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The implementation of the electromagnetic wave propagation algorithm in superlattices

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Analysis and modelling

ABSTRACT

Purpose: The subject of paper is the implementation of FDTD algorithm for study the electromagnetic wave propagation and to appoint the wavelength distribution of the electromagnetic waves leaving the structure for monochromatic incident wave in the case of a wavelength range of the band gap and in the case of full transmission.

Design/methodology/approach: In the paper is implemented algorithm to study the monochromatic electromagnetic wave propagation in the system of quasi one-dimensional aperiodic, lossless and isotropic Severin superlattice using finite-difference time domain method (FDTD) in the C programming language.

Findings: The FDTD simulation comparison of the results with those obtained using the matrix method demonstrate good correlation between the two methods. The use of the FDTD method and Fourier transforms (FFT) allows for a more complete picture of the observed phenomena, along with the distribution of time in which it takes place.

Research limitations/implications: The structures analyzed in the paper material consisted of quasi onedimensional lossless and non-dispersive isotropic material. An important would be analysis of the lossy materials with dispersion. Analysis of two-dimensional space would allow to study of propagation of the incident wave different angles.

Practical implications: The simulation allows to understand the temporal distribution of the electromagnetic wave propagation in the superlattice structure for the full transmission rate, and in the case of the occurrence of photonic band gap.

Originality/value: The novelty is to use FDTD algorithm with FFT to study the behavior of the electromagnetic wave in the electromagnetic wave wavelength of band gap range. **Keywords:** Propagation; Superlattice; FDTD; Optical filters

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<u>1. Introduction</u>

Photonic materials are used in many fields of science and industry [1-4]. Most often used in optoelectronics (fiber optics [5]), solid state physics [6], photonics (photonic crystals [7-11], quazicrystals [12-22]) and optics (as filters electromagnetic radiation [23], multilayer structures [24,27]).

Transmission properties of multilayer systems allow the use of them as a filter of electromagnetic radiation. Well-developed manufacturing technique of superlattices with specified thickness, layer sequence and type of material [28-31] allows to get structure with required filter characteristics. The internal structure of multilayer systems, a type of superlattice of the component materials, their spatial arrangement and the thickness of applied layers, resulting in lack of propagation of electromagnetic waves of specific wavelengths which incidents on an a given quazionedimmensional structure - the phenomenon of the photonic band gap. Emulation of properties of superlattice allows to examine the impact of structural parameters on the propagation of electromagnetic waves, which allows to adjust the system to the specific application and reduce the cost of performing a large number of test structures. To study the electromagnetic wave transmission the matrix method is used [32,33] and also the algorithm of finite-difference time domain (FDTD) [34].

The subject of this work is to implement the FDTD algorithm to study of the electromagnetic wave propagation and to determine the wavelength distribution of the electromagnetic waves leaving the structure for monochromatic incident wave in the case of a wavelength range of the band gap and in the case of full transmission. In order to present the FDTD method derived by Sullivan [35] characteristic of the system of equations describing the easiest way during the iterative in time t relationship between the intensity vectors of electric \vec{E} and magnetic \vec{H} fields was used.

$$\frac{\partial E}{\partial t} = \frac{1}{\varepsilon_r \varepsilon_0} \nabla \times \vec{H}$$
$$\frac{\partial \vec{H}}{\partial t} = -\frac{1}{\mu_0} \nabla \times \vec{E}$$
(1)

where ε_0 and μ_0 are, respectively, electric and magnetic permeability of vacuum, and ε_r is the relative permeability of the material. By limiting the amount of free states of intensities of electric and magnetic fields from the formula (1) to one state of freedom along the axis x of the vector of the electric field intensity and y respectively for the magnetic field intensity vector we obtain

$$\frac{\partial E_x}{\partial t} = -\frac{1}{\varepsilon_r \varepsilon_0} \frac{\partial H_y}{\partial z}$$
$$\frac{\partial H_y}{\partial t} = -\frac{1}{\mu_0} \frac{\partial E_x}{\partial z}$$
(2)

where the axis z indicates the direction of propagation of the electromagnetic wave. Denoting by $t = \Delta t \cdot n$ simulation time for

a time step Δt in the moment *n*, and by *k* specifying the point in space $z = \Delta x \cdot k$ discretized by step Δx and by replacing derivative to difference from equation (2) can be obtained

$$\frac{\frac{E_x^{n+\frac{1}{2}}(k) - E_x^{n-\frac{1}{2}}(k)}{\Delta t}}{\frac{H_y^{n+\frac{1}{2}}\left(k + \frac{1}{2}\right) - H_y^n\left(k + \frac{1}{2}\right)}{\Delta t}}{\frac{H_y^{n+\frac{1}{2}}\left(k + \frac{1}{2}\right) - H_y^n\left(k + \frac{1}{2}\right)}{\Delta t}} = -\frac{1}{\frac{1}{\mu_0}}\frac{E_x^{n+\frac{1}{2}}(k+1) - E_x^{n+\frac{1}{2}}(k)}{\Delta x}}{\frac{1}{2}}$$
(3)

According to the notation of FDTD method $H_y^n(k)$ determines for the time *n* in space *k* value of the magnetic field vector. In subsequent iterations, the value of $H_y^n\left(k+\frac{1}{2}\right)$ depends on the surrounding space values $E_x^{n-\frac{1}{2}}(k)$ and $E_x^{n-\frac{1}{2}}(k+1)$, which depend on the vectors of the surrounding meanetic field

which depend on the vectors of the surrounding magnetic field intensity. The structure of the subsequent iteration of the algorithm

shown in Fig. 1.



Fig. 1. Illustration of determining the value of intensity vectors of electric and magnetic fields in subsequent iterations of the algorithm [35]

Obtaining a distribution of electromagnetic wave wavelengths leaving the structure requires consideration of the Maxwell equations for electric induction vector \vec{D} . Normalization of the Gauss units of the electric field vector and the electric induction, according to equation (4), allows to simplify the calculations [36].

$$\widetilde{E} = \sqrt{\frac{\varepsilon_0}{\mu_0}} E$$
$$\widetilde{D} = \sqrt{\frac{1}{\varepsilon_0 \cdot \mu_0}} \cdot D$$
(4)

The value of the electric induction vector depends on the angular frequency $\omega = 2\pi f$ of electromagnetic wave, where f is

the frequency of electromagnetic wave propagating in the structure, according to the relation

$$\widetilde{D}(\omega) = \varepsilon_r \widetilde{E}(\omega) + \frac{\sigma}{j\omega\varepsilon_0} \widetilde{E}(\omega)$$
⁽⁵⁾

Taking into account (5) in equation (1) we get

$$\frac{\partial \widetilde{D}}{\partial t} = \frac{1}{\sqrt{\varepsilon_0 \mu_0}} \nabla \times \vec{H}
\widetilde{D}(\omega) = \varepsilon_r^*(\omega) \cdot \widetilde{E}(\omega)
\frac{\partial \vec{H}}{\partial t} = -\frac{1}{\sqrt{\varepsilon_0 \mu_0}} \nabla \times \widetilde{E}$$
(6)

where ε_r^* determines the dispersive size of the relative permeability of medium described by

$$\varepsilon_r^*(\omega) = \varepsilon_r + \frac{\sigma}{j\omega\varepsilon_0} \tag{7}$$

The σ is a coefficient describing the loss of an electromagnetic wave propagating in the material, and $j = \sqrt{-1}$. Magnetic induction vector can also be described as

$$\widetilde{D}(\omega) = \varepsilon_r \widetilde{E}(\omega) + \frac{\sigma}{j\omega\varepsilon_0} \widetilde{E}(\omega)$$
(8)

To be able to analyze by using the FDTD algorithm, equation (8) should be moved from the frequency domain to the time domain

$$\widetilde{D}(t) = \varepsilon_r \widetilde{E}(t) + \frac{\sigma}{\varepsilon_0} \int_0^t \widetilde{E}(t') \cdot dt'$$
⁽⁹⁾

Then, by replacing the integral for the sum of

$$D^{n} = \varepsilon_{r} E^{n} + \frac{\sigma \cdot \Delta t}{\varepsilon_{0}} \sum_{i=0}^{n} E^{i}$$
(10)

and by the use of additional auxiliary variable I we get

$$E^{n} = \frac{D^{n} - I^{n-1}}{\varepsilon_{r} + \frac{\sigma \cdot \Delta t}{\varepsilon_{0}}}$$

$$I^{n} = I^{n-1} + \frac{\sigma \cdot \Delta t}{\varepsilon_{0}} E^{n}$$
(11)

After the necessary transformations, the system of equations in the FDTD formalism describing the propagation of electromagnetic wave in a medium can be obtained

$$\begin{split} \widetilde{D}_{x}^{n+\frac{1}{2}}(k) &= \widetilde{D}_{x}^{n-\frac{1}{2}}(k) + \frac{1}{\sqrt{\varepsilon_{0} \cdot \mu_{0}}} \cdot \frac{\Delta x}{\Delta t} \bigg[H_{y}^{n} \bigg(k + \frac{1}{2} \bigg) - H_{y}^{n} \bigg(k - \frac{1}{2} \bigg) \bigg] \\ \widetilde{E}_{x}^{n+\frac{1}{2}}(k) &= \frac{1}{\varepsilon_{r} + \frac{\sigma_{r} \cdot \Delta t}{\varepsilon_{0}}} \cdot \bigg[\widetilde{D}_{x}^{n+\frac{1}{2}}(k) - I_{x}^{n+\frac{1}{2}}(k) \bigg] \\ I_{x}^{n+\frac{1}{2}}(k) &= I_{x}^{n-\frac{1}{2}}(k) + \frac{\varepsilon_{r} \cdot \Delta t}{\varepsilon_{0}} \cdot \widetilde{E}_{x}^{n+\frac{1}{2}}(k) \\ H_{y}^{n+1} \bigg(k + \frac{1}{2} \bigg) &= H_{y}^{n} \bigg(k + \frac{1}{2} \bigg) + \frac{1}{\sqrt{\varepsilon_{0} \cdot \mu_{0}}} \cdot \frac{\Delta x}{\Delta t} \bigg[\widetilde{E}_{x}^{n+\frac{1}{2}}(k) - \widetilde{E}_{x}^{n+\frac{1}{2}}(k+1) \bigg] \end{split}$$
(12)

In order to ensure the stability of the simulation time step Δt should be tied with spatial increment Δx and the speed of light in vacuum c_0 by the Courant's stability condition [37, 38]

$$\Delta t = \frac{\Delta x}{2 \cdot c_0} \tag{13}$$

To prevent the reflection of electromagnetic waves from the edge of the simulated area the boundary conditions must be defined. In this simulation the Absorbing Boundary Conditions (ABC) [39] were used defined by

$$E_x^n(0) = E_x^{n-2}(1) \tag{14}$$

To ensure stability of the simulation and good representation of the electromagnetic wave behavior the spatial step size should be selected according to

$$\Delta x = \frac{\lambda_0}{10}$$

$$\lambda_0 = \frac{c_0}{f} \tag{15}$$

In the paper a soft source of electromagnetic wave was used described for each run of the loop iterator i by

$$pulse = \sin(2\pi \cdot f \cdot \Delta t \cdot i)$$

$$E_x(k) = E_x(k) + pulse$$
(16)

In the time moment T for wave frequency f_m Fourier transformate can be obtained for electric field intensity vector E by

$$E(f_m) = \sum_{n=o}^{T} E(n \cdot \Delta t) \cos(2\pi \cdot f_m \cdot \Delta t \cdot n) - j \sum_{n=o}^{T} E(n \cdot \Delta t) \sin(2\pi \cdot f_m \cdot \Delta t \cdot n)$$
(17)

This is done by declaring two arrays in space k defining the real part rp(m,k) and imaginary part ip(m,k) of equation (17), which can be described as

$$rp(m,k) = rp(m,k) + E(k)\cos(2\pi \cdot f_m \cdot \Delta t \cdot n)$$

$$ip(m,k) = ip(m,k) + E(k)\sin(2\pi \cdot f_m \cdot \Delta t \cdot n)$$
(18)

and then determine the amplitude A(m,k) and phase F(m,k) for investigated frequency f_m , and thus the wavelength by

$$A(m,k) = \sqrt{(rp(m,k))^{2} + (ip(m,k))^{2}}$$

$$F(m,k) = 2 \arctan \frac{\sqrt{(rp(m,k))^{2} + (ip(m,k))^{2}} - rp(m,k)}{ip(m,k)}$$
(19)

2. Implementation

The following is a complete listing of a simple program written in C allowing to investigate the characteristics of electromagnetic wavelengths leaving the structure for a monochromatic incident wave. Each additional line of the program begins with a line number, and after the colon the correct code is placed. Program lines are interspersed with commentaries on the line below.

The load of standard libraries

1:#include <math.h> 2:#include <stdio.h> 3:#include <stdlib.h>

The size of the spatial units in ddx

4:#define KE 1300

Discretization of the frequency range for which the Fourier analysis is done

5:#define IC 90

Program's main function

6:int main(int argc, char *argv[]) 7:{

Block of variable definitions. Defined arrays specifying respectively the intensity of electric and magnetic fields, the two arrays defining the properties of space, arrays of electric induction and the auxiliary array.

8:float ex[KE], hy[KE], cb[KE], ca[KE], dx[KE], ix[KE];

Variables used to calculate the boundary conditions ABC

9:float ex_low_m1, ex_low_m2, ex_high_m1, ex_high_m2;

Auxiliary variables

10:int i, j, n, m, k, kc, s, kstart, NSTEPS;

Stores the simulation step

11:float T;

The relative permittivity of vacuum and materials A and B

12:float epsilon, epsilona, epsilonb;

The physical constants and auxiliary variables

13:float epsz, ddx, dt, freq_in, pi, sigma, eaf, sigmaa, sigmab;

Arrays used for determining the Fourier transform

14:float real_pt[IC][KE], imag_pt[IC][KE]; 15:float freq[IC], arg[IC], ampn[IC][KE], phasen[IC][KE]; 16:float real_in[IC], imag_in[IC], amp_in[IC], phase_in[IC]; 17:float mag[KE];

Variables used in file handling

18:FILE *fp, *fopen();

The physical constants. The permeability of vacuum and the number of π

19:epsz = 8.85419e-12; 20:pi = 3.14159;

Step in the space defined by the formula (15) in nanometers

21:ddx = 5.0e-9f;//nm Courant stability condition (13)

22:dt = ddx/(2*3e8);

The initial conditions of variables defining the boundary conditions ABC and material constants (sigma - vacuum loss factors and of materials A and B, epsilon - relative electric permittivity)

23:ex_low_m1 = 0.0f; 24:ex_low_m2 = 0.0f; 25:ex_high_m1 = 0.0f; 26:ex_high_m2 = 0.0f; 27:epsilon = 1.0f; 28:sigma = 0.0f; 29:sigmaa = 0.0f; 30:sigmab = 0.0f; 31:epsilona = 9.0f; 32:epsilonb = 1.0f;

The frequency of the electromagnetic wave incidenting on the structure

33: freq in = 937e + 12f;

Setting the startup variables

34:eaf = dt * sigma / (2 * epsz * epsilon); 35:for(k = 0; k < KE; k++){ 36: ex[k] = 0.0f; 37: hy[k] = 0.0f; 38: dx[k] = 0.0f; 39: cb[k] = 0.0f; 40: ix[k] = 0.0f; 41: ca[k] = 1.0f; 42: mag[k] = 0.0f; 43: for(m = 0; m < IC; m++){ 44: real_pt[m][k] = 0.;//real part 45: imag_pt[m][k] = 0.;//imaginary part 46: ampn[m][k] = 0.;//amplitude 47: phasen[m][k] = 0.;//phase 48: } 49: } 50:for(m = 0; m < IC; m++){ 51: real_in[m] = 0.; 52: imag_in[m] = 0.; 53: }

Determination of structure of the lattice and setting the initial values in the tables for considered model. Below aperiodic Severin's supergrid with L = 4. Determination of the structure is done by initiating tt matrix values, where material B is 2, and 1 is a material A

54:int tt[] = {2,2,1,2,2,2,1,2,1,2,1,2,2,2,1,2}; //B,B,A,B,B,B,A,B,A,B,A,B,A,B,B,B,A,B; A=1, B=2 55:for(i = 0; i < 15; i++) { 56: if(tt[i] == 1) { 57: for(k = 100 + i * 40; k < 140 + i * 40; k++) { 58: ca[k] = 1./(epsilona + sigmaa * dt / epsz); 59: cb[k] = sigmaa * dt / epsz; 60: } 61: }else { 62: for(k = 100 + i * 40; k < 140 + i * 40; k++) { 63: ca[k] = 1./(epsilonb + sigmab * dt / epsz); 64: cb[k] = sigmab * dt / epsz; 65: } 66: } 67: }

The scope of testing frequencies correspond to wavelengths in the range of 300-700 nanometers. Then determining the value of the tested frequencies.

68:float fmax = 1000e+12f; 69:float fmin = 430e+12f; 70:for(s = 0; s < IC; s++){ 71: freq[s] = fmin + (fmax - fmin) * (float)s / (float)(IC - 1); 72: } 73:for(m = 0; m < IC; m++){ 74: arg[m] = 2 * pi * freq[m] * dt; 75: printf("m = %2d\tFreq = %9.8f arg[m] = %7.5f\n", m, freq[m] * 1e-6, arg[m]); 76: }

Initialization of main loop

77:T = 0; 78:NSTEPS = 1; 79:while(NSTEPS > 0){

How many steps the user wants to perform before the value of electric and magnetic fields will be saved to the file

80: printf("NSTEPS --> "); 81: scanf("%d", andNSTEPS); 82: printf("%d \n", NSTEPS); 83: n = 0; 84: for(n = 1; n <= NSTEPS; n++){ 85: T = T + 1;

Determination of the electric induction

86: for(k = 1; k < KE; k++){ 87: dx[k] = dx[k] + 0.5 * (hy[k - 1] - hy[k]); 88: }

Soft source implementation (16)

89: pulse = sin(2 * pi * freq_in * dt * T); 90: dx[5] = dx[5] + pulse;

Determination of the value of the electric field and the auxiliary variable described by the formula (11)

91: for(k = 0; k < KE; k++){ 92: ex[k] = ca[k] * (dx[k] - ix[k]); 93: ix[k] = ix[k] + cb[k] * ex[k]; 94: }

The calculations necessary to determine the Fourier transform

95: for(k = 0; k < KE; k++){
96: for(m = 0; m < IC; m++){
97: real_pt[m][k] = real_pt[m][k] + cos(arg[m] * T) * ex[k];
98: imag_pt[m][k] = imag_pt[m][k] - sin(arg[m] * T) * ex[k];
99: }
100: }</pre>

The Fourier transform of the input signal determined for the first 100 iterations

101: if(T < 100){ 102: for(m = 0; m < IC; m++){ 103: real_in[m] = real_in[m] + cos(arg[m] * T) * ex[25]; 104: imag_in[m] = imag_in[m] - sin(arg[m] * T) * ex[25]; 105: } 106: }

Implementation of ABC boundary conditions

107: ex[0] = ex_low_m2; 108: ex_low_m2 = ex_low_m1; 109: ex_low_m1 = ex[1]; 110: ex[KE - 1] = ex_high_m2; 111: ex_high_m2 = ex_high_m1; 112: ex_high_m1 = ex[KE - 2];

Determination of magnetic field

113: for(k = 0; k < KE - 1; k++){ 114: hy[k] = hy[k] + 0.5f * (ex[k] - ex[k + 1]); 115: } End of main loop. Next display the intensity of electric and magnetic fields and then save them to files

```
116: }
116: }
117: for(k = 0; k < KE; k++){
118: printf("%3d %6.2f %6.2f\n", k, ex[k], hy[k]);
119: }
120: fp = fopen("Ex", "w");
121: for(k = 0; k < KE; k++){
122: fprintf(fp, "%6.2f\n", ex[k]);
123: }
124: fclose(fp);
125: fp = fopen("Hy", "w");
126: for(k = 0; k < KE; k++){
127: fprintf(fp, "%6.2f\n", hy[k]);
128: }
129: fclose(fp);</pre>
```

Calculation of the amplitude and phase of the input signal and the tested signal and save them to files.

```
130: for(m = 0; m < IC; m++){
131: amp in[m] = sqrt(pow(imag in[m], 2.) + pow(real in[m], 2.))
2.));
132: phase in[m] = atan2(imag in[m], real in[m]);
133: printf("%d: Re = \%8.4f, Im = \%8.4f, Amp = \%8.4f, Ph =
%7.2f\n",
134: m, real in[m], imag in[m], amp in[m], (180.0 / pi) *
phase in[m]);
135: for (k = 0; k < KE; k++)
136: ampn[m][k] = (1. / amp in[m]) * sqrt(pow(real pt[m][k], 2.))
+ pow(imag_pt[m][k], 2.));
137: phasen[m][k] = atan2(imag_pt[m][k], real_pt[m][k]) -
phase in[m];
138: }
139:
140: fp = fopen("Amp0", "w");
141: for(k = 0; k < KE; k++)
142: fprintf(fp, "%8.5f\n", ampn[0][k]);
143: }
144: fclose(fp);
145: fp = fopen("Amp1", "w");
146: for (k = 0; k < KE; k++)
147: fprintf(fp, "%8.5f\n", ampn[1][k]);
148: }
149: fclose(fp);
150: fp = fopen("Amp2", "w");
151: for (k = 0; k < KE; k++)
152: fprintf(fp, "%8.5f\n", ampn[2][k]);
153: }
154: fclose(fp);
155: fp = fopen("AmpAll", "w");
156: for(i = 0; i < IC; i++){
157: for(k = 0; k < KE; k++)
158: fprintf(fp, "%8.8f\n", ampn[i][k]);
159: }
160: }
161: fclose(fp);
162: fp = fopen("freq", "w");
163: for(k = 0; k < IC; k++)
```

164: fprintf(fp, "%8.8f\n", freq[k]); 165: } 166: fclose(fp); 167: printf("T = %5.0f\n", T); 168: } 169:return 0; 170:}

3. Research

In this study, isotropic, non-dispersive and lossless aperiodic Severin's supergrid of generation level number L=4 where the structure was defined by the formula

$$X_4^S = \{B, B, A, B, B, B, A, B, A, B, A, B, B, B, B, A, B\}.$$
 (20)

The refractive indices of the superlattice component materials are respectively $n_A = 3$, $n_B = 1$; refractive index of the medium $n_{in} = n_{out} = 1$; layer thicknes are $d_A = d_B = 200nm$; incident angle Θ relative to a normal to the quaziperiodic structure is set to zero. Calculations were performed for S - type polarization. Graph which has been designated using the matrix method, the transmission of wavelength for selected parameters is shown in Fig. 2.







Fig. 3. Characteristics of the wavelength propagating in the material for $\lambda_1 = 600nm$ and T = 1000

Determination of the transmission by the matrix method allows to notice the existence of a transmission for $\lambda_1 = 600 \text{ nm}$ and $f_1 = 5*10^{14}$ and the presence of a band gap for the wavelength $\lambda_2 = 500 \text{ nm}$ and the corresponding frequency $f_2 = 6*10^{14}$.



Fig. 4. Characteristics of the wavelength propagating in the material for $\lambda_1 = 600nm$ and T = 3000



Fig. 5. Characteristics of the wavelength propagating in the material for $\lambda_1 = 600nm$ and T = 8000



Fig. 6. Characteristics of the wavelength propagating in the material for $\lambda_2 = 500nm$ and T = 1000

Figs. 3, 4 and 5 show the characteristics of the wavelength obtained using the implemented algorithm for full transmission $\lambda_1 = 600nm$ and for the length of time of simulation *T* respectively 1000, 3000 and 8000.

In the diagrams from Figs. 6, 7 and 8 the wavelength characteristics of a band gap upon the occurrence of $\lambda_2 = 500nm$ and the length of simulation time *T* respectively 1000, 3000 and 8000 are shown. For processing the output files Mathematica software was used.



Fig. 7. Characteristics of the wavelength propagating in the material for $\lambda_2 = 500nm$ and T = 3000



Fig. 8 Characteristics of the wavelength propagating in the material for $\lambda_2 = 500 nm$ and T = 8000

4. Conclusions

In the paper is implemented algorithm to study the monochromatic electromagnetic wave propagation in the system quasi one-dimensional aperiodic, lossless and isotropic Severin superlattice using finite-difference time domain method (FDTD) in the C programming language.

FDTD simulation in comparison of the results with those obtained using the matrix method demonstrate good correlation between the two methods. The use of the FDTD method with the determination of the Fourier transform (FFT) allows for a more complete picture of the observed phenomena, along with the distribution of time in which it takes place.

The simulation allows us to understand temporal distribution of the electromagnetic wave propagation in the superlattice structure for the full transmission rate, and in the case of the occurrence of photonic band gap.

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