of a column with minimal norm in matrix of a system (or two-three columns, depending on eigenvalue multiplicity). And for solving the system of equations (20) in grating mode amplitudes, we have used the standard Gaussian method [20].

3. COMPUTATION RESULTS FOR PLANE WAVE DIFFRACTION MODEL

For all specific cases of computation, we use the same model of a dielectric grating with the following parameters. The grating period $\Lambda = 1.6\lambda$, the length of its grooves $\Lambda - l = 0.5\lambda$, the grating thickness $h = 1.25\lambda$, the substrate thickness $H = 0$ (a grating without a substrate) or $H = 10^3\lambda$. At the first of these two cases, a grating of infinite dielectric bars is considered. For planar dielectric gratings, parameters of period and thickness are assumed the same as those for relief ones, and the value of modulation of real dielectric permittivity μ in Eq. (3) is taken to be $\mu = 0.1$ (a purely phase gratings). The refractive index of grating grooves of a substrate and averaged index of refraction for planar grating are assumed to be 1.6; absorption is not taken into account.

For the chosen value of a grating period $\lambda/\Lambda = 0.625$, according to the condition (21), our gratings can have the following number of radiation diffraction orders: three at $0 \leq \beta_0 < 0.25$, namely the -1 st order, zero order (an incident wave), and the $+1$ st order; four orders at $0.25 < \beta_0 < 0.375$ because of additional appearance of the -2 nd order in the region of propagation, and again three orders at $0.375 < \beta_0 < 1$ owing to the $+1$ st order transition to the group of evanescent waves. Diffraction orders with other numbers n will attenuate in air on the output of a grating and a substrate. A total number of diffraction orders under consideration is 9, with the numbers from $n = -4$ to $n = +4$ (here, as usual, zero order is assigned to an incident wave). For a given grating geometry, this number of orders is optimal: this is the minimal number, for which increase in number of orders no longer significantly changes the intensity distribution between them.

Figure 3 shows the computation results for two spatial electric field components of two various polarizations in space inside a grating and in the vicinity of that with the absence of a substrate, and Figs. 4 and 5 display the intensities (diffraction efficiencies) of various reflection and transmission diffraction orders on the boundaries $x = 0$ and $x = h$ of planar and relief gratings without a substrate, in relation to the parameter of tangential propagation of diffracting wave $\beta_0 = \sin \vartheta$, where ϑ is the angle of wave incidence on a grating. We did not bring computations to the case of grazing incidence of a wave on a grating, because at great values of incident angle ($\beta_0 \rightarrow 1$), the presented theory can produce false results: this case needs special investigation.

It is visible from Figs. 4 and 5 that the relationship between intensity of various diffraction orders and the parameter of propagation of incident wave β_0 demonstrates the presence of regions showing rather slow growth or decrease with the values less than unity. Such regions are typical for radiation

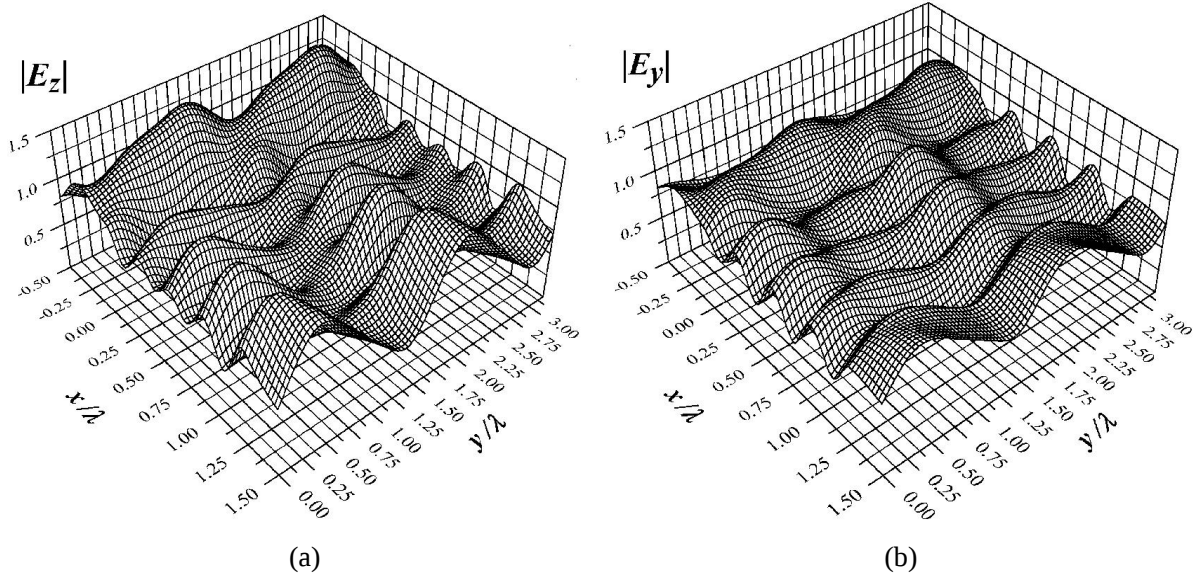


Figure 3. Spatial distribution pattern for the electric field amplitudes E_z and E_y of the TE and TM polarizations, respectively, in a planar sinusoidal grating without a substrate in the case of a plane diffracting wave.

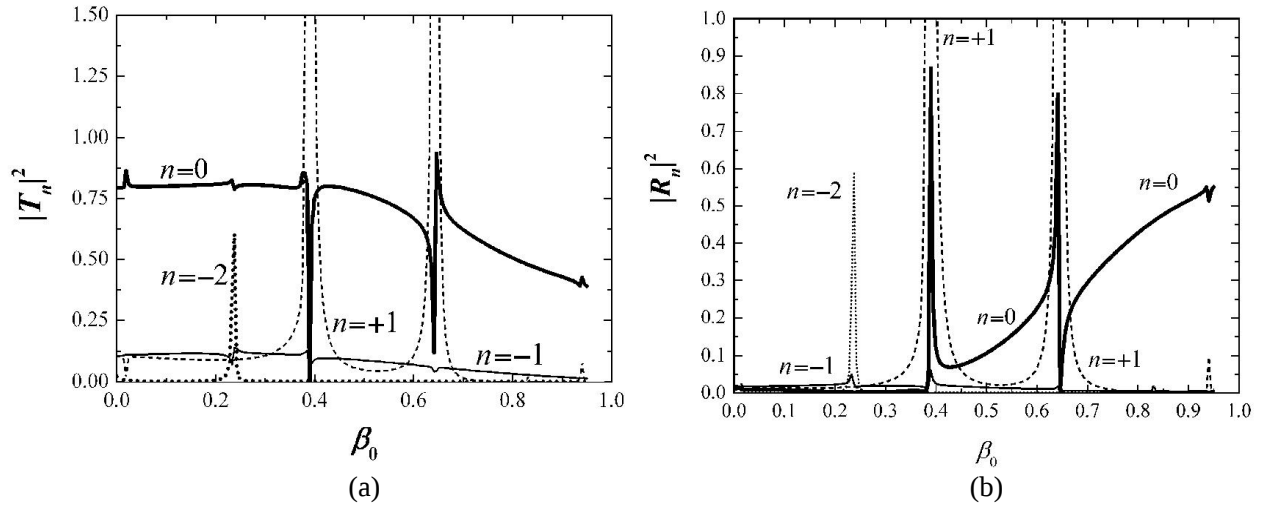


Figure 4. Intensities of the TE polarized (a) 4 transmitted $|T_n|^2$ and (b) 4 reflected $|R_n|^2$ radiation diffraction orders on the output of a planar sinusoidal grating without a substrate as functions of the parameter β_0 of incident wave tangential propagation.

diffraction orders, which satisfy the condition (21). However, when the boundary of these regions is reached with the change of β_0 for a certain n th order, i.e., when $\beta_n \rightarrow +1$ or $\beta_n \rightarrow -1$, the magnitude of intensity of the given order increases abruptly up to anomalously high values, and then it falls abruptly in magnitude again. In this case, the intensity of other diffraction orders also change very rapidly, although it remains less than unity for the propagating orders (for example, for the zero order). Thus, the transition of any diffraction order from propagation regime to waveguide one outside of a grating, or inversely, is accompanied by abrupt changes of intensity at once for all diffraction orders, and also by its anomalously high values for decaying orders. The values $\beta_0 = 0.25$ and $\beta_0 = 0.875$ can be examples of such transitions, when the -2 nd and -3 rd orders become propagating, or $\beta_0 = 0.375$, when the $+1$ st diffraction order turns into regime of attenuation. The similar phenomena, concerned with transitions

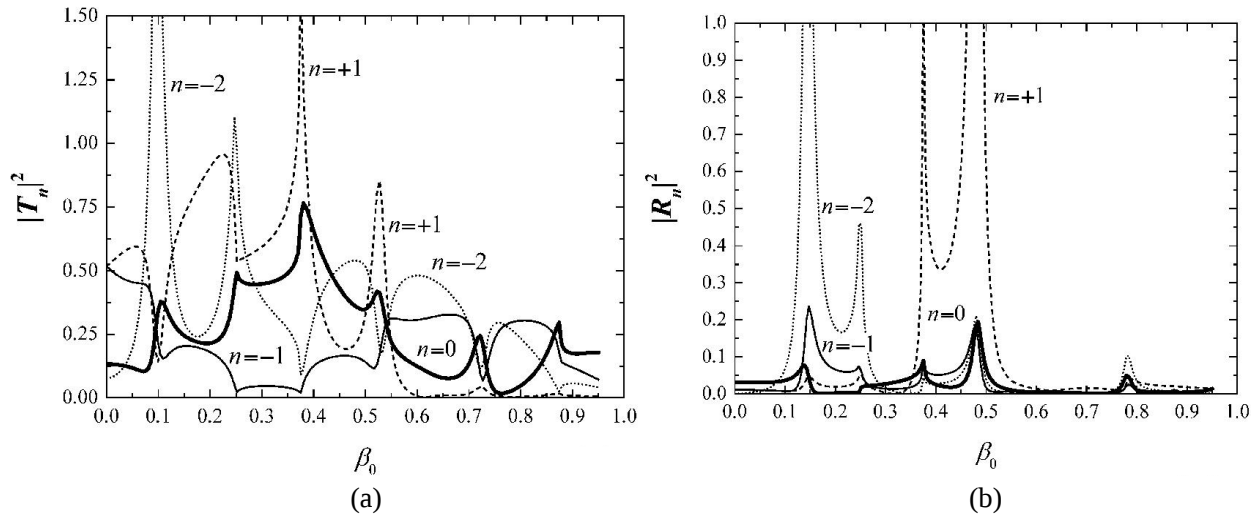


Figure 5. Intensities of the TE polarized (a) 4 transmitted $|T_n|^2$ and (b) 4 reflected $|R_n|^2$ radiation diffraction orders on the output of a rectangular relief grating without a substrate as functions of the parameter β_0 of incident wave tangential propagation.

of diffraction orders from one regime to the other, are called the Wood's anomalies [1, 3, 13].

Besides, note that coincidence of various eigenvalues of the matrix in Eq. (11) at $\beta_0 = 0.325$ and $\beta_0 = 0.625$, and satisfaction of the Bragg phase condition for the diffraction order $n = -2$ at the second value of β_0 , do not cause any great changes in intensities. Under this condition, we cannot consider the gratings with chosen parameters as thick and volume gratings.

4. GAUSSIAN BEAM DIFFRACTION BY DIELECTRIC GRATING WITHOUT A SUBSTRATE

The statement of diffraction problem for a Gaussian beam slightly differs from that for a plane wave. Suppose that a grating located in the region $0 \leq x \leq h$ is illuminated from negative x and y at the angle ϑ by a Gaussian beam, whose waist plane or the plane of minimal cross section is located at the distance L_0 from a grating (Fig. 6). Under these conditions, it is proposed to determine spatial field structure for every beam of various diffraction reflected and transmitted orders in the planes $x = -L$ and $x = h + H + L$ at the large distance L from a grating.

The method of diffraction Fourier-modes [7–9] allows us to pass naturally from the solution for one plane diffracting wave to the solution for a beam of electromagnetic waves. Transversely inhomogeneous beam field can be described by a Fourier integral, i.e., can be represented in the form of a superposition of a set of plane waves with continuously varying parameters of propagation. It provides the opportunity to use the one-wave solution to every plane-wave beam component and to sum all such solutions.

Let the field of the TE or TM polarization in the plane $x = 0$ be specified by means of the field function $u_0(y)$, then its propagation from the given plane to free space can be described, based on the field expansion in a Fourier integral:

$$u(x, y) = \int_{-\infty}^{+\infty} U(\beta) \exp(ik[\pm\alpha x + \beta y]) d\beta \quad (22)$$

where $U(\beta)$ is the Fourier transform of initial function, and the signs plus and minus are taken for the half-spaces $x > 0$ and $x < 0$, respectively,

$$\alpha = \sqrt{1 - \beta^2} \quad (23)$$

with nonnegative imaginary part. The exponential multiplier $\exp(\pm ik\alpha x)$ describes such propagation exactly, and the condition (23) provides the satisfaction of the wave Helmholtz Equation (2) for the

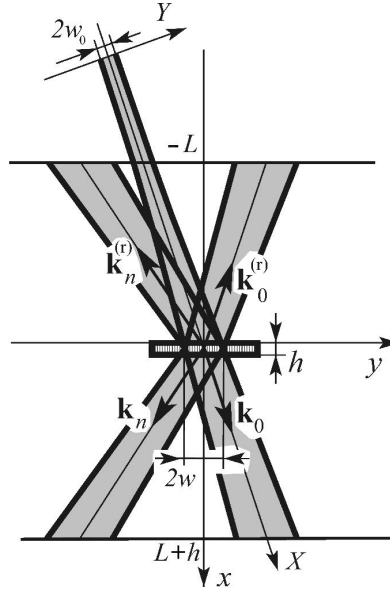


Figure 6. Diffraction of a Gaussian beam by a transmission dielectric grating. $\mathbf{k}_n$ is the wave vectors of n th diffraction order, determining its direction of propagation.

total field (22) as a whole and for every its plane-wave component separately. Expression (22) is mathematical appearance of the principal of superposition, which establishes that various components $\exp(ik[\pm\alpha x + \beta y])$ of the compound field (22) propagate in homogeneous linear medium independently of one another and conserve their starting amplitudes $U(\beta)$.

In order to use this method for description of radiation beams for various diffraction orders, one needs to relate their angular spectra at the output of a grating with spectrum of the initial Gaussian diffracting beam. If before inclined incidence on a grating, this beam covers the distance L_0 from the waist, then its Fourier-spectrum on the surface of a grating has the form [12, 19]:

$$U(\beta) = p\pi^{-1/2} \exp[-p^2(\beta - \beta_{b0})^2(1 + i\xi_0)] \quad (24)$$

where

$$p = kw/2 = p_0/\cos\vartheta \quad (25)$$

is the spectral parameter of a beam on the inclined boundary $x = 0$; $p_0 = kw_0/2$ is the same parameter; but on the beam cross-section plane, w_0 is the half-width of a beam in the most narrow place (in the waist, Fig. 6); β_{b0} is the parameter of tangential field propagation averaged over all plane-wave components, which determines the direction of propagation of a beam as a whole,

$$\xi_0 = L_0/(w_0 p_0) \quad (26)$$

is the parameter describing effects of Gaussian beam divergence under propagation on large distances [19].

The angular spectrum (24) uniquely determines the averaged parameter of tangential beam propagation of the value β_{b0} . It is natural to suppose that all remaining diffraction orders have similar angular spectra but with the corrections for various directions of propagation and various averaged parameters of tangential propagation, determined by analogy with Equation (10) for plane waves:

$$\beta_{bn} = \beta_{b0} + nK/k = \beta_{b0} + n\lambda/\Lambda \quad (27)$$

where the index n runs positive and negative integers. Hence, for the spectra of beams of various diffraction orders one can write by analogy of Eq. (24):

$$U_n(\beta) = p\pi^{-1/2} \exp[-p^2(\beta - \beta_{bn})^2(1 + i\xi_0)] \quad (28)$$

However, here the value of the spectral parameter p in Eq. (25) is the same for various diffraction orders, because all of them are caused by the same light spot of incident beam with the effective half-width w on the boundary $x = 0$ or $x = h + H$.

For every plane-wave component of every beam, the influences of the grating diffraction and also of the reflection with refraction on various interfaces are determined by the amplitude multipliers R_n in Eq. (17) or T_n in Eq. (18). Then, the principle of superposition provides the opportunity to write the fields of transmitted diffraction orders behind the grating in the form:

$$u_n^{(T)}(x, y) = \int_{-\infty}^{+\infty} T_n(\beta) U_n(\beta) \exp(ik[\alpha\bar{x} + \beta y]) d\beta \quad (29a)$$

($\bar{x} = x - h - H$), and to present the fields of reflected orders as follows:

$$u_n^{(R)}(x, y) = \int_{-\infty}^{+\infty} R_n(\beta) U_n(\beta) \exp(ik[-\alpha\bar{x} + \beta y]) d\beta \quad (29b)$$

($\bar{x} = x$), where the parameter of normal propagation of every plane-wave component of a beam α obeys Equation (23), and the spectra of beams of various diffraction orders are determined by Eq. (28).

It does not seem possible to calculate integrals (29) exactly, so we shall use the asymptotic method for their approximate calculation, which is based on the obvious assumption of a large width of the incident beam in comparison with the wavelength

$$w \gg \lambda, \quad \text{or} \quad p \gg 1 \quad (30)$$

Indeed, the length of light wave is less than a micron, but a laser beam diameter is usually a few mm. It means that the interval of integration in Eq. (29) is really very narrow, thanks to which the integrals in Eq. (29) are easily calculated asymptotically, if remaining integrands vary sufficiently slowly.

For the beam of every diffraction order (29), let express the function (23) in the form of a power series in argument β in the point $\beta = \beta_{bn}$, corresponding to the averaged value of parameter of tangential propagation of this beam:

$$\alpha \approx \alpha_{bn} - (\beta - \beta_{bn})(\beta_{bn}/\alpha_{bn}) - (\beta - \beta_{bn})^2/(2\alpha_{bn}^3) \quad (31)$$

where

$$\alpha_{bn} = \sqrt{1 - \beta_{bn}^2} \quad (32)$$

has meaning of the averaged parameter of normal beam propagation in the x coordinate (Fig. 6). It is obvious that the expansion in Eq. (31) is valid, when the given parameter is not too small, i.e., the propagation condition for the diffraction beam is not grazing in the grating output, and the value of β_{bn} is noticeably less than unity. And if the functions R_n in Eq. (17) and T_n in Eq. (18) does not substantially change in a small vicinity of the point $\beta = \beta_{bn}$, or

$$T_n(\beta) \approx T_n(\beta_{bn}), \quad R_n(\beta) \approx R_n(\beta_{bn}) \quad (33)$$

in the interval $\beta_{bn} - 2/p < \beta < \beta_{bn} + 2/p$, then the integrals (29) are reduced to calculation of the routine Fourier integral for a Gaussian beam [11]:

$$u_n^{(T)}(x, y) \approx \frac{T_n(\beta_{bn})}{\sqrt{1 + i\xi_n}} \exp \left\{ ik(\alpha_{bn}\bar{x} + \beta_{bn}y) - \frac{1}{1 + i\xi_n} \left(\frac{y}{w} - \frac{\bar{x}}{w} \frac{\beta_{bn}}{\alpha_{bn}} \right)^2 \right\} \quad (34a)$$

$$u_n^{(R)}(x, y) \approx \frac{R_n(\beta_{bn})}{\sqrt{1 + i\xi_n}} \exp \left\{ ik(-\alpha_{bn}\bar{x} + \beta_{bn}y) - \frac{1}{1 + i\xi_n} \left(\frac{y}{w} + \frac{\bar{x}}{w} \frac{\beta_{bn}}{\alpha_{bn}} \right)^2 \right\} \quad (34b)$$

where

$$\xi_n = (L_0 + |\bar{x}|/\alpha_{bn})/(w_0 p_0) \quad (35)$$

is the parameter of diffraction divergence in view of the distance L_0 , travelling before a grating, and of the distance $|\bar{x}|/\alpha_{bn}$, traversed after leaving it (geometrically, the real value α_{bn} equals cosine of the beam propagation angle), the linear combination of coordinates $\pm\alpha_{bn}\bar{x} + \beta_{bn}y$ determines a coordinate axis of reflected or transmitted beam propagation, and a straight line $y \mp \bar{x}\beta_{bn}/\alpha_{bn}$ is the axis, orthogonal to that and determining the direction of beam amplitude change in the transverse cross-section.

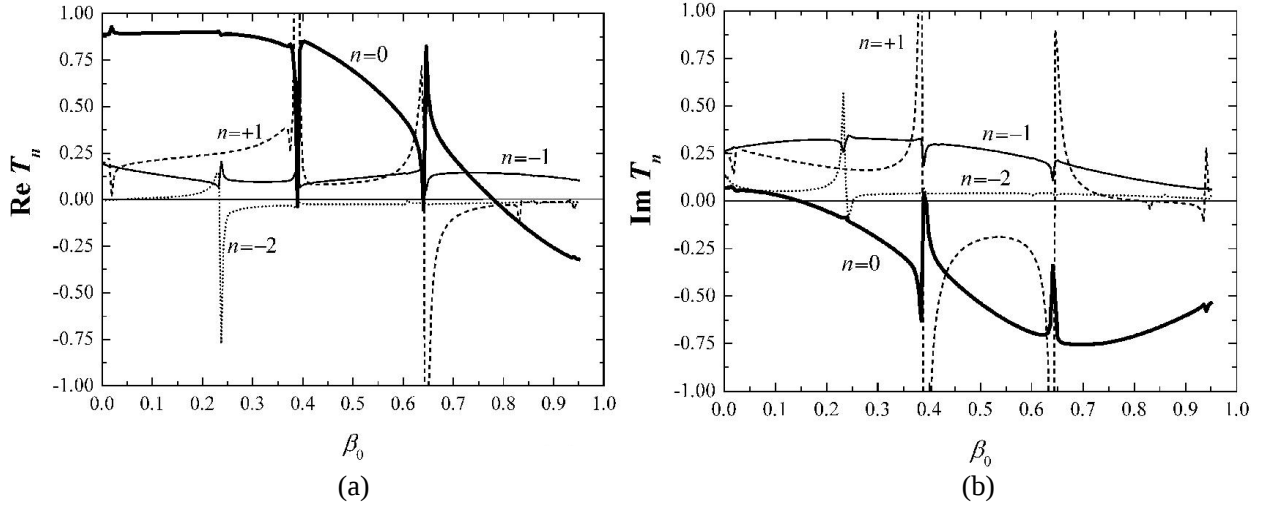


Figure 7. (a) Real and (b) imaginary parts of the complex amplitude transmission coefficient T_n of a planar sinusoidal grating for 4 diffraction orders as functions of the parameter β_0 of tangential propagation of the TE polarized plane incident wave.

Thus, in interval of slow change of the waves reflection and transition coefficients, depending on parameter of incident Gaussian beam propagation, all transmitted and reflected diffraction orders (34) also represent beams of inclined propagation with the proper Gaussian profile, whose amplitudes are determined by the complex amplitude coefficients of transmission T_n in Eq. (18) and reflection R_n in Eq. (17), computed for a plane diffracting wave. However, if integrands (the pointed coefficients) in the integrals (29) become very fast varying functions, as in several points on Figs. 4 and 5, then a similar approximation is inapplicable. Near such points, one should take into account possible variations in integrands under variations of argument of integration β . Here, the pattern of variations of the functions T_n and R_n (see Fig. 7) can be approximated by the inversely proportional dependence with a complex coefficient

$$z(x) = [1 + i(\xi + i\eta)x]^{-1} \quad (36)$$

i.e., with two real parameters ξ and η . But one of them, say, ξ , can be interpreted as scaling of the argument x ; by such a way, only one parameter η/ξ equal to the ratio of two initial parameters will influence on pattern of the function (36). Fig. 8 and its comparison with Fig. 7 show that the function (36) describes well the pattern of the functions R_n in Eq. (17) and T_n in Eq. (18) in the points of anomalous behavior. Then for the integrals (29) one can use the following representation

$$u_n^{(T,R)}(x, y) = \int_{-\infty}^{+\infty} \frac{U_n(\beta)}{D(\beta)} \exp(ik[\pm\alpha\bar{x} + \beta y]) d\beta \quad (37)$$

where $\bar{x} = x - h - H$ and the sign plus used for transmitted diffraction orders (T), but $\bar{x} = x$ and the sign minus correspond to reflected orders (R),

$$D(\beta) = [T_n(\beta)]^{-1} \quad \text{or} \quad D(\beta) = [R_n(\beta)]^{-1} \\ D(\beta) \approx D(\beta_{bn}) + D'(\beta_{bn})(\beta - \beta_{bn}) = \Gamma_n(\beta - \beta_{bn} - \sigma_n/p) \quad (38)$$

Here, prime denotes the derivative with respect to the argument β ,

$$\Gamma_n = D'(\beta_{bn}) \quad \sigma_n = -pD(\beta_{bn})[D'(\beta_{bn})]^{-1} \quad (39)$$

and the spectral parameter p for all diffraction orders is the same as for the incident beam (25).

For the parameter of normal propagation α in Eq. (23) of every plane-wave component of a beam, we shall use the previous expansion in Eq. (31) on the bases of the assumption that the condition of propagation for the given diffraction order is far from grazing. Then, after the substitution of variable

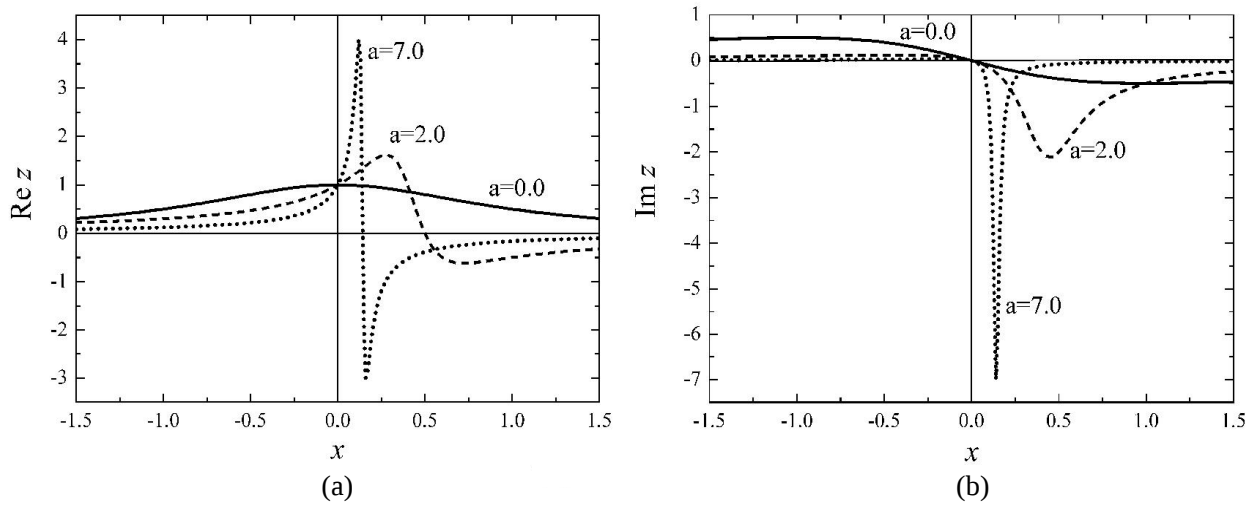


Figure 8. (a) Real and (b) imaginary parts of the inversely proportional function $z = [1 + i(1 + ia)x]^{-1}$ at various values of the parameter a .

of integration $\zeta = p(\beta - \beta_{bn})$, the integral expression (37) for the beam of n th diffraction order can be represented as follows:

$$u_n^{(T,R)}(x, y) \approx p\Gamma_n^{-1} \exp[ik(\pm\alpha_{bn}\bar{x} + \beta_{bn}y)]W(\rho_n, \sigma_n) \quad (40)$$

where the upper sign (plus) and lower one (minus) are related to transmitted and reflected diffraction orders, respectively,

$$W(\rho_n, \sigma_n) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \exp[-\zeta^2(1 + i\xi_n) + 2i\rho_n\zeta] \frac{d\zeta}{\zeta - \sigma_n} \quad (41)$$

$$\rho_n = \frac{k}{2p} \left(y \mp \bar{x} \frac{\beta_{bn}}{\alpha_{bn}} \right) = \frac{y}{w} \mp \frac{\bar{x}}{w} \frac{\beta_{bn}}{\alpha_{bn}} \quad (42)$$

As in expressions (34), the choice of the sign in Eq. (42) completely corresponds to the sign of the phase term in the index of exponent in Eq. (40) with the multiplier $\bar{x}$. The integral (41) plays an important part in the theory of Gaussian beam propagation through multilayer dielectric media [12], and therefore, we present the result of its calculation in a general form:

$$W(\rho_n, \sigma_n) = i\sqrt{\pi}\theta_n \exp\left(\bar{S}_n^2 - \frac{\bar{\rho}_n^2}{1 + i\xi_n}\right) [1 - \operatorname{erf}(\bar{S}_n)] \quad (43a)$$

where erf is the error function [21],

$$\bar{S}_n = \bar{Q}_n \sqrt{1 + i\xi_n} - \frac{\bar{\rho}_n}{\sqrt{1 + i\xi_n}}; \quad Q_n = -i\sigma_n = ip \frac{D(\beta_{bn})}{D'(\beta_{bn})}; \quad \Gamma_n = D'(\beta_{bn}) \quad (43b)$$

$$\bar{Q}_n = Q_n; \quad \bar{\rho}_n = \rho_n; \quad \theta_n = +1 \quad \text{at} \quad \operatorname{Re} Q_n \geq 0 \quad (43c)$$

$$\bar{Q}_n = -Q_n; \quad \bar{\rho}_n = -\rho_n; \quad \theta_n = -1 \quad \text{at} \quad \operatorname{Re} Q_n < 0 \quad (43d)$$

ξ_n is the parameter of diffraction divergence of the field (35).

Thus, the approximate expressions (40), (43) for computation of the fields of various diffraction orders provide the opportunity to take into consideration inhomogeneity of the amplitude coefficients of wave transformation (reflection and transmission) over the spectrum of every order. Here, as approximate values for constant parameters Q_n in Eq. (43b), one can use their values in the beam centers $\beta = \beta_{bn}$, and the derivatives $D'(\beta_{bn})$ can be calculated using the differences of values $D(\beta)$ in the symmetric points of a beam spectrum $\beta = \beta_{bn} + 1/p$ and $\beta = \beta_{bn} - 1/p$.

Behavior of the solution, described by the analytical expressions (40) and (43), essentially depends on the value Q_n (43b). If it is great in magnitude, which is provided by a small value of the derivative

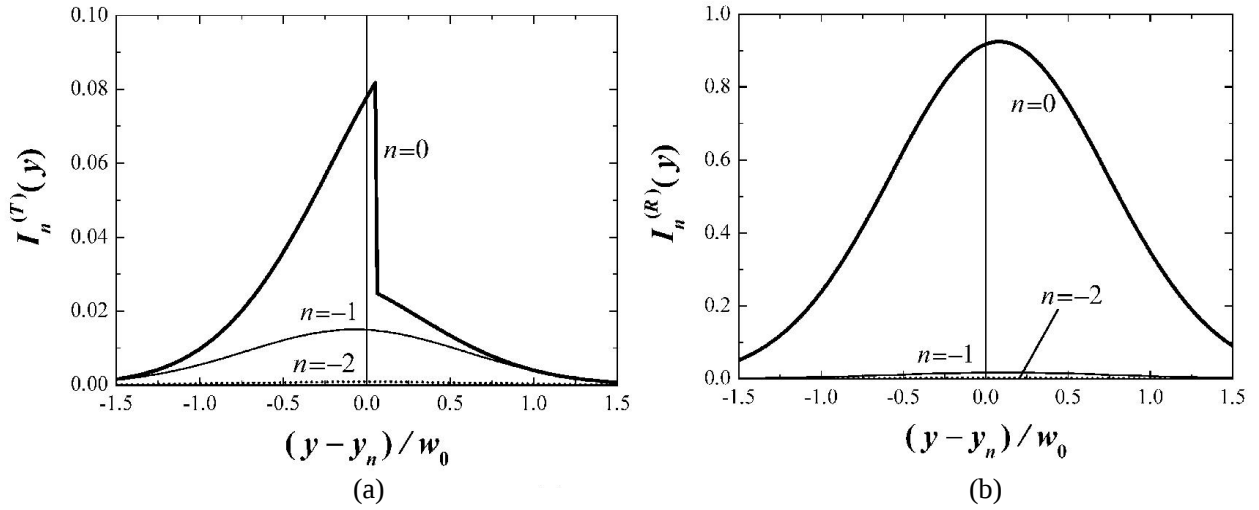


Figure 9. Transverse intensity structure of (a) transmitted $I_n^{(T)}(y)$ and (b) reflected $I_n^{(R)}(y)$ beams of various diffraction orders in the planes $x = h + L$ and $x = -L$, respectively, computed relative to the middle of every beam y_n at the diffraction of the TE polarized beam with the parameter of tangential propagation $\beta_0 = 0.64275$ by a planar sinusoidal grating without a substrate.

Γ_n over a spectrum of a Gaussian beam, this function permits a simple asymptotic expansion [12], whose substitution into Eq. (40) yields the Gaussian function (34). However, if the derivative over the spectrum is sufficiently great, then the value Q_n becomes small in magnitude, and in this case expressions (40), (43) can describe spatial field structure, which differs from that of the initial Gaussian beam. For example, Figs. 9 and 10 display the results of computation of transverse cross-structure (40), (43) for various diffraction orders. In these figures, the value $I_n^{(T,R)}$ denotes the squared absolute value of the field function $u_n^{(T,R)}$ (40), which has a sense of relative local beam energy density. For convenience, the graphs of transverse cross-structure for various beams are displayed with reference to one beam center, although in fact the beams centers y_n in the detection plane $x = h + L$ or $x = -L$ are spatially separated on the large distances:

$$y_{-2}/w_0 = -76.43; \quad y_{-1}/w_0 = 1.775; \quad y_0/w_0 = 83.90$$

It is supposed that the distance from the waist to a grating $L_0 = 10$ cm, from that to the plane of detection $L = 5$ cm $= 100w_0$, and the wavelength $\lambda = 500$ nm. However, here the effect of beams diffraction divergence specified by parameters ξ_n (35) does not appear practical, because the magnitude of distances L_0 and L of beams propagation is insufficient for this. The graphs of Figs. 9 and 10 depict intensities of radiation beams, and the fields undergoing total internal reflection on the grating boundaries are not shown. For them, expression (43) yields false results, because this expression is based on the approximate representation in Eq. (31) of the parameter of normal propagation for plane-wave beam components, and such representation is inoperable in the cases of grazing propagation and of total internal reflection with very small $|\alpha_{bn}|$. The structure of diffraction fields, being under these conditions, requires special consideration.

While certain diffraction orders undergo transition from radiation regime to waveguide conditions of diffraction (or inversely) with great abrupt change of intensity, remaining radiation orders also show abrupt variations of intensity (Fig. 9(a)), but not so great, and these variations take place not uniformly over all beam front, but locally with wide crevasses and outliers in separated regions of cross-section.

So, the transverse structure of diffraction beams on the output of a dielectric grating without a substrate reproduces largely the structure of an incident beam or looks much like that. But in those anomalous cases, when the transverse profile of propagating beam differs noticeably from a Gaussian one, its effective width remains the same as for the incident field.

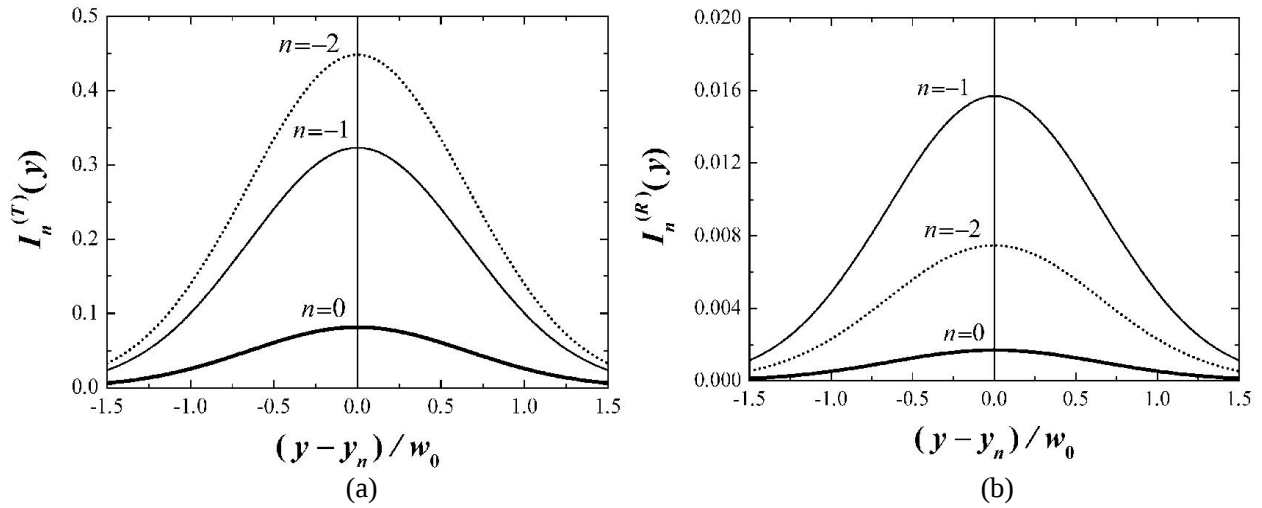


Figure 10. Transverse intensity structure of (a) transmitted $I_n^{(T)}(y)$ and (b) reflected $I_n^{(R)}(y)$ beams of various diffraction orders in the planes $x = h + L$ and $x = -L$, respectively, computed relative to the middle of every beam y_n at the diffraction of the TE polarized beam with the parameter of tangential propagation $\beta_0 = 0.64275$ by a rectangular relief grating without a substrate.

5. DIFFRACTION OF BEAMS BY DIELECTRIC GRATINGS ON A SUBSTRATE

Up to this point we have considered the results of computations for dielectric gratings without a substrate. However, it is a rare case, because a thin optical diffraction grating, for reliability, is produced usually on a thick dielectric substrate, and if we study properties of transmission gratings, then the influence of a thick substrate on passing diffraction orders should be taken into consideration.

In the above presented theoretical model, the possibility of investigation of diffraction by a grating with a thick dielectric substrate has already been provided. In Figs. 11 and 12, we display the dependences of intensities of two radiation diffraction orders on the parameter of tangential propagation for a plane incident wave, and for the same parameters of a planar and relief grating as previously, but

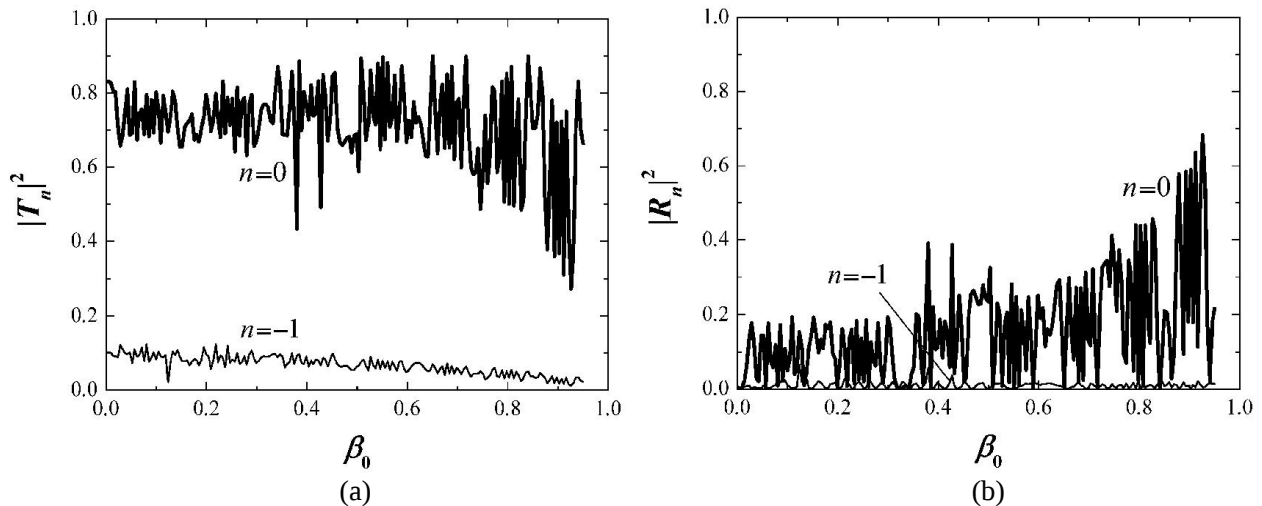


Figure 11. Intensities of the TE polarized (a) two transmitted $|T_n|^2$ and (b) two reflected $|R_n|^2$ radiation diffraction orders on the output of a planar sinusoidal grating located on a substrate of the thickness $10^3\lambda$, in dependence of the parameter β_0 of incident plane wave tangential propagation.

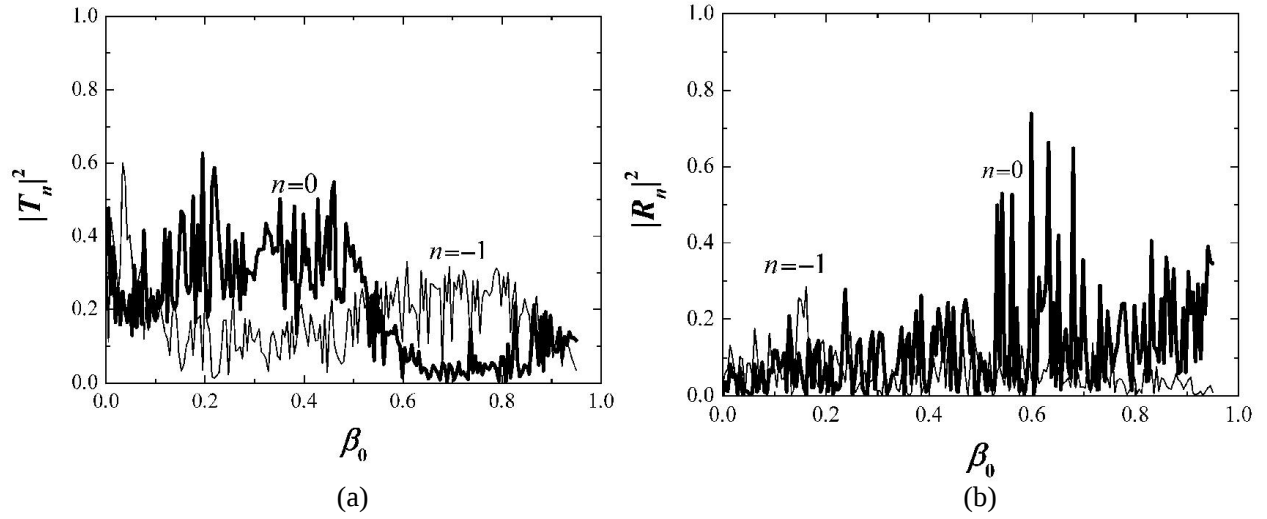


Figure 12. Intensities of the TE polarized (a) two transmitted $|T_n|^2$ and (b) two reflected $|R_n|^2$ radiation diffraction orders on the output of a rectangular relief grating located on a substrate of the thickness $10^3\lambda$, in dependence of the parameter β_0 of incident plane wave tangential propagation.

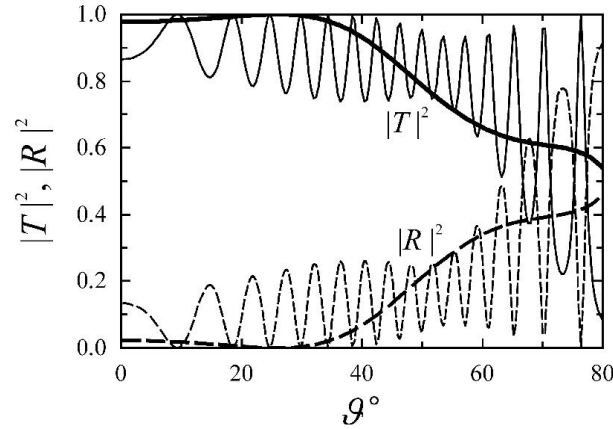


Figure 13. Intensities of transmitted (solid lines) and reflected (dashed curves) waves at the incidence of the TE polarized plane wave on a thin dielectric layer without (thick lines) and with (thin curves) a substrate of the thickness 20λ . The thickness of a layer $h = 1.2\lambda$, its real dielectric permittivity $\varepsilon = 1.75$, permittivity of a substrate $\varepsilon_s = 2.5$.

placed on a substrate of the thickness $10^3\lambda$ with the same refractive index 1.6, as for the grating material. Here, the appearance of very fast oscillations of intensity under varying value of the angle of incidence stands out. This is the effect of additional reflection of radiation on the substrate boundaries. It is illustrated well by Fig. 13, where the intensities of reflected and transmitted waves are shown for a thin dielectric layer without a substrate and on that. For obviousness, the thickness of a substrate here is assumed to be only 20λ , because for large substrate thickness the swing and frequency of oscillations rapidly increase.

The presence of strong oscillations of the reflection and transmission coefficients for waves near grating leads to disappearance of the regions where these coefficients vary slowly under change of the angle of incidence (the parameter of propagation) of diffracting wave, and consequently at any angles of incidence, the given coefficients demonstrate their noticeable inhomogeneity over the spectrum even for a Gaussian beam with very narrow spectrum of spatial frequencies. By this reason, the initial Gaussian

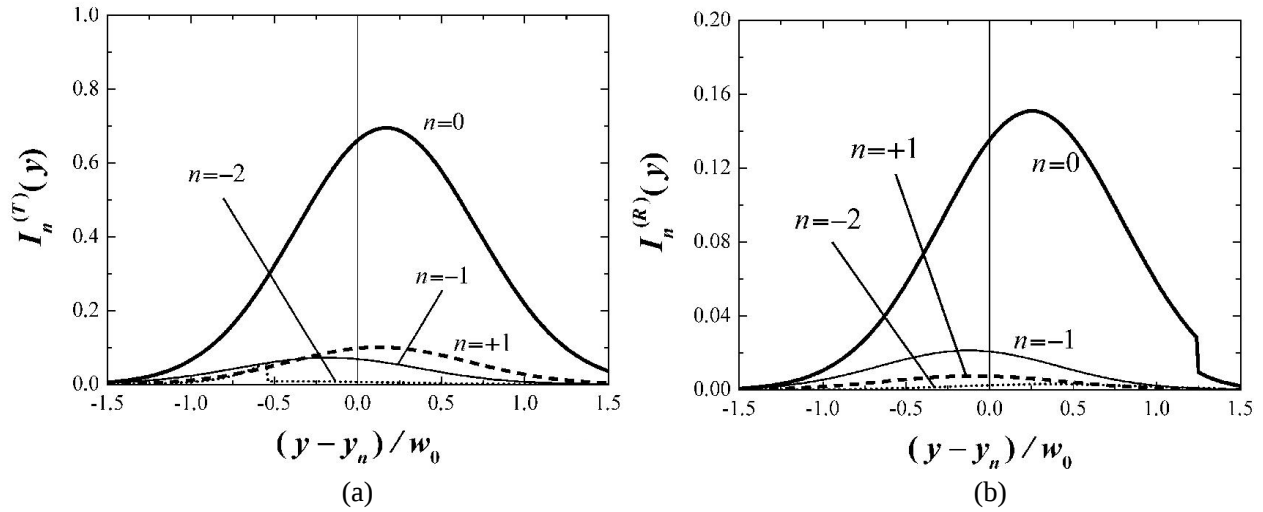


Figure 14. Transverse intensity structure of (a) transmitted $I_n^{(T)}(y)$ and (b) reflected $I_n^{(R)}(y)$ beams of various diffraction orders in the planes $x = h + H + L$ and $x = -L$, respectively, computed relative to the middle of every beam y_n at the diffraction of the TE polarized beam with the parameter of tangential propagation $\beta_0 = 0.320$ by a planar sinusoidal grating located on a substrate with the thickness $10^3\lambda$.

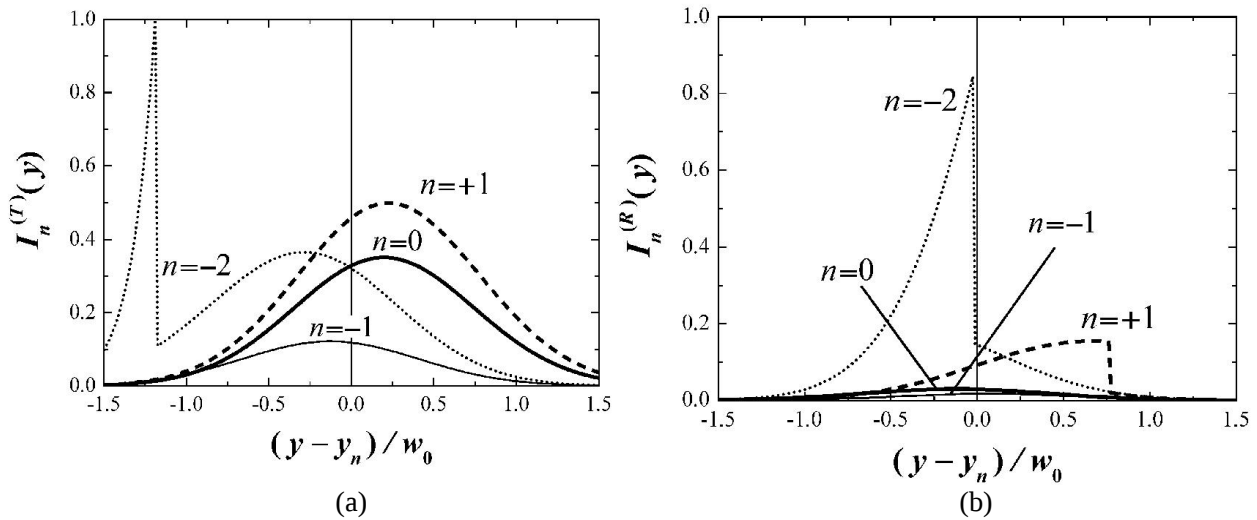


Figure 15. Transverse intensity structure of (a) transmitted $I_n^{(T)}(y)$ and (b) reflected $I_n^{(R)}(y)$ beams of various diffraction orders in the planes $x = h + H + L$ and $x = -L$, respectively, computed relative to the middle of every beam y_n at the diffraction of the TE polarized beam with the parameter of tangential propagation $\beta_0 = 0.320$ by a rectangular relief grating located on a substrate with the thickness $10^3\lambda$.

profile of diffraction beam cross-section will be not reproduced by reflection and transmission diffraction orders, including the zero order in itself corresponding to an incident field. Displaying the transverse spatial structure of various radiation diffraction orders for a grating with a substrate, computed by Equations (40), (43), is clear from Figs. 14, 15. It is visible that distortions of the shape of the Gaussian profile of an initial beam are available everywhere.

Strictly speaking, in addition to waveguide modes of a grating, taking into account by the present theory, waveguide modes of a substrate can also exist, whose field propagates along the normal in a grating and in a substrate, but undergoes total internal reflection on the lower boundary of a substrate with air. There is a special technique for solving diffraction problems with the participation of waveguide

modes in a plane dielectric layer [22], which is reduced to the regularization of integral expressions for the fields inside a layer. However, the amplitudes of such modes are negligibly small because of large thickness of a dielectric layer (a substrate), in which they are excited. It is known [19] that increase of the thickness of a guiding dielectric layer produces fast increase of the number of its waveguide modes owing to the decrease of spectral distance between modes, and causes decrease in their intensity. Besides, the energy of waveguide mode of a substrate is not concentrated near a thin layer, as in the case of thin waveguide films and does not propagate in the form of a narrow beam, as fields of radiation modes, but spreads over all thickness of a substrate. Moreover, it propagates as a whole parallel to the surface of a layer. It follows that waveguide modes in thick substrates can be safely ignored.

6. CONCLUSION

We have considered an advanced mode theory of plane electromagnetic wave diffraction by a dielectric grating, and on its basis we have constructed a diffraction model for a more complex light field structure, represented as a superposition of plane waves with close spatial-frequency characteristics, such as Gaussian beams. At the same time, it turned out that the transfer to inhomogeneous fields of bounded cross-section allows for natural interpretation of many anomalous effects inherent in a plane-wave approximation, which display as abrupt changes of amplitude of various diffraction orders at the angles of diffracting field incidence corresponding to transfers from propagation regime to regime of total internal reflection, and inversely. It was found that such amplitude changes produce distortions of spatial beam shape for radiation diffraction orders on the output of a grating. Our model gives an expression that provides the computation of a spatial structure of such radiation diffraction beams and estimation of their distortions in comparison with the spatial shape of diffracting beam. For the Gaussian structure, these distortions display as violation of symmetry, displacement of an intensity maximum from the middle of a beam, and also as appearance of separated narrow peaks of amplitude. For a grating without a substrate, such distortions of the shape of spatial structure occur very seldom, for special values of the angle of diffracting beam incidence, but for a transmitting grating on a thick dielectric substrate, the distortions of spatial shape of diffraction beams turn out occurring everywhere because of strong oscillations of field amplitudes at reflections on the boundaries of a substrate. Here, for completeness we would present an additional equation describing the amplitudes of diffraction orders, undergoing total internal reflection on the boundaries of a grating, or being very close to this condition, but the derivation of such an equation and its discussion need special consideration.

ACKNOWLEDGMENT

This work is supported by the State Program of Scientific Research of the Republic of Belarus “Convergence-2025”.

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