

Diffraction analysis by periodic structures using a method of coupled waves

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The coupled-wave method (CWM) has been used to analyse diffraction on some periodic structures, i.e., on relief gratings including metallized ones having sinusoidal relief as well as on one-dimensional and two-dimensional photonic crystals. Exact boundary conditions were taken into account in numerical calculations. Grating polarizers have been analysed, properties of dielectric gratings wherein coupled-mode resonance occurs have been studied, diffraction efficiency has been calculated for sinusoidal relief metallized gratings. Calculations were carried out for TE and TM polarizations. Band structure of a two-dimensional photonic crystal has been calculated using CWM.

Keywords: grating, diffraction, coupled-wave resonance, photonic crystal.

1. Introduction

There is a great number of papers and monographs devoted to the study of light propagation in periodic structures (volume gratings, interference mirrors, photonic crystals, thin holograms, relief gratings including relief gratings on metal). Among them there are two monographs that can be mentioned here, one concerning volume gratings [1] and the other concerning photonic crystals [2]. The monograph [1] summarized the results of theoretical and experimental studies of volume gratings by means of approximation methods and the main attention has been focused on TE-polarization wave diffraction. Kogelnik's paper [3] that dealt with all types of volume holograms and yielded good results, when the modulation factor of dielectric constant of a periodic medium is much less than one ($\ll 1$), was the most characteristic and popular work of that time. However, approximation methods are not suitable to analyse periodic structures having significant modulation factors of dielectric constant. Therefore accurate systems of equations were obtained and accurate initial conditions were defined using the Bloch-Floquets theorem based on Maxwell's equations [4]. One can deem that the exact theory of diffraction on volume gratings [5], interference mirrors [6], and relief gratings [7,8] has received completion in the works by Moharam and Gaylord. These works have not received wide publicity since the solution of the system of differential equations can be only obtained using powerful computers which were not available to the wide community of scientists and engineers in the 1980s. In general, those calculation methods were called the coupled-wave methods (CWM). An interest in exact solutions of diffraction problems

by means of numerical methods appeared in the 1990s when high-speed PCs became reality. The modal method by Fourier expansion and the modal method by modal expansion were developed [9]. In these methods, an infinite dimensional system of linear differential equations with constant or variable coefficients can be obtained on the basis of Maxwell's equations and the difference between them is due to exact boundary conditions being taken into account using different techniques. Therefore, these methods are considered to be identical and are called depending on the author of a paper either CWM [10] or the Fourier expansion methods [11]. In Refs. 12 and 13, the systems of first-order linear differential equations are formulated that are identical to the equations given in Ref. 11 but which are obtained by a way of variable amplitude plane wave expansion of the electromagnetic field. The Bloch-Floquets theorem is not used to obtain these equations and, therefore, we believe that this method is more universal and can be used in other problems. The initial conditions are used in a different way and we suppose that this approach is simpler and clearer than the approaches of other authors [10,14–17]. Whereas there are no particular problems when studying diffraction of TM-polarized light on periodic structures using CWM (even for the case of metallized gratings), it is necessary to take into account a great number of diffraction orders because of slow convergence in order to make an exact calculation. In order to improve convergence (in order to get the desired calculation accuracy one should use a system of differential equations of the least possible dimension) for TM-polarized waves a little modified system of equations was proposed in Refs. 15, 16, 17, and 18, which has been obtained using Fourier expansion of permittivity and its reciprocal. A strict mathematical substantiation for such modification of the system of equations for TM-polarized light diffraction is

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given in Ref. 11. A special attention should be given to Ref. 18 where the system of differential equations was obtained which provides rapid convergence of solution for relief gratings including the metallized ones for the case of TM-polarization. The C-method or coordinate transformation method was proposed to accelerate the analysis of TM-polarized light diffraction for metallized relief gratings (e.g., with a sinusoidal profile) [19,20]. All those methods are based on numerical solution of the system of differential equations that can take into account hundreds of diffraction orders. It is possible to say that at the moment there are efficient methods to analyse diffraction of light on various periodic structures, and these methods are used to design various optical devices such as polarizers with periodic arrangement of metallic bands [21], narrow-band optical filters on the basis of coupled mode resonance [22–26], and diffraction relief gratings [27]. Analysis of diffraction gratings using CWM foresees that the periodic structure is boundless in two directions, and in the third direction it is bounded by two parallel planes, the media beyond the grating are homogeneous, and the boundary conditions are defined from the continuity of the tangential components of the strength of electric and magnetic fields on the planes that bound the grating. For analysis of photonic crystals it is foreseen that they are extended to infinity in three dimensions and permittivity may depend periodically from one, two and three variables (one-dimensional, two-dimensional or three-dimensional photonic crystals, respectively) [2]. In this case, a traditional analysis consists in solving of wave equation relative to the magnetic field strength, the solution is reduced to eigenvalues, and, for instance, a matrix equation with dimensions of more than 1000×1000 is used to analyse a three-dimensional photonic crystal [28,29]. After finding a solution, the frequencies of electromagnetic waves that can propagate in a photonic crystal with the given value of the wave vector are defined. It is obvious that high-speed computers are needed to solve such problems. But even in this case the calculation accuracy is low. On the other hand, when the coupled wave equations [11–13] is carefully examined, one can conclude that these equations can also describe the propagation of allowed electromagnetic waves in a boundless photonic crystal with periodic initial conditions.

Thus, the purpose of this work is as follows: to formulate the initial conditions for solving the diffraction problems and to show the efficiency of analysing various types of diffraction gratings using our method [12,13], to find methods of rapid search for submatrices of fundamental solution matrix using spatial symmetry of the diffraction problem, to show that it is possible to calculate the band structure of one-dimensional and two-dimensional photonic crystals using the CWM, and to for analysis of one-dimensional photonic crystals it is sufficient to solve a system of two first-order differential equations (exact solution), and for two-dimensional photonic crystals it is necessary to solve a truncated system consisting of the 2*n* first-order differential equations that is equivalent to a system of *n*² in the traditional method [2].

2. A system of differential equations for a diffraction grating. Initial conditions

A generalized diffraction grating is shown in Fig. 1. The grating has the thickness *d* in the direction of *z*-axis and is boundless in the *xoy* plane; its permittivity varies periodically along the *x*-axis with period Λ and can be also dependent on *z* (e.g., for a sinusoidal relief grating). The first medium that fills the whole space above grating (*z* < 0) has permittivity ϵ_1 , it is real and more than zero, the second medium (grating) has dielectric constant $\epsilon_2(x, z)$ and can be a complex quantity, and the third medium (*z* > 0) is characterized with the constant ϵ_3 .

In the first medium, in *xoz* plane, a plane wave falls onto the grating at the angle θ_{10} to *z*-axis. As a result of light diffraction in the grating, secondary plane waves with the amplitudes *R_n* (reflection amplitudes) propagate in the first medium, and waves with the amplitudes *T_n* (transmission amplitudes) propagate in the third medium. The initial equations [30] in the partial derivatives which are used to obtain common linear systems of differential equations [31] that describe diffraction on periodic structures are as follows

$$\text{rot } \mathbf{E} = -j \frac{\omega}{c} \mathbf{H} \tag{1}$$

$$\text{rot } \mathbf{H} = -j \epsilon_2(x, z) \frac{\omega}{c} \mathbf{E}$$

where **E**, **H** are the electric and magnetic vectors of electromagnetic field, respectively, *c* is the velocity of light in a vacuum, $\omega = k_0 c$ is the cyclic frequency, $k_0 = 2\pi/\lambda$, and λ is the wavelength in a vacuum.

Besides, the permittivity of the second medium and its reciprocal are expanded into complex Fourier series with the following coefficients

$$\epsilon_p(z) = \frac{1}{\Lambda} \int_0^\Lambda \epsilon_2(x, z) \exp\left(-i \frac{2\pi}{\Lambda} px\right) dx, \tag{2}$$

$$a_p(z) = \frac{1}{\Lambda} \int_0^\Lambda \frac{1}{\epsilon_2(x, z)} \exp\left(-i \frac{2\pi}{\Lambda} px\right) dx. \tag{3}$$

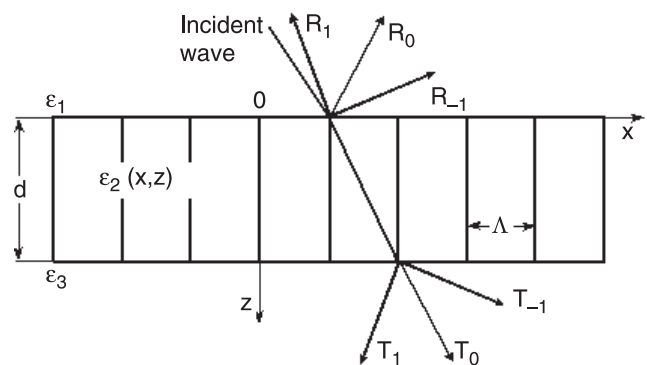


Fig. 1. A generalized diffraction grating $\epsilon(x, z) = \epsilon(x + \Lambda, z)$.

2.1. Equations and initial conditions for TE-polarization

It is expedient to expand the electric and magnetic fields as follows [12]

$$\begin{aligned} \mathbf{E}(x, z) &= \mathbf{e}_y \sum_n G_n(z) \exp(-jk_{nx}x) \\ \mathbf{H}(x, z) &= \sum_n [-\mathbf{e}_x F_{nx}(z) + \mathbf{e}_z F_{nz}(z)] \exp(-jk_{nx}x) \end{aligned} \quad (4)$$

where $\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$ are the unit vectors along $x, y,$ and z are the axes, respectively, $G_n(z)$ is the electric field of a coupled wave having index $n, F_{nx}(z), F_{nz}(z)$ are the x and z components of the magnetic field of a coupled wave having the index $n.$

The wave vector k_{nx} is related to the wave vector k_{0x} as follows

$$k_{nx} = k_{0x} - n \frac{2\pi}{\Lambda}, \quad (5)$$

where $k_{0x} = (2\pi\sqrt{\epsilon_1}/\lambda) \sin \theta_{10}$ and n is the integer.

Substituting Eq. (4) into Eq. (1), taking into account Eqs. (2) and (5), and equalizing coefficients before each factor $\exp\left(jn \frac{2\pi}{\Lambda} x\right)$ to zero we obtain the following system of differential equations

$$\begin{aligned} \dot{G}_n(z) &= -jk_0 F_n(z), \\ \dot{F}_n(z) &= j \frac{k_{nx}^2}{k_0} G_n(z) - jk_0 \sum_p \|\epsilon_2\|_{np}(z) G_p(z). \end{aligned} \quad (6)$$

Since the system of Eq. (6) contains the first derivatives G_n and F_{nx} and a simple algebraic relationship exists between G_n and $F_{nz}(k_{nx}G_n = k_0F_{nz}),$ we can exclude F_{nz} from the system of equations and omit the lower index x in $F_{nx}.$ In a general case, n varies from $-\infty$ to $+\infty.$ In a certain case of calculations, we must restrict ourselves to a finite dimensional system, i.e., we must take into account N diffraction orders, and as result we shall have system Eq. (6) of $2N$ equations. The number of diffraction orders determines the calculation accuracy.

The system of differential equations, Eq. (6), can be written as a matrix

$$\begin{pmatrix} \dot{\mathbf{G}} \\ \dot{\mathbf{F}} \end{pmatrix} = \begin{pmatrix} \mathbf{0} & \mathbf{B}_1 \\ \mathbf{B}_2 & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{G} \\ \mathbf{F} \end{pmatrix}, \quad (7)$$

where $\mathbf{B}_1 = -jk_0 \mathbf{I}, \mathbf{B}_2 = j \frac{1}{k_0} \|k\|_n^2 - jk_0 \|\epsilon_2\|_{np}, \mathbf{I}$ is the unit matrix, $\|k\|_n^2$ is the diagonal matrix whose elements are equal to $k_{nx}^2. \|\epsilon_2\|_{np}$ is the Toeplitz matrix formed from Fourier expansion coefficients $\epsilon_n(z)$ in conformity with the rule

$$\|\epsilon_2\|_{np} = \begin{pmatrix} \epsilon_0(z) & \epsilon_1(z) & \dots & \epsilon_N(z) \\ \epsilon_{-1}(z) & \epsilon_0(z) & \dots & \epsilon_{N-1}(z) \\ \dots & \dots & \dots & \dots \\ \epsilon_{-N}(z) & \epsilon_{-N+1}(z) & \dots & \epsilon_0(z) \end{pmatrix}.$$

It should be noted here that matrices \mathbf{B}_1 and \mathbf{B}_2 are connected one with other.

In accordance with Ref. 31, the solution of the system of Eq. (7), may be represented as

$$\begin{pmatrix} \mathbf{G}(z) \\ \mathbf{F}(z) \end{pmatrix} = A \begin{pmatrix} \mathbf{G}(0) \\ \mathbf{F}(0) \end{pmatrix} = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{G}(0) \\ \mathbf{F}(0) \end{pmatrix}, \quad (8)$$

where the matrix \mathbf{A} is the solution of a corresponding matrix Eq. (7) in the interval $[0, z]$ for initial unit matrix in the point $z = 0.$ Since the matrix trace in Eq. (7) is zero, $\det(\mathbf{A}) = 1$ accordingly to Ref. 31. This result may be used efficiently to monitor the accuracy of calculation. If the dielectric constant of periodic medium does not depend on $z,$ the following relation is valid

$$A(z) = \exp \left[\begin{pmatrix} 0 & \mathbf{B}_1 \\ \mathbf{B}_2 & 0 \end{pmatrix} z \right] = \exp(\mathbf{B}z). \quad (9)$$

Thus, accordingly to Eq. (8) we may write the following matrix equations

$$\begin{aligned} \mathbf{G}(d) &= \mathbf{A}_{11} \mathbf{G}(0) + \mathbf{A}_{12} \mathbf{F}(0), \\ \mathbf{F}(d) &= \mathbf{A}_{21} \mathbf{G}(0) + \mathbf{A}_{22} \mathbf{F}(0) \end{aligned} \quad (10)$$

Completing algebraic system of Eq. (10) with a supplementary system of equations that follow from the equality of the tangential components of the electric and magnetic field at the boundaries ($z = 0$ i $z = d$) of the periodic and homogeneous media, we may uniquely calculate R_n and $T_n.$ The wave amplitudes R_n and T_n of corresponding diffraction orders, which propagate into the first and third media, we will regulate and write in the vectorial form \mathbf{R} and $\mathbf{T}.$ The algebraic systems of equations that arise from the conditions at the boundaries are in vector form as follows [13]

$$\begin{aligned} \mathbf{R} - \mathbf{G}(0) &= -\mathbf{V} \\ \mathbf{C}_1 \mathbf{R} - \mathbf{F}(0) &= -\mathbf{C}_1 \mathbf{V} \\ \mathbf{T} - \mathbf{G}(d) &= 0 \\ \mathbf{C}_3 \mathbf{T} - \mathbf{F}(d) &= 0 \end{aligned} \quad (11)$$

where \mathbf{V} is the column vector whose components are equal to $V_n = \delta_{0n},$ i.e., to Kroneckers symbol when one index is zero, \mathbf{C}_1 and \mathbf{C}_3 are the diagonal matrices whose elements are equal to $C_{1n} = \sqrt{\epsilon_1} \cos \theta_{1n}$ and $C_{3n} = \sqrt{\epsilon_3} \cos \theta_{3n},$ respectively.

Cosines of propagation angles of diffracted wave in the first and the third media can be expressed using corresponding sines as follows

$$\begin{aligned} \cos \theta_{1n} &= j \sqrt{\sin^2 \theta_{1n} - 1} \\ \cos \theta_{3n} &= -j \sqrt{\sin^2 \theta_{3n} - 1} \end{aligned}$$

This notation enables selection of proper signs before the cosines even when the propagated waves in the first and the third media are damped waves ($|\sin \theta_{1n}| > 1, |\sin \theta_{3n}| > 1$). Using Eqs. (10) and (11) we can find all the unknown vectors

$$\begin{aligned} \mathbf{F}(0) &= 2(\mathbf{C}_3 \mathbf{A}_{11} \mathbf{C}_1^{-1} + \mathbf{C}_3 \mathbf{A}_{12} - \mathbf{A}_{21} \mathbf{C}_1^{-1} - \mathbf{A}_{22})^{-1} \\ &\quad \times (\mathbf{A}_{21} - \mathbf{C}_3 \mathbf{A}_{11}) \mathbf{V}, \\ \mathbf{G}(0) &= \mathbf{C}_1^{-1} \mathbf{F}(0) + 2\mathbf{V}, \\ \mathbf{R} &= \mathbf{G}(0) - \mathbf{V}, \mathbf{T} = \mathbf{G}(0) \end{aligned} \quad (12)$$

Thus, in accordance with Eq. (12), knowing the submatrices $\mathbf{A}_{11}, \mathbf{A}_{12}, \mathbf{A}_{21}, \mathbf{A}_{22}$ of the matrix $\mathbf{A}(d)$ one can calculate the amplitudes of all diffracted plane waves in the first and the third media by means of matrix algebra and, consequently, to determine diffraction efficiencies of all diffraction orders. The most complex problem for computer-aided calculations is finding the matrix $\mathbf{A}(d)$, which, for the case when the dielectric constant ε_2 does not depend on coordinate z , is reduced to finding the proper numbers and proper vectors of a matrix from Eq. (7), whose dimension is $2N \times 2N$, where N is the number of diffraction orders taken into account. The situation is a little bit simplified when the system of the first-order, Eq. (7), is reduced to a system of the second-order equations, however, with the dimension N . These systems which are equivalent will be as follows

$$\begin{aligned} \ddot{\mathbf{F}} &= \mathbf{B}_2 \mathbf{B}_1 \mathbf{F}, \\ \ddot{\mathbf{G}} &= \mathbf{B}_1 \mathbf{B}_2 \mathbf{G} \end{aligned} \quad (13)$$

When eigenvalues of the matrix $\mathbf{B}_1 \mathbf{B}_2$ which are equal to γ_n^2 and the corresponding eigenvectors that form matrix \mathbf{S} are found, the solution of Eq. (13) may be written as

$$\begin{aligned} \mathbf{G}(z) &= \exp(\mathbf{A}_1 z) \mathbf{C}_{g+} + \exp(-\mathbf{A}_1 z) \mathbf{C}_{g-}, \\ \mathbf{F}(z) &= \exp(\mathbf{A}_1 z) \mathbf{C}_{f+} + \exp(-\mathbf{A}_1 z) \mathbf{C}_{f-}, \end{aligned} \quad (14)$$

where $\mathbf{C}_{g+}, \mathbf{C}_{g-}, \mathbf{C}_{f+}, \mathbf{C}_{f-}$, are the vectors that are related to integration constants and are determined by $\mathbf{F}(0)$ and $\mathbf{G}(0)$.

The matrix \mathbf{A}_1 can be calculated as follows: $\mathbf{A}_1 = \mathbf{S} \mathbf{\Gamma} \mathbf{S}^{-1}$, where $\mathbf{\Gamma}$ is the diagonal matrix formed on the basis of array of eigenvalues $\gamma_n = \sqrt{\gamma_n^2}$. If $\mathbf{C}_{g+}, \mathbf{C}_{g-}, \mathbf{C}_{f+}, \mathbf{C}_{f-}$, are determined from the condition when $z = 0$ and Eqs. (8) and (14) are compared, the following relations can be written

$$\begin{aligned} \mathbf{A}_{11} &= \mathbf{A}_{22} = \frac{1}{2} [\exp(\mathbf{A}_1 z) + \exp(-\mathbf{A}_1 z)], \\ \mathbf{A}_{12} &= \frac{1}{2} [\exp(\mathbf{A}_1 z) - \exp(-\mathbf{A}_1 z)] \mathbf{A}^{-1} \mathbf{B}_1 \\ \mathbf{A}_{21} &= \frac{1}{2} [\exp(\mathbf{A}_1 z) - \exp(-\mathbf{A}_1 z)] \mathbf{A} \mathbf{B}_1^{-1} \end{aligned} \quad (15)$$

where $\exp(\pm \mathbf{A}_1 z) = \mathbf{S} \exp(\pm \mathbf{\Gamma} z) \mathbf{S}^{-1}$.

Between the submatrices $\mathbf{A}_{11}, \mathbf{A}_{12}, \mathbf{A}_{21}, \mathbf{A}_{22}$, the following relation is valid

$$\mathbf{A}_{11} \mathbf{A}_{22} - \mathbf{A}_{12} \mathbf{A}_{21} = \mathbf{I}, \quad (16)$$

that can be used to monitor the accuracy of calculation. Thus, the finding of eigenvalues and eigenvectors of the matrix $\mathbf{B}_1 \mathbf{B}_2$ is the most cumbersome operation in calculating of \mathbf{R} and \mathbf{T} vectors. All the other calculations take substantially less time. We believe that this procedure is sufficiently clear and rational.

The situation becomes more complicated when the dielectric constant of the second medium depends on z (e.g., in relief gratings with sinusoidal relief). In this case, the whole grating thickness d is divided into r layers, the thickness of each layer being $h = d/r$ [5], and r can be more than 50. Within each layer we solve Eqs. (7) or (13) using the matrix algebra methods, and after that we match the solutions at the layer boundaries and between the grating and the homogeneous media. In this case, it is necessary to solve a linear algebraic system of equations where the number of unknown values are $N[6 + 4(r - 1)]$. In other words, the problem becomes rather cumbersome, especially for TM polarization. Therefore, a little bit different algorithm is proposed to solve such problems. The matrix $\mathbf{A}(d)$ for the grating can be represented as the product of matrices of the corresponding layers

$$\begin{aligned} \mathbf{A}(d) &\cong \mathbf{A}[h, (r - 1/2)h] \mathbf{A}[h, (r - 1 - 1/2)h] \dots \\ \dots \mathbf{A}(h, h/2) &= \prod_{m=1}^r \mathbf{A}[h, (m - 1/2)h] \end{aligned} \quad (17)$$

In turn, the matrix $\mathbf{A}[h, (m - 1/2)h]$ can be written as

$$\begin{aligned} \mathbf{A}[h, (m - 1/2)h] &= \exp[\mathbf{B}(mh - h/2)h] \\ &\cong \sum_{s=0}^L [\mathbf{B}(mh - h/2)h]^s / s! \end{aligned}, \quad (18)$$

where L is determined by the calculation accuracy. It can be shown that the modulus of a maximal eigenvalue of the matrix \mathbf{B} is commensurable with $k_{\max} = \sqrt{|(k_{nx}^2)_{\max} - \varepsilon_0 k_0^2|}$, and, if $\Lambda > \lambda$, they are quite close if the number of diffraction orders taken into account is more than 10. Thus, for rapid series convergence Eq. (18) the step length of grating decomposition can be taken from the condition $h > 1/k_{\max}$. Obviously, there should be an optimal step length of grating decomposition. The time needed for calculations using Eq. (18) grows as h falls, but the time needed for calculations using Eq. (17) simultaneously increases together with increase in accuracy of defining of matrix $\mathbf{A}(d)$.

2.2. Equations and initial conditions for TM-polarization

The system of differential equations for TM-polarization obtained in Refs. 10, 11, 12, and 13 is the following

$$\begin{aligned} \dot{G}_n(z) &= -jk_0 F_n(z) + j \frac{k_{nx}}{k_0} \sum_p \|\varepsilon_2\|_{np}^{-1}(z) k_{px} F_p, \\ \dot{F}_n(z) &= -jk_0 \sum_p \|\varepsilon_2\|_{np}(z) G_p(z) \end{aligned} \quad (19)$$

For better convergence of calculation results, it was proposed in Refs. 16 and 17 to change insignificantly the system of differential equations. The modified system of equations is as follows

$$\begin{aligned} \dot{G}_n(z) &= -jk_0 F_n(z) + j \frac{k_{nx}}{k_0} \sum_p \|\varepsilon_2\|_{np}^{-1}(z) k_{px} F_p, \\ \dot{F}_n(z) &= -jk_0 \sum_p \left\| \frac{1}{\varepsilon_2} \right\|_{np}^{-1}(z) G_p(z) \end{aligned} \quad (19a)$$

The electric and magnetic fields will be written as

$$\begin{aligned} \mathbf{H}(x, z) &= \mathbf{e}_y \sum_n F_n(z) \exp(-jk_{nx}x), \\ \mathbf{E}(x, z) &= \sum_n [\mathbf{e}_x G_{nx}(z) - \mathbf{e}_z G_{nz}(z)] \exp(-jk_{nx}x), \end{aligned} \quad (20)$$

where G_{nz} is determined from the algebraic equation $k_{nx} F_n = \frac{2\pi}{\lambda} \sum_p \|\varepsilon_2\|_{np} G_{pz}$. At the same time G_{nx} has been obtained through G_n .

System of Eqs. (19a) can be also written in a matrix form like Eq. (7), and the matrices \mathbf{B}_1 and \mathbf{B}_2 will be the next

$$\mathbf{B}_1 = -jk_0 \mathbf{I} + k_0^{-1} \|k\|_n \|\varepsilon_2\|_{np}^{-1} \|k\|_n, \quad \mathbf{B}_2 = -jk_0 \left\| \frac{1}{\varepsilon_2} \right\|_{np}^{-1}.$$

In a general case, these matrices do not commute, but the products of $\mathbf{B}_1 \mathbf{B}_2$ and $\mathbf{B}_2 \mathbf{B}_1$ have the same set of eigenvalues, and, respectively, the matrices \mathbf{S} , that diagonalize these two matrix products are different. The solution of Eq. (19a) also can be presented in form of Eqs. (9) and (10). The initial conditions at the boundary of media 1 and 2, and media 2 and 3, are taken into account by means of the following algebraic systems of equations

$$\begin{aligned} \cos \theta_{1n} R_n - G_n(0) &= \cos \theta_{1n} \delta_{n0}, \\ \sqrt{\varepsilon_1} R_n - F_n(0) &= -\sqrt{\varepsilon_1} \delta_{n0}, \\ \cos \theta_{3n} T_n - G_n(d) &= 0, \\ \sqrt{\varepsilon_3} T_n - F_n(d) &= 0. \end{aligned} \quad (21)$$

Solving the algebraic systems of Eqs. (10) and (21) jointly, we obtain

$$\mathbf{G}(0) = (\mathbf{C}_3 \mathbf{A}_{11} + \mathbf{C}_3 \mathbf{A}_{12} \mathbf{C}_1 - \mathbf{A}_{22} \mathbf{C}_1 - \mathbf{A}_{21}), \quad (\mathbf{A}_{22} - \mathbf{C}_3 \mathbf{A}_{12}) \mathbf{V} \quad (22)$$

where:

$$C_{1n} = \sqrt{\varepsilon_1} / \cos \theta_{1n}, C_{3n} = \sqrt{\varepsilon_3} / \cos \theta_{3n}, V_n = 2\sqrt{\varepsilon_1} \delta_{n0}.$$

Using Eqs. (21), (22), and (10) we can calculate R_n and T_n , and also diffraction efficiencies of all the orders of diffraction. The equivalent systems, relative to the intensities of magnetic and electric fields are as follows

$$\begin{aligned} \ddot{\mathbf{F}} &= \mathbf{B}_2 \mathbf{B}_1 \mathbf{F}, \\ \ddot{\mathbf{G}} &= \mathbf{B}_1 \mathbf{B}_2 \mathbf{G} \end{aligned} \quad (23)$$

After finding the eigenvalues of the matrix $\mathbf{B}_1 \mathbf{B}_2$, which are equal to γ_n^2 , and the corresponding eigenvectors that form the matrix \mathbf{S}_g , and the corresponding eigenvectors of the matrix $\mathbf{B}_2 \mathbf{B}_1$ that form the matrix \mathbf{S}_f , the solution of Eq. (25) can be written as

$$\begin{aligned} \mathbf{G}(z) &= \exp(\mathbf{A}_{1g} z) \mathbf{C}_{g+} + \exp(-\mathbf{A}_{1g} z) \mathbf{C}_{g-}, \\ \mathbf{F}(z) &= \exp(\mathbf{A}_{1f} z) \mathbf{C}_{f+} + \exp(-\mathbf{A}_{1f} z) \mathbf{C}_{f-}, \end{aligned} \quad (24)$$

where $\mathbf{C}_{g+}, \mathbf{C}_{g-}, \mathbf{C}_{f+}, \mathbf{C}_{f-}$, are the vectors that are related to the integration constants and are determined by $\mathbf{F}(0)$ and $\mathbf{G}(0)$.

Matrix \mathbf{A}_{1g} can be calculated as follows: $\mathbf{A}_{1g} = \mathbf{S}_g \mathbf{\Gamma} \mathbf{S}_g^{-1}$, where $\mathbf{\Gamma}$ is the diagonal matrix formed on the basis of ordered sequence of eigenvalues $\gamma_n = +\sqrt{\gamma_n^2}$. Respectively, matrix \mathbf{A}_{1f} is defined by $\mathbf{A}_{1f} = \mathbf{S}_f \mathbf{G} \mathbf{S}_f^{-1}$. Having determined $\mathbf{C}_{g+}, \mathbf{C}_{g-}, \mathbf{C}_{f+}, \mathbf{C}_{f-}$, from condition when $z = 0$ and compared Eqs. (19a) and (26) we can write the following relationships

$$\begin{aligned} \mathbf{A}_{11} &= \frac{1}{2} [\exp(\mathbf{A}_{1g} z) + \exp(-\mathbf{A}_{1g} z)], \\ \mathbf{A}_{22} &= \frac{1}{2} [\exp(\mathbf{A}_{1f} z) + \exp(-\mathbf{A}_{1f} z)], \\ \mathbf{A}_{12} &= \frac{1}{2} [\exp(\mathbf{A}_{1g} z) - \exp(-\mathbf{A}_{1g} z)] \mathbf{A}_{1g}^{-1} \mathbf{B}_1, \\ \mathbf{A}_{21} &= \frac{1}{2} [\exp(\mathbf{A}_{1f} z) - \exp(-\mathbf{A}_{1f} z)] \mathbf{A}_{1f}^{-1} \mathbf{B}_2 \end{aligned} \quad (25)$$

where:

$$\begin{aligned} \exp(\pm \mathbf{A}_{1g} z) &= \mathbf{S}_g \exp(\pm \mathbf{\Gamma} z) \mathbf{S}_g^{-1}, \\ \exp(\pm \mathbf{A}_{1f} z) &= \mathbf{S}_f \exp(\pm \mathbf{\Gamma} z) \mathbf{S}_f^{-1}. \end{aligned}$$

If $\varepsilon(z, x)$ is symmetric function relative to x , then between submatrices $\mathbf{A}_{11}, \mathbf{A}_{12}, \mathbf{A}_{21}, \mathbf{A}_{22}$ the following relationships are valid

$$\mathbf{A}_{11} = \overline{\mathbf{A}_{22}}, \mathbf{A}_{11} \overline{\mathbf{A}_{22}} - \mathbf{A}_{12} \overline{\mathbf{A}_{21}} = \mathbf{I}, \quad (26)$$

where the horizontal bar is the sign of transposition.

Thus, if in our solution we consider N diffraction orders, the problem is reduced using matrix algebra methods to finding eigenvalues and eigenvectors of matrices of $N \times N$ dimension, which is the most cumbersome operation from the point of view of computer-aided calculations. Other operations are reduced to reversion, multiplication, and addition of matrices of the same order. Whereas in the

diffraction problem in addition to symmetry $\varepsilon_2(x, z)$ there is also a supplementary symmetry, i.e., the plane wave incidence angle onto the grating in the first medium is zero, in a case when N is an odd number the diffraction problem can be reduced to solving a system of equations of the type of Eqs. (13) and (23) of the dimension $(N + 1)/2$.

3. Photonic crystals

Calculation of a band structure of photonic crystals using the traditional method [2] is rather difficult problem, calculations becoming especially difficult for two-dimensional and three-dimensional periodic structures. The traditional method is mainly used to specify the wave vector components in the first Brillouin zone and to find the allowed frequencies at which the optical wave can propagate through the photonic crystal without damping. When light propagates in a reflecting-only grating [13] (one-dimensional photonic crystal) or when studying diffraction on a grating whose dielectric constant periodically depends on x and z , in general, we search for the matrix $\mathbf{A}(\Lambda_z)$, where Λ_z is the period of photonic crystal along z coordinate. From the theory of photonic crystals it follows [2] that a wave can propagate in a photonic crystal without damping if the following condition is satisfied

$$\mathbf{A}(\Lambda_z) \begin{pmatrix} \mathbf{G}(0) \\ \mathbf{F}(0) \end{pmatrix} = \begin{pmatrix} \mathbf{G}(\Lambda_z) \\ \mathbf{F}(\Lambda_z) \end{pmatrix} = \exp(-ik_z \Lambda_z) \begin{pmatrix} \mathbf{G}(0) \\ \mathbf{F}(0) \end{pmatrix} = \rho \begin{pmatrix} \mathbf{G}(0) \\ \mathbf{F}(0) \end{pmatrix}. \quad (27)$$

Thus, if the modulus of eigenvalue ρ of matrix $\mathbf{A}(\Lambda_z)$ is equal to one, then for the specified frequency (wavelength) and for the specified wave vector k_{0x} the corresponding wave vector k_{0z} exists with which the optical wave propagates through the photonic crystal without damping. Accordingly, the eigenvector of matrix $\mathbf{A}(\Lambda_z)$ determines components of the field, using which the electromagnetic field of the allowed mode can be calculated. Thus, the vector k_{0z} is

$$k_{0z} = \frac{1}{\Lambda_z} \arccos[\text{Re}(\rho)]. \quad (28)$$

So, the analysis of photonic crystal using our method is reduced to finding of matrix $\mathbf{A}(\Lambda_z)$ and its eigenvalues and eigenvectors, for which in the case of one-dimensional photonic crystal it is necessary to solve a system of two first-order differential equations [13], and for two-dimensional photonic crystals, as revealed by practice, it is sufficient to find matrix $\mathbf{A}(\Lambda_z)$ of dimension 20×20 .

The systems of differential equations that describe optical wave propagation in one-dimensional photonic crystals for TE and TM polarized waves are the following [13] TE-polarization

$$\begin{aligned} \dot{G} + ik_0 F &= 0, \\ \dot{F} - i \frac{k_x^2}{k_0} G + ik_0 \varepsilon(z) G &= 0. \end{aligned} \quad (30)$$

TM-polarization

$$\begin{aligned} \dot{G} - i \frac{k_x^2}{k_0 \varepsilon(z)} F + ik_0 F &= 0, \\ \dot{F} + ik_0 \varepsilon(z) G &= 0. \end{aligned} \quad (31)$$

The matrix $\mathbf{A}(\Lambda_z)$ for one-dimensional photonic crystal has dimension 2×2 and can be expressed by

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}.$$

When take into account that $\mathbf{A} = 1$ [31], we can see that the eigenvalues of this matrix by a module are equal to one if $|(a_{11} + a_{22})/2| \leq 1$, a_{11} and a_{22} are the real numbers for a non-absorbing periodic medium [13]. Thus, in order to find eigenvalues, it is necessary to know only the trace of the matrix $\mathbf{A}(\Lambda_z)$. The band structure of the photonic crystal taken from Ref. 2 was calculated using the proposed method. The calculation results are completely coincident with those given in Fig. 4 of Chapter 4 in Ref. 2.

In order to analyse two-dimensional photonic crystal, it is necessary to have the matrix $\mathbf{A}(\Lambda_z)$, whose dimension is determined by the number of diffraction orders taken into account in calculations. For non-absorbing periodic structures and for both polarizations, it is quite sufficient to consider only 11 orders of diffraction, i.e., matrix dimension in this case is 22×22 and it has 22 eigenvalues. The eigenvalues can be divided into two groups, and each value of the first group is related to a corresponding value of the second group whose product is equal to one. This correspondence between eigenvalues means that a wave can propagate into opposite directions relative to z -axis. In other words, we can have an even number of eigenvalues equal to one by module that are mutually complex conjugated. Thus, the problem of calculation of the band structure is reduced to finding the matrix $\mathbf{A}(\Lambda_z)$. If the period Λ_z can be divided into two or more intervals in which $\varepsilon(z, x)$ does not depend on z , then it is expedient to find the matrix \mathbf{A} in each interval and to find the general matrix as the product of matrices of individual intervals. To find the matrix $\mathbf{A}(\Lambda_z)$ it is expedient to use the methods described in Sec. 2 of this paper.

4. Numerical calculations of analysis of periodic structures

Using Eqs. (6), (19), and (19a), the calculations for various periodic structures and for a two-dimensional photonic crystal of a simple structure were carried out. The corresponding periodic structures are shown in Fig. 2.

For the periodic structure in Fig. 2(a), for TE- and TM-polarized waves, the grating parameters have been re-

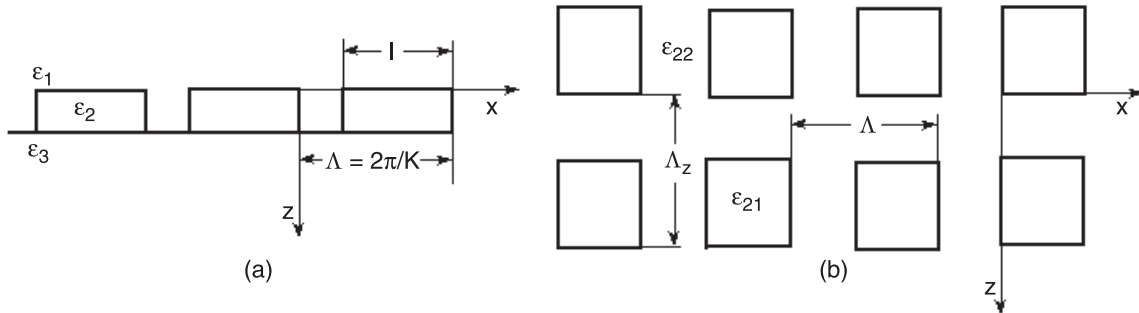


Fig. 2. Schematic representation of periodic structures, (a) a diffraction grating and (b) a two-dimensional photonic crystal.

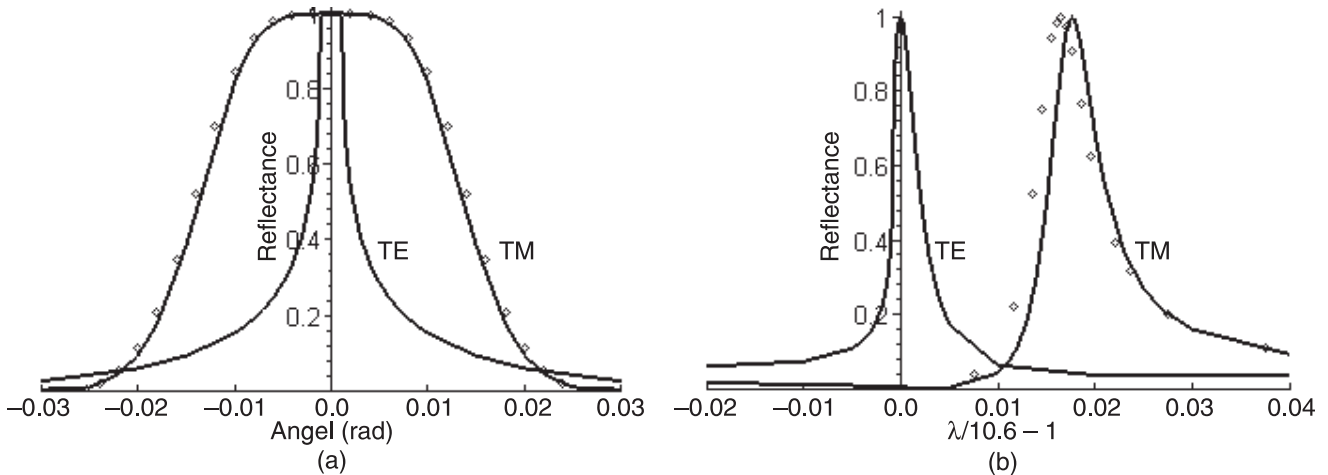


Fig. 3. Dependence of reflectivity for a grating with coupled mode resonance. S is TE polarization, P is TM polarization. Fig. 3(a) is dependence of reflectivity from incidence angle of plane wave onto a grating. Fig. 3(b) is dependence of reflectivity from wavelength.

ceived at which the reflectivity from such a grating is practically equal to 1 (coupled mode resonance). All 11 orders of diffraction were taken into account in the calculation. The calculation was carried out for the grating with parameters $\epsilon_1 = 1$, $\epsilon_2 = 3.61$, $\epsilon_3 = 2.25$, $\Lambda = 7.06117 \mu\text{m}$, and $d = 3.0798 \mu\text{m}$. The received coefficient of reflection is 0.9999973 for TE polarization at $10.6 \mu\text{m}$ wavelength. The maximum of reflection for TM-polarized waves moves a little towards the long wavelengths. Figure 3 shows the dependence of reflectivity from an incidence angle and a relative wavelength. For TM polarization, the solid curves were calculated using Eq. (19), and the results shown with dots were obtained using Eq. (19a). It follows from Fig. 3, that there is no difference in the calculation results for TM-polarized waves obtained using Eqs. (19) and (19a). In other words, to calculate completely phase gratings (without absorption), it is possible to use both systems of equations and they yield almost the same results even in the case of relatively low number of diffraction orders.

Figure 4 shows the dependences of grating transmission from grating spacing for both polarizations. These gratings are consisting of periodically spaced metallic bands on a dielectric substrate (grating polarizers). The calculations were carried out for $\lambda = 0.85 \mu\text{m}$, the metal was silver ($\epsilon_2 = -35 - i1.2$), the mark-to-space ratio was 0.5, the thickness of metallic film was $0.1 \mu\text{m}$. Eleven diffraction orders

were taken into account in calculations of TE-polarized waves, and for TM-polarized waves, the calculations were made for 11 diffraction orders using Eqs. (19) and (19a), and for 25 diffraction orders using Eq. (19a).

The dependences in Fig. 4 have essentially different characters of grating transmission for various polarizations. When Λ/λ ratio is small, the TE wave is completely reflected from the grating, and transmission of TM-polarized waves is close to 0.9. The calculations have indicated that the results obtained using Eqs. (19) and Eq. (19a) taking into account 11 diffraction orders differ greatly, whereas there is less difference between the results obtained using Eq. (19a) taking into account 11 (solid curve) and 25 (dots) diffraction orders.

Using Eqs. (19) and taking into account 11 orders of diffraction, the dependence of grating transmission from Λ/λ in the range of 0.05 to $2/3$ has smooth character without valleys near $\Lambda/\lambda = 0.4$ and passes essentially lower than the curves obtained using Eqs. (19a). The curves received using Eqs. (19a) and taking into account 11 and 25 orders of diffraction are a little bit different. When take into account only 11 orders, the curve is smooth but it has one deep valley near $\Lambda/\lambda = 0.4$, and when take 25 orders, there are many valleys but they are rather shallow. It means, the system of Eqs. (19a) has to be used to analyze such a grating for the case of TM polarization. This conclusion is coincident with the results of Refs. 16 and 17.

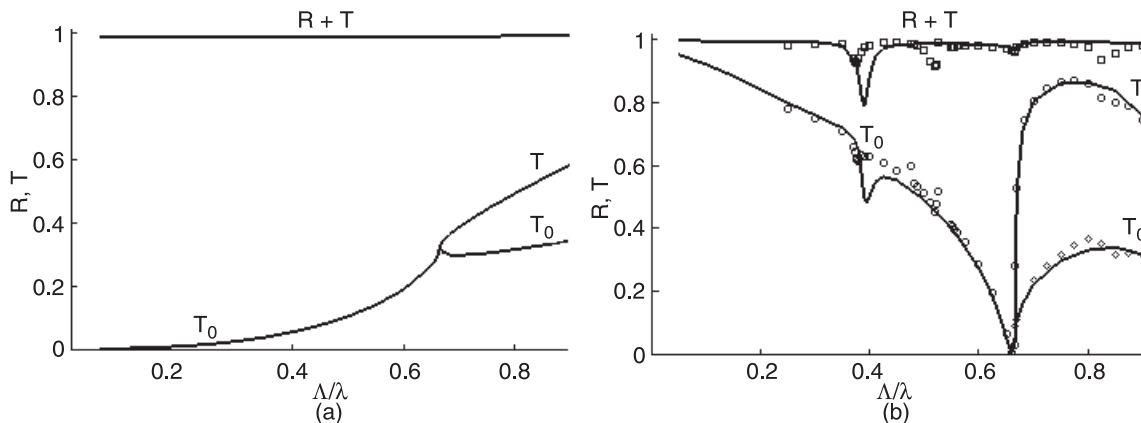


Fig. 4. Dependence of transmission of relief metallized gratings from grating spacing, T_0 is the transmission in zero order of diffraction, T is the total grating transmission, $R + T$ is the total coefficient of grating transmission and reflection. Fig. 4(a) is TE polarization and Fig. 4(b) is TM polarization.

Figure 5 shows the dependence of diffraction efficiency of an aluminium metallized grating from a wavelength. The grating has a $0.1 \mu\text{m}$ deep sinusoidal relief and the groove frequency of 1800 gr/mm , i.e., its parameters coincide with those of the grating produced by Richardson Grating Laboratory [32, Fig. 8].

The calculations were made for Littrow scheme diffraction taking into account 11 diffraction orders. For TE-polarized waves, the coincidence with the experimental curve [31] is very good, the difference between the two curves within the whole wavelength range is 0–3% of diffraction efficiency. For TM-polarized waves, the coincidence is only qualitative, the calculated dependence of diffraction efficiency is by 20–25% different of the experimental curve. Using Eqs. (19a) made the results even worse. Therefore, to improve the accuracy of calculation of diffraction of metallized relief gratings for TM-polarized waves it is necessary to increase the number of diffraction orders taken into account and it is advisable to use Eqs. (19) or the system of equations given in Ref. 18. The system of Eqs. (19) yields better results than (19a) for the same number of diffraction orders taken into account, what is logically explained in Ref. 18 as a result of the

fact that the grating relief depth is less than the grating spacing.

Calculation of the photonic crystal band structure shown in Fig. 6 has been carried out only for TE-polarized waves taking into account 11 orders of diffraction. A two-dimensional crystal of a simple structure (Fig. 26) with the same period of $1 \mu\text{m}$ along both axes was selected for calculation. The dimensions of square rod were $4 \times 4 \mu\text{m}^2$. Calculating the band structure when 11 orders of diffraction are taken into account it is necessary to find the eigenvalues of matrix 22×22 . In order to achieve the same calculation accuracy using the traditional method [2] it is necessary to find the eigenvalues of matrix with dimensions 121×121 , that lead to increasing of calculation time. To confirm the calculation accuracy, k_z was determined for the values of $k_x = m2\pi/a$, where m is the integer and varies in the range from -4 to $+4$. For $v = 0.02$, k_z is equal to $0.189164 \mu\text{m}^{-1}$, i.e., variations were observed in the 7th symbol after the point, and for $v = 0.2 - k_z = 2.010 \mu\text{m}^{-1}$, i.e., variations appeared in the 4th symbol. Thus, taking into account only 11 orders of diffraction gives a sufficient accuracy of calculation of band structure of two-dimensional photonic crystals.

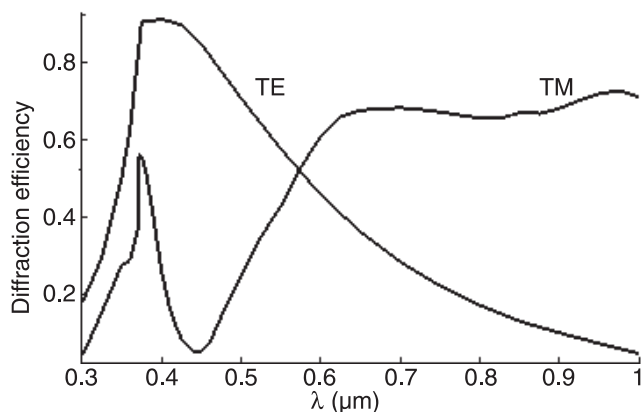


Fig. 5. Dependence of diffraction efficiency of a metallized grating with sinusoidal relief from wavelength.

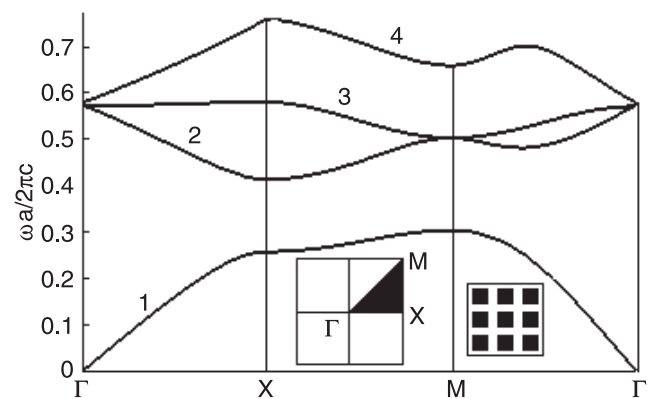


Fig. 6. Band structure of a photonic crystal, $\epsilon_{21} = 1$, $\epsilon_{22} = 8.9$, $a = \Lambda = \Lambda_x = 1 \mu\text{m}$.

5. Conclusions

This paper offers a description of the method for analysing light diffraction on periodic structures. The analysis is based on solving a linear system of differential equations taking into account exact boundary conditions. The system of equations is obtained on the basis of the Maxwell equation. The structure of equations for describing TM polarized wave diffraction is more complex than the system of equations for TE polarized waves. Respectively, for analysing of TM polarized wave diffraction of the higher number of diffraction orders have to be taken into account. This is especially important for metallic diffraction grating. The results of the diffraction analysis of TE and TM polarized waves for various types of periodic structures such as grating polarizers, gratings with coupled wave resonance and sinusoidal relief metallized gratings are given. The band structure for a two-dimensional photonic crystal of a simple form has been constructed.

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