The creation and shifts of band gaps in binary superlattices

INTRODUCTION

Superlattices are intensively tested materials [1÷24], the filtering capabilities are particularly attractive [21]. Multilayers are characterized by the presence of the photonic band gap, so that electromagnetic waves (EMW) at the specific frequencies does not propagate them. Using emulation properties of multilayer systems allows pre-testing of the structure and the design to get the specific characteristics of the electromagnetic wave transmission bands. This reduces the number of samples performed and reduces the cost of examinations.

Transmission superlattices are calculated using the matrix method [18÷21] and by the method of finite-difference in the time domain for one-dimensional structures (1D FDTD) [22, 25].

MATRIX METHOD

The transmission of the multilayer structure is calculated from the following equation:

\[ T = \frac{n_{in} \cos \Theta_{in}}{n_{out} \cos \Theta_{out}} \left| X_{11} \right|^2 \]  

(1)

where: \( n_{in}, n_{out} \) – respectively the refractive index of the electromagnetic wave falling on the multilayer structure and which goes after passing, \( \Theta_{in} \) – angle of falling of the EMW for superlatticet, \( \Theta_{out} \) – the angle at which EMW leaves multilayers, \( X_{11} \) – the first word of the characteristic matrix diagonal \( X \) superlattice described the relation:

\[ X = \left[ \begin{array}{cc} 1 & r_{i,j} \cdot e^{i \theta_{j,j}} \\ 0 & 1 \\ \end{array} \right] \]

(2)

where: \( n_j \) – refractive index of the layer \( j \), \( d_j \) – thickness of the layer \( j \), \( \theta_j \) – determined from Snell's law angle of falling of EMW for the layer \( j \), \( \lambda \) – the wavelength of falling wave. Depending on the type of polarization \( t \) and \( r \) determine the amplitude Fresnel ratios respectively for transmittance and reflectance [20]. For the polarization \( P \) are defined as:

\[ t_{j,j+1} = \frac{2 n_j \cos \Theta_j}{n_j \cos \Theta_{j+1} + n_{j+1} \cos \Theta_j} \]

\[ r_{j,j+1} = \frac{n_j \cos \Theta_{j+1} - n_{j+1} \cos \Theta_j}{n_j \cos \Theta_{j+1} + n_{j+1} \cos \Theta_j} \]

(3)

while for S type of polarization they take the form:

\[ t_{j,j+1} = \frac{2 n_j \cos \Theta_j}{n_j \cos \Theta_{j+1} + n_{j+1} \cos \Theta_j} \]

\[ r_{j,j+1} = \frac{n_j \cos \Theta_{j+1} - n_{j+1} \cos \Theta_j}{n_j \cos \Theta_{j+1} + n_{j+1} \cos \Theta_j} \]

(4)

1D FDTD

Using Maxwell's laws, we can determine the equations [23, 24]:

\[ \frac{\partial D}{\partial t} = \nabla \times \vec{H} \]

\[ \frac{\partial \vec{E}}{\partial t} = -\frac{1}{\mu_0} \nabla \times \vec{E} \]

(5)

which involve together the electric field \( \vec{E} \), magnetic field \( \vec{H} \) and the electric induction vector \( \vec{D} \). \( \varepsilon_0, \mu_0 \) are electric and magnetic permeability in a vacuum, and \( \varepsilon_r \) is a relative permittivity of the medium.

In order to simplify calculation of the electric field and the electric induction vector are normalized according to the relation:

\[ \vec{E} = \frac{\varepsilon_0}{\mu_0} \vec{E}, \quad \vec{D} = \frac{1}{\varepsilon_0 \mu_0} \vec{D} \]

(6)

Another transformation allows to obtain necessary for analyzing the propagation of EMW the system of equations in the formalism of the FDTD method:

\[ \vec{H} \left[ \frac{n}{k} \right] + \vec{D} \left[ \frac{n}{k} \right] = \vec{D} \left[ \frac{n}{k} \right] + \vec{H} \left[ \frac{n}{k} \right] \]

(7)

where \( n \) is a step in the one-dimensional \( k \)-space, \( I \) is an auxiliary matrix, and \( \Delta x, \Delta t \) describe respectively discretization of coordinates of the position and time, and are related for the stability of the simulation by Courant condition [25]

\[ \Delta t \leq \frac{\Delta x}{\sqrt{N \cdot c_0}} \]

(8)

where \( N \) is the dimension of the simulation, and \( c_0 \) is the EMW velocity of the material. Simulation used a soft source of EMW, the area has been limited by absorbing boundary conditions (ABC), and a wavelength characteristic was prepared using FFT [25].
RESEARCH

In this study the behaviour of the electromagnetic wave passing through the superlattice ABABAB binary structure composed of lossless materials whose properties do not depend on the frequency of the electromagnetic wave, using the matrix method and the FDTD algorithm. Electromagnetic wave fell perpendicular to the sample surface by what the type of polarization does not affect the properties of transmission. Binary superlattice symmetry makes the structure ABABAB transmission is the same as transmission of the structure BABBAB. Due to the use multilayers as a filters of visible light the calculation performed for the wavelength range of 300 to 750 nm. The refractive indexes materials of the layers are \( n_A = 3 \), \( n_B = 2 \). And a value of the thickness varies in the range from 100 to 200 nm.

**Influence of the amount of clusters AB in the transmission properties**

Figure 1 shows how the transmission properties of the multilayer changes with increasing number of pairs of layers AB. Thicknesses of the individual layers are \( d_A = d_B = 200 \) nm what gives a sample thickness increase 400 nm with each increase of the parameter \( n_{kl} \) determining the number of repetitions of cluster AB. The structures in Figures 1 and 2 was surrounded by air so that the refractive index before \( n_{in} \) and after \( n_{out} \) the structure was equal to 1.

In Figures 1a and 1b, respectively, for samples with the structures of AB and ABAB it can be seen changes in transmission as a function of the size of the wavelength of light, but has not yet outlines the structure of band gaps. By increasing the number of consecutive pairs of layers (Fig. 1c÷j) can be seen at wavelengths near the 340, 500 and 670 nm clearly the formation of photonic band gaps.

Figure 2 was created by the imposition of all the graphs in Figure 1. It can be seen that increasing the number of layers influences on the formation and stabilization of the band gaps for given, specific to the structure, electromagnetic wavelengths.

Influence of the environment on the superlattice transmission

The graphs in Figure 3 describe the EMW transmission in wavelength function for the parameters of binary superlattice: \( n_A = 3 \), \( n_B = 2 \), \( d_A = d_B = 200 \) nm, \( n_{kl} = 10 \). The following graphs show how it changes the structure of the transmission according to the refractive index of the medium in which is placed the multilayer.

The environment has no effect on the structure of band gaps, but influences of the nature of the interband (Fig. 3).

It should be noted that the most interesting filtration properties of superlattice have refraction indexes close to the value of refractive index of the environment where the fluctuations in the transmission are smaller interband.

Influence of layer thickness on the shift and broadening of band gaps

Figure 4 shows the influence of increasing the thickness of the cluster on the occurrence of band gaps shift towards higher wavelengths. Shift was observed for the band gap in Figure 4a near a wavelength of 340 nm, and the results are summarized in Figure 5, which shows the linear nature of the change. In Figure 6 can be seen how to change the width of the control band gap as a function of the thickness of a single layer.
Analysis of the behaviour of electromagnetic waves in binary superlattice using the FDTD algorithm

In order to examine the behaviour of a monochromatic electromagnetic wave having a wavelength equal to the wavelength of the band gap analysis was performed using the FDTD algorithm, during which were determined by FFT (Fast Fourier Transform) wavelength characteristics. Layer thicknesses were equal to 200 nm, and 5 nm was the resolution of simulation (test area divided into 1300 equal parts). The time step was $8.3391 \times 10^{-15}$ s and was selected to fulfill the Courant stability condition. The refractive indexes of the layers were respectively $n_A = 3$, $n_B = 2$.

The calculations were conducted for 8000 time steps when the outgoing electromagnetic wave structure has been stabilized [22].

EMW penetrating the superlattice structure, for each boundary layer is partially reflected and partially passes. Another part of the electromagnetic wave reflected inside the structure interfere with each other, which involves a change in the output wavelength and causes the formation of superlattice band gaps.

Figures 7 and 8 illustrate the characteristics of the wavelength of the monochromatic electromagnetic wave with wavelengths of 500 and 337 nm corresponding to photonic band gaps. Interference within the material changes the wavelength distribution and creates peaks around the gap area.

Figure 9 shows the behaviour of the electromagnetic wave when it is illuminated by a wave length corresponding to full transmittance. It is important that at each of the figures from 7 to 9 we can see, all the band gaps.
Based on the study it can be concluded that the matrix method and

Fig. 9. The wavelengths characteristic in the FDTD simulation of the structure illumination of monochromatic light with a wavelength 640 nm

Rys. 9. Charakterystyka długości fali w symulacji FDTD dla struktury oświetlanej światłem monochromatycznym o długości fali 640 nm

CONCLUSIONS

Based on the study it can be concluded that the matrix method and FDTD very well complement the study of photonic properties of multilayer structures. It has been found that the presence of the photonic band gap depends strongly on the number of superlattice layers.

The environment of the multilayer structure does not affect the existence of band gaps, but it strongly influences the interband areas. Increasing the thickness of the superlattice layers shifts in a linear photonic band gaps toward the higher wavelength and the influences of their size.

The use of the FDTD method has allowed to illustrate the behaviour of electromagnetic waves in areas of high and low transmission.

REFERENCES