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The Propagation of Polarized Monochromatic Light in Periodic Media

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The work is dedicated to analysis of photonic band gaps of one-dimensional photonic crystal and simulating diffraction on one-dimensional binary diffraction grating using RCWA method. The results of simulating diffraction using RCWA are compared with spectrophotometrical data.

Key words and phrases: RCWA, periodic media, diffraction, photonic crystal, Bloch-waves.

1. Introduction

Periodic structures as photonic crystals are widely used in modern laser devices, communication technologies and for creating various beam splitters and filters. Diffraction gratings are applied for creating 3D television sets, DVD and Blu-ray drives and reflective structures (Berkley mirror). It is important to simulate diffraction on such structures to design optical systems with predetermined properties based on photonic crystals and diffraction gratings. Methods of simulating diffraction on periodic structures uses theory of Floquet-Bloch and rigorous coupled-wave analysis (RCWA) [1,2]. Current work is dedicated to analysis of photonic band gaps and simulating diffraction on one-dimensional binary diffraction grating using RCWA. The Maxwell's equations for isotropic media and constitutive relations based on the cgs system were used as a model.

2. One-Dimensional Photonic Crystal

The photonic crystal is a dielectric structure with periodical refractive index along one or more directions. A distinctive feature of these structures is the presence of so-called photonic band gaps, preventing the propagation of waves of a certain frequency. Due to this property, with the help of photonic crystals it's possible to create devices that can reflect or transmit light with fixed wavelength.

We consider the formation of photonic band gaps by example of monochromatic waves propagating along z-axis, which is perpendicular to the direction of periodicity of one-dimensional photonic crystal. Its dielectric permittivity is a periodic function of z:

$$\varepsilon\left(z\right)=\begin{cases}\varepsilon_1, & (n-1)d<z<nd-a,\\ \varepsilon_2, & nd-a<z<nd,\end{cases} \tag{1}$$

where n is a number of the cell and $\varepsilon\left(z\right)=\varepsilon\left(z+d\right)$, where d is a period and a is the width of layer with dielectric permittivity ε_1.

Since the mediums are isotropic, the TE and TM polarizations propagate independently and they can be considered separately. Consider the case of waves of TE polarization. We can reduce Maxwell's equations to the following wave equation:

$$\partial^2 E_y/\partial z^2+k_0^2\beta E_y=0,\quad \left(\beta=\varepsilon-k_x^2/k_0^2\right). \tag{2}$$

From this equation, we find a general solution for the field components in a uniform layer, and then obtain the system considering the condition that the tangential field

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components at the interface between two media with $z = (n-1)d$ and $z = nd - a$, from which we find equations relating the undetermined coefficients from $(n-1)$-th cell with n-th cell in a layer with a dielectric constant ε_2:

$$\begin{pmatrix} A_{n-1}^{(2)} \\ B_{n-1}^{(2)} \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} A_n^{(2)} \\ B_n^{(2)} \end{pmatrix}, \tag{3}$$

where m_ij depends of geometrical and optical properties of layers of each crystal cell.

Next, we find the general periodic solution for TE polarized waves using the theory of Floquet-Bloch [1], according to which a decision of wave equation in a layered periodic medium can be found in the form $E(z) = \tilde{E}(z)\, e^{i(Kz-k)}$, where $\tilde{E}(z)$ is a periodic function with the period of d. Constant K is called the Bloch wave number.

From (3) and the condition of periodicity, we obtain the following system:

$$\begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} A_n^{(2)} \\ B_n^{(2)} \end{pmatrix} = e^{iKd} \begin{pmatrix} A_n^{(2)} \\ B_n^{(2)} \end{pmatrix}, \tag{4}$$

In this system, the factor of e^{iKd} is an eigenvalue of the coefficient matrix. Then solving the characteristic equation of this system with respect to factor e^{iKd}, given that the coefficient matrix is unimodular, we obtain:

$$2\cos Kd = m_{11} + m_{22}. \tag{5}$$

Substituting the values of the coefficient matrix to the (5), we obtain the dispersion equation in implicit form, which establishes the relationship between the Bloch wave number K, frequency ω, and x-component k_x of wave vector. The dispersion equation for TE waves:

$$\cos Kd = \cos\left(k_0\sqrt{\beta_1}b\right)\cos\left(k_0\sqrt{\beta_2}a\right) - \frac{1}{2}\frac{\beta_1+\beta_2}{\sqrt{\beta_1\beta_2}}\sin\left(k_0\sqrt{\beta_1}b\right)\sin\left(k_0\sqrt{\beta_2}a\right). \tag{6}$$

If $|(m_{11}+m_{22})/2| > 1$, K takes complex values, the Bloch wave is evanescent, and the propagation of electromagnetic waves is impossible in this region, it is called band gap. If $|(m_{11}+m_{22})/2| < 1$, K is real, this is the case of permitted zones, in this area Bloch waves will propagate.

The dependence of the wave vector k_x and frequency ω is shown below in fig. 1. Dark areas correspond to areas of transmission. Wave frequencies with the value of this area will be distributed in the environment. Bright areas correspond to the band gaps. These frequencies are forbidden and light cannot propagate in the medium. Such waves will be reflected from the structure.

3. One-Dimensional Binary Diffraction Grating

A linearly polarized electromagnetic field incident at Λ-periodic binary grating at an angle Θ (Fig.1.). The wave-vector of the incident field is obtained from the geometry: $\mathbf{k_I} = k(\sin\theta,\, 0,\, \cos\theta) = n_I k_0 (\sin\theta,\, 0,\, \cos\theta)$ with $k_0 = \dfrac{2\pi}{\lambda_0}$ and n_I — refractive index in region I. The wave-vectors of reflected and transmitted diffracted orders can be determined from the Floquet condition:

$$k_{xj} = k_0\left(n_I\sin\theta - j\frac{\lambda_0}{\Lambda}\right), \tag{7}$$

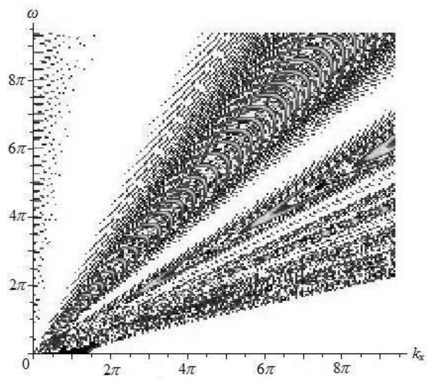

Figure 1. **The Band Structure for TE-waves**

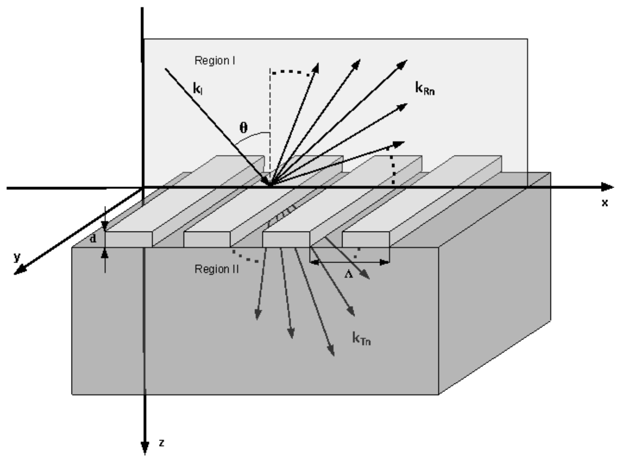

Figure 2. **Geometry for the Diffraction Problem**

$$k_{L,zj} = \begin{cases} \sqrt{\left(k_0 n_L\right)^2 - k_{xj}^2}, & \operatorname{Re}\left(\left(k_0 n_L\right)^2 - k_{xj}^2\right) \geqslant 0 \\ -i\sqrt{k_{xj}^2 - \left(k_0 n_L\right)^2}, & \operatorname{Re}\left(\left(k_0 n_L\right)^2 - k_{xj}^2\right) < 0, \end{cases} \quad L = I,\, II. \tag{8}$$

The grating is bound by two media: input media with refractive index $n_I = \sqrt{\varepsilon_I}$, as a rule vacuum, and output media with refractive index $n_{II} = \sqrt{\varepsilon_{II}}$, which corresponds to substrate. Relative permittivity in the grating region is a Λ-periodic function $\varepsilon(x) = \varepsilon(x + m\Lambda)$, $m = 0, \pm 1, \pm 2, \ldots$, which is expandable in a Fourier series. Electromagnetic fields in regions I and II are satisfied to Rayleigh expansion on the form:

$$u = \exp\left(-ik_0 n_I\left(\sin\theta x + \cos\theta z\right)\right) + \sum_{j=-\infty}^{\infty} R_j \exp\left(-i\left(k_{xj}x - k_{I,zj}z\right)\right), \tag{9}$$

$$u = \sum_{j=-\infty}^{\infty} T_j \exp\left(-i\left(k_{xj}x - k_{II,zj}(z-d)\right)\right), \tag{10}$$

where u corresponds to E_y in TE case and H_y in TM case, R_j and T_j are amplitudes of the reflected and transmitted diffracted orders, which corresponds to E_y in TE case and H_y in TM case.

The problem of planar diffraction is decomposed into two independent problems: TE- and TM-polarization. The general problem is to find R_j and T_j.

The case of TE-polarization is fully described in article [2]. We will consider the case of TM-polarization. Main steps of algorithm are presented below.

1. Fourier series for tangential electric and magnetic fields in the grating region:

$$H_y = \sum_j U_{yj}\left(z\right)\exp\left(-ik_{xj}x\right), \quad E_x = i\sum_j S_{xj}\left(z\right)\exp\left(-ik_{xj}x\right). \tag{11}$$

2. Substituting Fourier series for tangential electric and magnetic fields into corresponding equations:

$$\sum_p \bar{\varepsilon}_{j-p}\frac{\partial U_{yp}}{\partial z} = k_0 S_{xj}, \quad \frac{1}{k_0}\frac{\partial S_{xj}}{\partial z} = \frac{k_{xj}}{k_0}\left(\sum_p \bar{\varepsilon}_{j-p}\frac{k_{xp}}{k_0}U_{yp}\right) - U_{yj}. \tag{12}$$

3. Previous coupled-wave equations can be reduced to:

$$\left[\partial^2 \mathbf{U}_y/\partial(z')^2\right] = \left[\mathbf{FB}\right]\left[\mathbf{U}_y\right], \tag{13}$$

where $z' = k_0 z$, $\mathbf{B} = \mathbf{K}_x\mathbf{F}^{-1}\mathbf{K}_x - \mathbf{I}$, $\mathbf{K}_x = diag\left\{k_{x\,-N}/k_0, \ldots, k_{x\,0}/k_0, \ldots k_{x\,N}/k_0\right\}$, $\mathbf{I}$ — identity matrix, $\mathbf{F}^{-1}$ — is a toeplitz matrix of components of the Fourier series of function $1/\varepsilon\left(x\right)$, $\mathbf{F}$ — inverse to $\mathbf{F}^{-1}$.
4. Solving previous equation we obtain:

$$U_{yj}\left(z\right) = \sum_{m=1}^{n} w_{jm}\left\{c_m^+\exp\left(-k_0 q_m z\right) + c_m^-\exp\left[k_0 q_m\left(z-d\right)\right]\right\}, \tag{14}$$

$$S_{xj}\left(z\right) = \sum_{m=1}^{n} v_{jm}\left\{-c_m^+\exp\left(-k_0 q_m z\right) + c_m^-\exp\left[k_0 q_m\left(z-d\right)\right]\right\}, \tag{15}$$

where w_{jm} and q_m are the elements of the eigenvector matrix $\mathbf{W}$ and the positive square root of the eigenvalues of matrix $\mathbf{FB}$; v_{jm} is the element of the matrix $\mathbf{V} = \mathbf{F}^{-1}\mathbf{WQ}$, $\mathbf{Q} = diag\left\{q_1, q_2, \ldots, q_n\right\}$.
5. Using boundary conditions at the input boundary we obtain:

$$\delta_{j0} + R_j = \sum_{m=1}^{n} w_{jm}\left[c_m^+ + c_m^-\exp\left(-k_0 q_m d\right)\right], \tag{16}$$

$$i\left[\frac{\cos\theta}{n_I}\delta_{j0} - \frac{k_{I,zj}}{k_0 n_I^2}R_j\right] = \sum_{m=1}^{n} v_{jm}\left[c_m^+ - c_m^-\exp\left(-k_0 q_m d\right)\right], \tag{17}$$

and at the output boundary:

$$\sum_{m=1}^{n} w_{jm}\left[c_m^+\exp\left(-k_0 q_m d\right) + c_m^-\right] = T_j, \tag{18}$$

$$\sum_{m=1}^{n} v_{jm}\left[c_m^+\exp\left(-k_0 q_m d\right) - c_m^-\right] = i\left(\frac{k_{II,zj}}{k_0 n_{II}^2}\right)T_j. \tag{19}$$

6. Eliminating R_j and T_j from previous equations we obtain:

$$i\delta_{j0}\left(\frac{k_{I,zj}}{k_0 n_I^2}+\frac{\cos\theta}{n_I}\right)=\sum_{m=1}^{n}c_m^+\left[i\frac{k_{I,zj}}{k_0 n_I^2}w_{jm}+v_{jm}\right]+ \\ +\sum_{m=1}^{n}c_m^-\exp\left(-k_0 q_m d\right)\left[i\frac{k_{I,zj}}{k_0 n_I^2}w_{jm}-v_{jm}\right], \quad (20)$$

$$\sum_{m=1}^{n}c_m^+\exp\left(-k_0 q_m d\right)\left[-i\frac{k_{II,zj}}{k_0 n_{II}^2}w_{jm}+v_{jm}\right]+ \\ +\sum_{m=1}^{n}c_m^- w_{im}\left[-i\frac{k_{II,zj}}{k_0 n_{II}^2}w_{jm}-v_{jm}\right]=0. \quad (21)$$

7. Solving the system of linear equations we obtain c_m^+ and c_m^-. Substituting c_m^+ and c_m^- into corresponding equations we determine R_j and T_j. The efficiencies of the diffracted orders are given by:

$$\mathbf{R}_j=\left|R_j\right|^2\mathrm{Re}\left(\frac{k_{I,zj}}{k_0 n_I\cos\theta}\right), \\ \mathbf{T}_j=\left|T_j\right|^2\mathrm{Re}\left(\frac{k_{II,zj}}{n_{II}^2}\right)/\left(\frac{k_0\cos\theta}{n_I}\right). \quad (22)$$

The results of comparison between simulation and spectrophotometrical data for copper binary grating with period 200000nm, spike width 110000nm and spike height 187nm in the case of TM-polarization with incidence angle 8° are presented below.

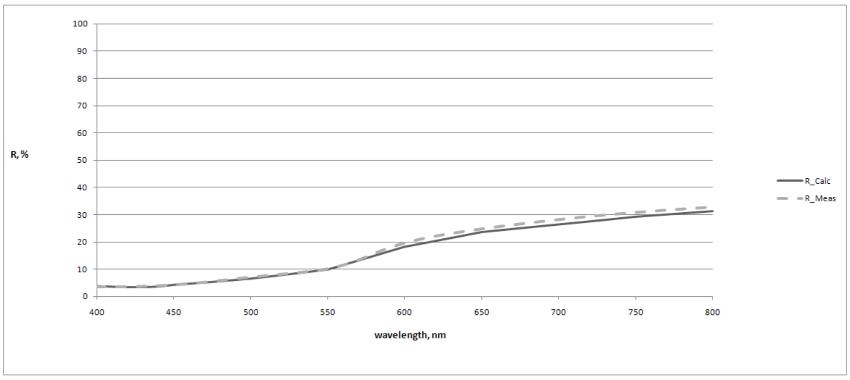

Figure 3. **Comparison Between Simulation and Spectrophotometrical Data**

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Распространение поляризованного монохроматического света в периодических структурах

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Работа посвящена анализу запрещённых зон одномерного фотонного кристалла и моделированию дифракции света на одномерной бинарной дифракционной решётке методом RCWA. Метод RCWA описан для одномерных фотонных кристаллов и одномерных бинарных дифракционных решёток. Приведено сравнение результатов моделирования со спектрофотометрическими данными.

Ключевые слова: RCWA, периодические среды, дифракция, фотонный кристалл, блоховские волны.