Diffraction of polarized light on periodic structures

V. Bukanina¹, D. Divakov², A. Tyutyunnik³, A. Hohlov⁴

¹ Student, Peoples Friendship University of Russia, Moscow, Russia
² Student, Peoples Friendship University of Russia, Moscow, Russia
³ Student, Peoples Friendship University of Russia, Moscow, Russia
⁴ PhD in physics, Peoples Friendship University of Russia, Moscow, Russia

E-mail: aaxoxlov@sci.pfu.edu.ru

Abstract. 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). 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.

1. One-dimensional photonic crystal

The photonic crystal is a dielectric structure with periodic 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:

\[ \varepsilon(z) = \begin{cases} \varepsilon_1, & (n-1)d < z < nd - a \\ \varepsilon_2, & nd - a < z < nd \end{cases} \]  

(1)

where \( n \) is a number of the cell, \( a \) is the width of layer with dielectric permittivity \( \varepsilon_2 \) and \( \varepsilon(z) = \varepsilon(z + d) \), where \( d \) is a period.

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:

\[ \frac{\partial^2 E_y}{\partial z^2} + k_0^2 \beta E_y = 0, \quad (\beta = \varepsilon \frac{k_y^2}{k_0^2}) \]  

(2)
From this equation, we find a general solution for the field components in a uniform layer, we obtain considering

\[
E_y(z) = A e^{i k_0 \sqrt{\beta} (z - nd)} + B e^{-i k_0 \sqrt{\beta} (z - nd)}
\]
\[
H_x(z) = A \sqrt{\beta} e^{i k_0 \sqrt{\beta} (z - nd)} - B \sqrt{\beta} e^{-i k_0 \sqrt{\beta} (z - nd)}.
\]

Then we obtain the system considering the condition that the tangential field components at the interface between two media with \( z = n - 1 \) \( d \) and \( z = nd - a \)

\[
\begin{align*}
A_{n-1}^2 + B_{n-1}^2 &= A_n^1 e^{-i k_0 \sqrt{\beta} d} + B_n^1 e^{i k_0 \sqrt{\beta} d} \\
A_n^2 \sqrt{\beta}_2 - B_n^2 \sqrt{\beta}_2 &= A_n^1 \sqrt{\beta}_1 e^{-i k_0 \sqrt{\beta} d} - B_n^1 \sqrt{\beta}_1 e^{i k_0 \sqrt{\beta} d} \\
A_n^1 e^{-i k_0 \sqrt{\beta} d} + B_n^1 e^{i k_0 \sqrt{\beta} d} &= A_n^2 e^{-i k_0 \sqrt{\beta} d} + B_n^2 e^{i k_0 \sqrt{\beta} d} \\
A_n^1 \sqrt{\beta}_1 e^{-i k_0 \sqrt{\beta} d} - B_n^1 \sqrt{\beta}_1 e^{i k_0 \sqrt{\beta} d} &= A_n^2 \sqrt{\beta}_2 e^{-i k_0 \sqrt{\beta} d} - B_n^2 \sqrt{\beta}_2 e^{i k_0 \sqrt{\beta} d}.
\end{align*}
\]

\[(4)\]

where \( A^1, B^1 \) and \( A^2, B^2 \) are indefinite coefficients in the layers with dielectric permittivity \( \varepsilon_1 \) and \( \varepsilon_2 \).

From (4) we find equations relating the indefinite coefficients from \( n-1 \) –th cell with \( n \)-th cell in a layer with a dielectric permittivity \( \varepsilon_2 \):

\[
\begin{pmatrix}
A_{n-1}^2 \\
B_{n-1}^2
\end{pmatrix} =
\begin{pmatrix}
m_{11} & m_{12} \\
m_{21} & m_{22}
\end{pmatrix}
\begin{pmatrix}
A_{n}^2 \\
B_{n}^2
\end{pmatrix}
\]

\[(5)\]

where

\[
\begin{align*}
m_{11} &= e^{-i k_0 \sqrt{\beta}_1 d} \left( \cos k_0 \sqrt{\beta}_1 b - i \frac{\beta_1 + \beta_2}{2 \sqrt{\beta_1 \beta_2}} \sin k_0 \sqrt{\beta}_1 b \right) \\
m_{12} &= e^{i k_0 \sqrt{\beta}_1 d} \left( \frac{i}{2} \frac{\beta_2 - \beta_1}{\sqrt{\beta_1 \beta_2}} \sin k_0 \sqrt{\beta}_1 b \right) \\
m_{21} &= e^{-i k_0 \sqrt{\beta}_2 d} \left( -i \frac{\beta_2 - \beta_1}{2 \sqrt{\beta_1 \beta_2}} \sin k_0 \sqrt{\beta}_2 b \right) \\
m_{22} &= e^{i k_0 \sqrt{\beta}_2 d} \left( \cos k_0 \sqrt{\beta}_2 b + i \frac{\beta_1 + \beta_2}{2 \sqrt{\beta_1 \beta_2}} \sin k_0 \sqrt{\beta}_2 b \right)
\end{align*}
\]

\[(6)\]

For the case of TM polarization done a similar action.

Next we use the Floquet-Bloch theorem, according to which the periodic solution in a layered periodic medium has the form \( E_z(z) = \tilde{E}_0 e^{i K z} \), where \( \tilde{E}_0 \) is a periodic function with the period of \( d \). Constant \( K \) is called the Bloch wave number.

Considering \( E_{n-1}(z - d) e^{i K (z - d)} = E_n(z) e^{i K z} \) we write the condition of periodicity for the Bloch wave in the form:
From (3) and (7) we obtain the following system:

$$
\begin{pmatrix}
A_n^2 \\
B_n^2
\end{pmatrix} = e^{iKd} \begin{pmatrix}
A_{n-1}^2 \\
B_{n-1}^2
\end{pmatrix}
$$

(7)

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:

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

(8)

Substituting the values of the coefficient matrix to the (9), we obtain the dispersion equation in implicit form, which establishes the relationship between the Bloch wave number $K$, frequency $\omega$, and $x$-component $k_x$ of wave vector. The dispersion equation for TE waves:

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

(10)

The dispersion equation for TM waves has the following form:

$$
\cos Kd = \cos k_0 \sqrt{\beta_1 b} \cos k_0 \sqrt{\beta_2 a} - \frac{1}{2} \left( \frac{\varepsilon_2}{\varepsilon_1} \frac{\beta_1 + \beta_2}{\beta_1 \beta_2} \right) \sin k_0 \sqrt{\beta_1 b} \sin k_0 \sqrt{\beta_2 a}
$$

(11)

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.

So the reflection coefficient tends to 1 in the band gap. The graph below represents the reflection coefficient for a one-dimensional photonic crystal of 125 layers (fig. 1).
The wavelengths for which the reflection coefficient reaches 100% correspond to the band gaps. The reflection coefficient is the closer to unit the more is number of layers.

2. One-dimensional binary diffraction grating

Let us assume that a linearly polarized electromagnetic field with wavelength $\lambda$ incidents at $\Lambda$-periodic binary grating at an angle $\theta$ (fig. 2).

![Fig. 2 Geometry for the binary diffraction problem](image)

Wave-vector of the incident field can be obtained from the geometry as $\mathbf{k}_i = k \sin \theta \hat{x}, \cos \theta \hat{y} = n_i k_0 \sin \theta \hat{x}, \cos \theta \hat{y}$, where $k_0 = 2\pi / \lambda_0$, $n_i$ - refractive index of region I (fig.2). Wave-vectors of the reflected and transmitted fields are defined from Floquet-condition and geometry:

$$k_{yL,j} = n_j \sin \theta - j \lambda_0 / \Lambda,$$

$$k_{L,j} = \begin{cases} \sqrt{k_0 n_L^2 - k_{yL,j}^2}, & \text{Re } k_0 n_L^2 - k_{yL,j}^2 \geq 0 \\ -i \sqrt{k_0 n_L^2 - k_{yL,j}^2}, & \text{Re } k_0 n_L^2 - k_{yL,j}^2 < 0 \end{cases}, \quad L = I, II.$$

Grating region is bounded by two media with constant relative permittivity. Region I is the input media with $\epsilon_i = n_i^2 = 1$. Region II corresponds to the output media, where $\epsilon_{II} = n_{II}^2 > 1$. Relative permittivity in the grating region is a $\Lambda$-periodic function $\epsilon(x) = \epsilon(x + m\Lambda), m = 0, \pm 1, \pm 2, \ldots$.

Electromagnetic fields in regions I and II are satisfied to Rayleigh expansion:

$$u = \exp(-ik_0 n_i \sin \theta x + \cos \theta z) + \sum_{j=-\infty}^{\infty} R_j \exp(-i k_{yL,j}x - k_{L,j}z).$$
\[ u = \sum_{j=-\infty}^{\infty} T_j \exp(-i k_y x - k_{zj} z - d) . \]  

where \( u \) corresponds to \( E_y \) in TE-case and \( H_y \) in TM-case.

Electromagnetic field in the grating region satisfies to Maxwell’s equations, which can be reduced to the system:

\[ -ik_0 H_x = \frac{\partial E_y}{\partial z}, \quad -ik_0 H_y = \frac{\partial E_x}{\partial x} - \frac{\partial E_z}{\partial z}, \quad -ik_0 H_z = \frac{\partial E_y}{\partial x}, \]

\[ ik_0 \varepsilon(x) E_x = \frac{\partial H_y}{\partial z}, \quad ik_0 \varepsilon(x) E_y = \frac{\partial H_x}{\partial x} - \frac{\partial H_z}{\partial z}, \quad ik_0 \varepsilon(x) E_z = \frac{\partial H_y}{\partial x}. \]

The system **Error! Reference source not found.** defines electromagnetic field in the grating region. Binary diffraction problem consists of definition electromagnetic fields in regions I, II and grating region.

We will solve the problem according to the plan:

Expansion of the tangential electric and magnetic fields in Fourier series in the grating region;

Substitution of the expanded tangential fields into the system (16), (17) to become two systems differential equations of the first order with normalized amplitudes of the tangential fields in the grating region as a variable;

Reduction of two systems differential equations of the first order to one system differential equations of the second order;

General solution of system differential equations of the second order through eigenvalues and eigenvectors;

Using boundary conditions at the input and output boundaries to obtain quantities for the general solution of system differential equations of the second order;

Substitution quantities into general solution to determine electromagnetic field in the grating region;

2.1. TE-case

Fourier series for tangential electric and magnetic fields:

\[ E_y = \sum_j S_{yj} z \exp(-i k_y x), \]

\[ H_x = -i \sum_j U_{xj} z \exp(-i k_y x). \]

Substitution of the expanded tangential fields into the system (18), (19) to become two systems differential equations of the first order:

\[ \frac{\partial S_{yj}}{\partial z} = k_0 U_{xj}, \]

\[ \frac{\partial U_{xj}}{\partial z} = \left( \frac{k_y^2}{k_0} \right) S_{yj} - k_0 \sum_p \varepsilon_{j-p} S_{yp}. \]

Equations (20), (22) can be written in matrix form using \( z' = k_0 z \):

\[ \begin{bmatrix} \frac{\partial S_y}{\partial z'} \\ \frac{\partial U_x}{\partial z'} \end{bmatrix} = \begin{bmatrix} 0 & I \\ A & 0 \end{bmatrix} \begin{bmatrix} S_y \\ U_x \end{bmatrix}, \]

where \( A = K^2 - F \);

\( I \) - identity matrix;
\[
K_x = \begin{bmatrix}
k_{1,0} & 0 & \cdots & 0 \\
0 & \ddots & \ddots & \vdots \\
\vdots & \ddots & k_{i,0} & \vdots \\
0 & \cdots & 0 & k_{N,0}
\end{bmatrix}
\]

\( F \) - matrix for the coefficients of Fourier series for \( x \).

Previous systems can be reduced to:

\[
\begin{bmatrix}
\frac{\partial S_x}{\partial z} \\
\frac{\partial U_x}{\partial z}
\end{bmatrix} = \begin{bmatrix}
0 & 1 \\
A & 0
\end{bmatrix} \begin{bmatrix}
S_x \\
U_x
\end{bmatrix},
\]

(23)

General solution of system differential equations of the second order:

\[
S_{yz} z = \sum_{m=1}^{n} w_{jm} c_m^+ \exp -k_0 q_m z + c_m^- \exp [k_0 q_m z - d],
\]

(24)

\[
U_{yz} z = \sum_{m=1}^{n} v_{jm} c_m^- \exp -k_0 q_m z + c_m^+ \exp [k_0 q_m z - d],
\]

(25)

where \( w_{jm} \) and \( q_m \) are the elements of the eigenvector matrix \( W \) and the positive square root of the eigenvalues of the matrix \( A \), \( v_{jm} \) - elements of the matrix \( V = WQ \), \( Q \) - diagonal matrix with elements \( q_m \).

Using conditions on the boundary \( z = 0 \):

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

(26)

\[
i \left[ n_j \cos \theta \delta_{j0} - k_{1,j} / k_0 \right] R_j = \sum_{m=1}^{n} v_{jm} \left[ c_m^- - c_m^+ \exp -k_0 q_m d \right],
\]

(27)

where \( \delta_{j0} = \begin{cases} 
1, & j = 0 \\
0, & j \neq 0
\end{cases} \).

Using conditions on the boundary \( z = d \):

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

(28)

\[
\sum_{m=1}^{n} v_{jm} \left[ c_m^- \exp -k_0 q_m d - c_m^+ \right] = i k_{1,j} / k_0 T_j.
\]

(29)

Eliminating \( R_j \) and \( T_j \) we become system of linear equations to obtain \( c_m^+, c_m^- \):

\[
\begin{align*}
i \delta_{j0} & k_{1,j} / k_0 + n_j \cos \theta = \sum_{m=1}^{n} c_m^+ w_{jm} \left[ i k_{1,j} / k_0 + q_m \right] + \\
&+ \sum_{m=1}^{n} c_m^- w_{jm} \exp -k_0 q_m d \left[ i k_{1,j} / k_0 - q_m \right].
\end{align*}
\]

(30)
\[ \sum_{m=1}^{n} c_m^+ w_{jm} \exp \left( -i k_x zj / k_0 + q_m \right) + \]
\[ + \sum_{m=1}^{n} c_m^- w_{jm} \left[ -i k_y zj / k_0 - q_m \right] = 0. \]

Substituting \( c_m^+ \), \( c_m^- \) into (26), (28) we determine \( R_j \) and \( T_j \). The efficiencies of the diffracted orders are given by:

\[ R_j = \left| R_j \right|^2 \Re \left( \frac{k_{j,yj}}{k_y n_y \cos \theta} \right). \]

\[ T_j = \left| T_j \right|^2 \Re \left( \frac{k_{j,yj}}{k_y n_y \cos \theta} \right). \]

2.2. TM-case

Fourier series for tangential electric and magnetic fields:

\[ H_y = \sum_j U_{sj} \exp (-i k_y x), \]

\[ E_x = i \sum_j S_{sj} \exp (-i k_y x). \]

Substitution of the expanded tangential fields into the system (16), (17) to become two systems differential equations of the first order:

\[ \sum_p \bar{e}_{j-p} \frac{\partial U_{zp}}{\partial z} = k_0 S_{sj}, \]

\[ \frac{1}{k_0} \frac{\partial S_{sj}}{\partial z} = \frac{k_{j,yj}}{k_0} \sum_p \bar{e}_{j-p} \frac{k_{p,xj}}{k_0} U_{zp}. \]

Equations (26), (28) can be written in matrix form using \( z' = k_0 z \):

\[ \begin{bmatrix} \partial U_{sj} / \partial z' \\ \partial S_{sj} / \partial z' \end{bmatrix} = \begin{bmatrix} 0 & F \\ B & 0 \end{bmatrix} \begin{bmatrix} U_{sj} \\ S_{sj} \end{bmatrix}, \]

where \( \mathbf{B} = \mathbf{K}_x \mathbf{F}^{-1} \mathbf{K}_x \mathbf{I} \);

\( \mathbf{I} \) - identity matrix;

\[ \mathbf{K}_x = \begin{bmatrix} k_x / k_0 & 0 & \cdots & 0 \\ 0 & \ddots & \vdots & \vdots \\ \vdots & \ddots & k_x / k_0 & 0 \\ 0 & \cdots & 0 & k_x \end{bmatrix}; \]

\( \mathbf{F}^{-1} \) - matrix for the coefficients of Fourier series for \( 1 / \varepsilon \ x \);

\( \mathbf{F} \) - inverse to \( \mathbf{F}^{-1} \).
Previous systems can be reduced to:

\[
\left[ \frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial z}\frac{\partial}{\partial z} + \mathbf{U}_y \right] = \mathbf{FB} \left[ \mathbf{U}_y \right]
\]

(39)

General solution of system differential equations of the second order:

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

(40)

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

(41)

where \( w_{jm} \) and \( q_m \) are the elements of the eigenvector matrix \( \mathbf{W} \) and the positive square root of the eigenvalues of the matrix \( \mathbf{A} \), \( v_{jm} \) - elements of the matrix \( \mathbf{V} = \mathbf{F}^i \mathbf{W} \mathbf{Q} \), \( \mathbf{Q} \) - diagonal matrix with elements \( q_m \).

Using conditions on the boundary \( z = 0 \):

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

(42)

\[
i \left[ \frac{\cos \theta}{n_{\|}} \delta_{j0} \frac{k_{l,j}}{k_0 n_{\|}^2} R_j \right] = \sum_{m=1}^{n} v_{jm} \left[ c_m^+ - c_m^- \exp \left( -k_0 q_m d \right) \right],
\]

(43)

where \( \delta_{j0} = \begin{cases} 1, & j = 0 \\ 0, & j \neq 0 \end{cases} \).

Using conditions on the boundary \( z = d \):

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

(44)

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

(45)

Eliminating \( R_j \) and \( T_j \) we become system of linear equations to obtain \( c_m^+, c_m^- \):

\[
i \delta_{j0} \left( \frac{k_{l,j}}{k_0 n_{\|}^2} + \frac{\cos \theta}{n_{\|}} \right) = \sum_{m=1}^{n} c_m^+ \left[ i \frac{k_{l,j}}{k_0 n_{\|}^2} w_{jm} + v_{jm} \right] +
\]

\[
+ \sum_{m=1}^{n} c_m^- \exp \left( -k_0 q_m d \right) \left[ i \frac{k_{l,j}}{k_0 n_{\|}^2} w_{jm} - v_{jm} \right] +
\]

\[
\sum_{m=1}^{n} c_m^+ \exp \left( -k_0 q_m d \right) \left[ -i \frac{k_{l,j}}{k_0 n_{\|}^2} w_{jm} + v_{jm} \right] +
\]

\[
+ \sum_{m=1}^{n} c_m^- w_{jm} \left[ -i \frac{k_{l,j}}{k_0 n_{\|}^2} w_{jm} - v_{jm} \right] = 0.
\]

(46)

(47)

Substituting \( c_m^+, c_m^- \) into (42), (44) we determine \( R_j \) and \( T_j \). The efficiencies of the diffracted orders are given by:
\[ R_j = |R_j|^2 \text{Re} \left( \frac{k_{1,j}}{k_{0,n_1} \cos \theta} \right) \]  \hspace{1cm} (48)

\[ T_j = |T_j|^2 \text{Re} \left( \frac{k_{n,j}}{n^2_n} \right) \left( \frac{k_{0} \cos \theta}{n_j} \right) \]  \hspace{1cm} (49)

2.3. Simulation

The results of comparison between simulation and spectrophotometric data for copper binary grating with period 200000nm, spike width 110000nm and spike height 187nm are presented below.

**Fig. 3 TE-case, angle of incidence 8°**

**Fig. 4 TM-case, angle of incidence 8°**
According to the results (fig. 3 – 6) we can conclude that simulation results and experimental data differs for less than 4.5% which proves the accuracy of the method.