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A Study of the Propagation of Electromagnetic Pulses through Photonic Crystal Structures

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Abstract—A mathematical model for the study of two- and three-dimensional photonic crystals and of waveguide systems based on them was designed and applied. The numerical algorithm for the construction of the solution was built using such numerical methods as the method of finite differences in the time domain (FDTD), the TS/SF method, and the method of a perfectly matched layer (PML), which makes it possible to apply the algorithm under consideration to the study of other waveguide systems as well. The results of the simulation of particular waveguide systems are presented.

Keywords: photonic crystals, mathematical modeling, parallel computing.

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INTRODUCTION

A mathematical model for the investigation of waveguide systems based on photonic crystals was designed and applied in this study. The concept of photonic crystals (PC) was first suggested in 1987 by Eli Yablonovich [1, 2]. In the general case, a photonic crystal is a material whose structure features periodic variation of the refractive index. It is well known that crystals of all types can effectively scatter certain kinds of radiation under the condition that the parameters of the crystal lattice are on the same order of magnitude as the wavelength of the radiation. Likewise, photonic crystals that are transparent to a broad spectrum of electromagnetic radiation do not transmit light with a wavelength comparable to the period of photonic crystal structure. These areas of the spectrum received the name photonic bandgaps (PBGs). When the bandgaps for all the directions in a crystal taken together overlap, this is referred to as a complete bandgap. The existence of a complete bandgap implies that within a certain range of the spectrum, no kind polarized light can propagate through the PC in either direction in one, two, or three dimensions.

1. THE NUMERICAL ALGORITHM

The propagation of an electromagnetic field in a photonic crystal system is described by Maxwell's equations. The algorithm used in the study consists of the combined application of the method of finite differences in the time domain (the FDTD method), to solve Maxwell's equations, the method of a perfectly matched layer (the PML method), to implement the boundary conditions, and the method of total and scattered fields (the TF/SF method), to drive the field source.

We demonstrate the numerical algorithm for solving the problem with a two-dimensional rectangular domain $S = \{(x, z): 0 \le x \le a, 0 \le z \le b\}$ (Fig. 1).

The algorithm is built upon the FDTD method [3, 4]. We introduce a difference net $\omega_h = \{x_i = ih_x, z_j = jh_z, i = 0, 1, ..., N_x, j = 0, 1, ..., N_z\}$ in the specified domain [5]. A net $\omega_s = \{t_s = s\tau, s = 0, 1, ...\}$ with respect to the time variable is introduced as well. We designate the value of net-point function F at some point (x_i, z_j) of the net at an instant of time t_s as $F^s_{i,j} = F(ih_x, jh_z, s\tau)$. In accordance with the FDTD method the E_y component of

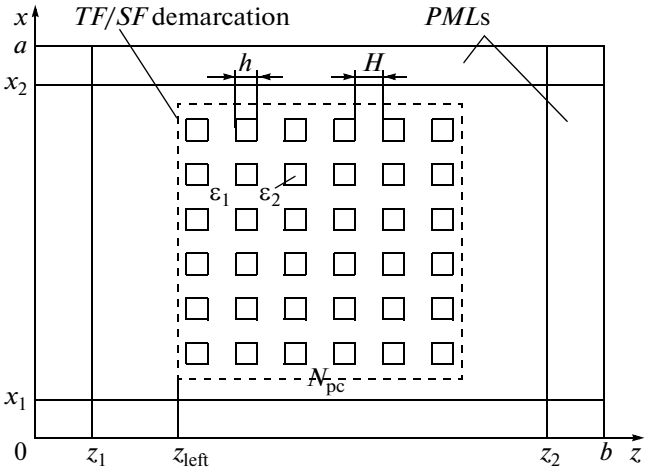

Fig. 1. A diagram of the computation domain.

the field is considered at net points (i, j) of the domain at instants of time t_s, whereas the H_x and H_z components, at intermediate points $(i, j + 1/2)$ and $(i + 1/2, j)$ and at intermediate instants of time $s + 1/2$, i.e., at fractional net points and fractional instants of time. This approximation makes it possible to write spatial and time derivatives from Maxwell's equations in terms of central differences and obtain a difference approximation to the solution. To take one example, for the E_y component

$$(E_y)_{i,j}^{s+1} = (E_y)_{i,j}^{s} + \frac{\tau}{\varepsilon_0\varepsilon_{i,j}h_z}[(H_x)_{i,j+1/2}^{s+1/2} - (H_x)_{i,j-1/2}^{s+1/2}]$$

$$- \frac{\tau}{\varepsilon_0\varepsilon_{i,j}h_x}[(H_z)_{i+1/2}^{s+1/2} - (H_z)_{i-1/2,j}^{s+1/2}].$$

The absorbing boundary conditions, which are determined using the method of a perfectly matched layer, or the PML method, are used in the developed algorithm to restrict the domain [6, 7]. In this method each component of an electromagnetic field is decomposed into two terms that satisfy certain equations. For example, in the two-dimensional case with a transverse magnetic (TM) field for the E_y component

$$\varepsilon_0\varepsilon\frac{\partial E_{yz}}{\partial t} + \sigma_z E_{yz} = \frac{\partial H_x}{\partial z},$$

$$\varepsilon_0\varepsilon\frac{\partial E_{yx}}{\partial t} + \sigma_x E_{yx} = -\frac{\partial H_z}{\partial x}.$$

The values of parameters σ_x, σ_z, σ_x^*, and σ_z^* depend on the position of a point in the domain; that is to say, within the PML, an area adjacent to the boundaries, they are nonzero and increase as the boundary of the domain of computation is approached, while in the rest of the domain of computation they are zero.

The method of a total field and a scattered field (the TF/SF method) [8] is employed in the algorithm under discussion to drive the waveguide system. This method consists in breaking down the domain of computation into two subdomains, the domain of a total field and the domain of a scattered field. Since Maxwell's equations are linear, the electromagnetic field can be expressed as the sum of incident and scattered fields; either of these also satisfies Maxwell's equations.

Only the scattered field is considered in the domain of the scattered field, and both the scattered and incident ones are considered in the domain of the total field. Special boundary conditions are laid down at the boundary between these domains. For instance, in the transverse electromagnetic (TE) case at the left boundary $z_{\text{left}} = h_z j_{\text{left}}$ these conditions have the following form:

$$(E_{y,\text{tot}})_{i,j_{\text{left}}}^{s+1} = (E_{y,\text{tot}})_{i,j_{\text{left}}}^{s} + \frac{\tau}{\varepsilon_0\varepsilon h_z}[(H_{x,\text{tot}})_{i,j_{\text{left}}+1/2}^{s+1/2}$$

$$- (H_{x,\text{scat}})_{i,j_{\text{left}}-1/2}^{s+1/2} - (H_{x,\text{inc}})_{i,j_{\text{left}}-1/2}^{s+1/2}].$$

Specifying the incident field in a particular way, one can consider the scattering of electromagnetic waves on an object located in the domain of total field. The incident field can be obtained, among other objects, by solving an auxiliary one-dimensional problem with the field established by current:

$$j(x, t) = \exp(0.2\pi(f_{\max} - f_{\min})t - 2)\sin(\omega t),$$

where $w = \pi(f_{\max} + f_{\min})$, $f_{\max}$, and $f_{\min}$ are variable parameters.

The algorithm is also designed for waveguide systems based on nonlinear photonic crystals with the constitutive equations

$$\mathbf{D} = \varepsilon_0\varepsilon\mathbf{E} + \varepsilon_0\chi|\mathbf{E}|^2\mathbf{E},$$

$$\mathbf{B} = \mu_0\mu\mathbf{H}.$$

The application of the FDTD method results in difference equations that do not allow the explicit expression of values of field components in the next time layer in terms of their values in the previous layer. Therefore, first the components of vectors **D**, **B**, and **H** are computed and then the solution of the equation for components of vector **E** is constructed using Newton's method [9]. The iterative schemes used to determine these components are the following:

$$(E_{yx})_{i,j}^{s+1}\Big|^{k+1} = (E_{yx})_{i,j}^{s+1}\Big|^{k}$$

$$- \frac{\varepsilon_0\varepsilon_{i,j}(E_{yx})_{i,j}^{s+1}\Big|^{k} + 4\varepsilon_0\chi^{(3)}[(E_{yx})_{i,j}^{s+1}\Big|^{k}]^3 - (D_{yx})_{i,j}^{s+1}}{\varepsilon_0\varepsilon_{i,j} + 12\varepsilon_0\chi^{(3)}[(E_{yx})_{i,j}^{s+1}\Big|^{k}]^2},$$

$$(E_{yz})_{i,j}^{s+1}\Big|^{k+1} = (E_{yz})_{i,j}^{s+1}\Big|^{k}$$

$$- \frac{\varepsilon_0\varepsilon_{i,j}(E_{yz})_{i,j}^{s+1}\Big|^{k} + 4\varepsilon_0\chi^{(3)}[(E_{yz})_{i,j}^{s+1}\Big|^{k}]^3 - (D_{yz})_{i,j}^{s+1}}{\varepsilon_0\varepsilon_{i,j} + 12\varepsilon_0\chi^{(3)}[(E_{yz})_{i,j}^{s+1}\Big|^{k}]^2}.$$

where k is the number of iteration. The values of the components of vector E at the preceding instant of time are taken as the zero approximation.

2. THE RESULTS OF COMPUTATION FOR TWO-DIMENSIONAL WAVEGUIDE SYSTEMS

First, the developed algorithm was applied in the computation of the passage of an electromagnetic pulse through a photonic crystal of a two-dimensional structure (Fig. 1). The values of parameters for the domain of computation were the following: $a = 1.9 \times 10^{-5}$, $b = 2.5 \times 10^{-5}$, $h_x = h_z = 5 \times 10^{-8}$, $\tau = 8 \times 10^{-17}$, $H = 3 \times 10^{-7}$, $h = 2 \times 10^{-7}$, $a = 5 \times 10^{-7}$, $\varepsilon_1 = 1$, $\varepsilon_2 = 11.56$, and $N_{\text{pc}} = 30$. The thicknesses of PMLs along the x and z axes were 1.9×10^{-6} and 2.5×10^{-6}, respectively.

The incident electromagnetic pulse features a central frequency of $0.5c/a$ and a halfwidth of $0.4c/a$. The spectrum of this pulse has the form shown in Fig. 2 as a dashed line.

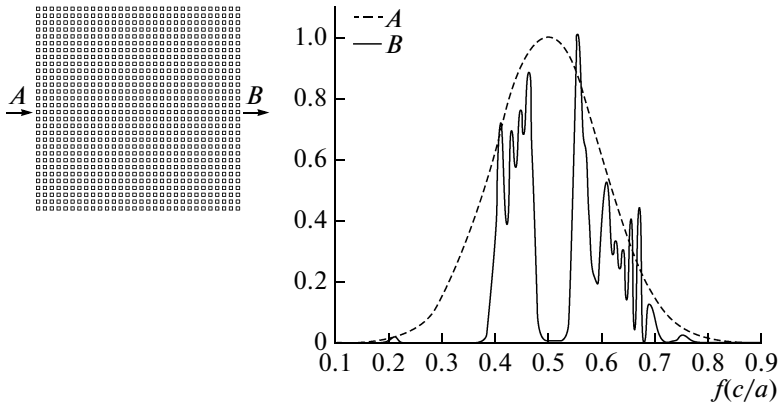

Fig. 2. The model of a two-dimensional photonic crystal and its spectral characteristics. Here *A* is the incident pulse and *B* is the transmission spectrum of the PC.

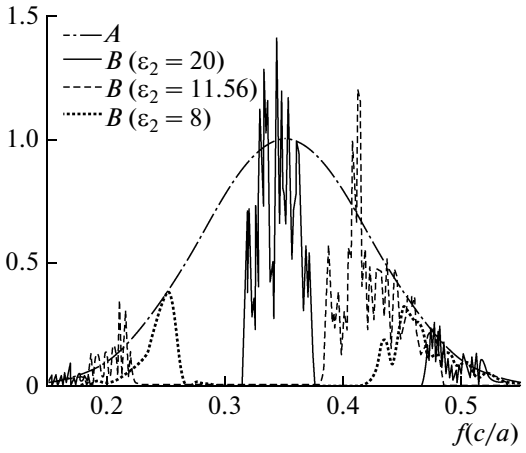

Fig. 3. The spectral characteristics of photonic crystals with different dielectric constants.

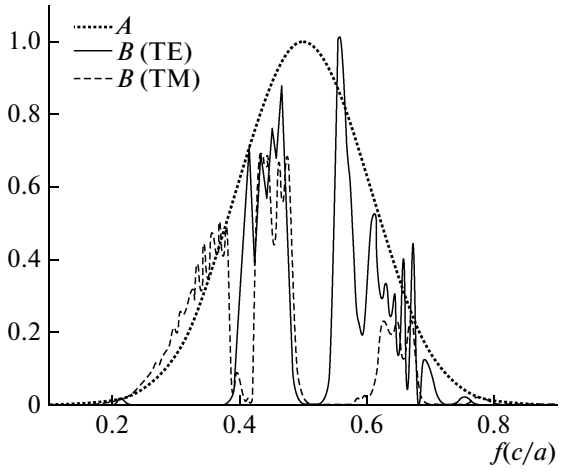

Fig. 4. The spectral characteristics of a photonic crystal for TE and TM waves.

As seen from Fig. 2, after the pulse traverses the photonic crystal, bandgaps, i.e., regions with near-zero transmittance, occur in the spectrum. A change in the dielectric constant of the crystal results in the displacement of bandgaps. The frequency $f_1 = \frac{\pi}{\sqrt{\varepsilon}}\frac{c}{a}$, where $\varepsilon = \varepsilon_1 v + \varepsilon(1 - \nu)$ and ν is the relative share of the medium with dielectric constant ε_1 in terms of volume, corresponds to the center of the first bandgap. For the parameters used, the value of this frequency is $f_1 = 0.305c/a$, which is confirmed in Fig. 2.

We reduce the dielectric constant of a crystal, that is to say, let $\varepsilon_2 = 8$. Then the frequency that corresponds to the center of the first bandgap will increase and assume the value $f_1 = 0.343c/a$. The spectral characteristic of such a crystal are displayed in Fig. 3, where it is evident that the bandgap shifted to the right, in the direction of increasing frequency. For a crystal with $\varepsilon_2 = 20$, the frequency corresponding to the center of the first bandgap is $f_1 = 0.249c/a$, i.e., the bandgap is to the left of the one for the original crystal.

Bandgaps exist for different polarizations. The computations described above were performed for the case of TE-polarization (when the vector of an electric field is parallel to the axes of rods). The spectral characteristics of a photonic crystal in the TM case (when the vector of the magnetic field is parallel to the axes of rods) are also shown in Fig. 4. From the figure it is evident that after they traverse the photonic crystal, electromagnetic pulses of different polarizations have spectra that share common bandgaps. Frequencies whose bandgaps are the same produce a complete bandgap, a frequency range wherein light of no polarization can propagate through the PC in either direction.

A photonic crystal waveguide can be obtained by removing a number of rods from the photonic crystal. Because there are bandgaps in a photonic crystal, the range wherein such waveguides operate is the same as

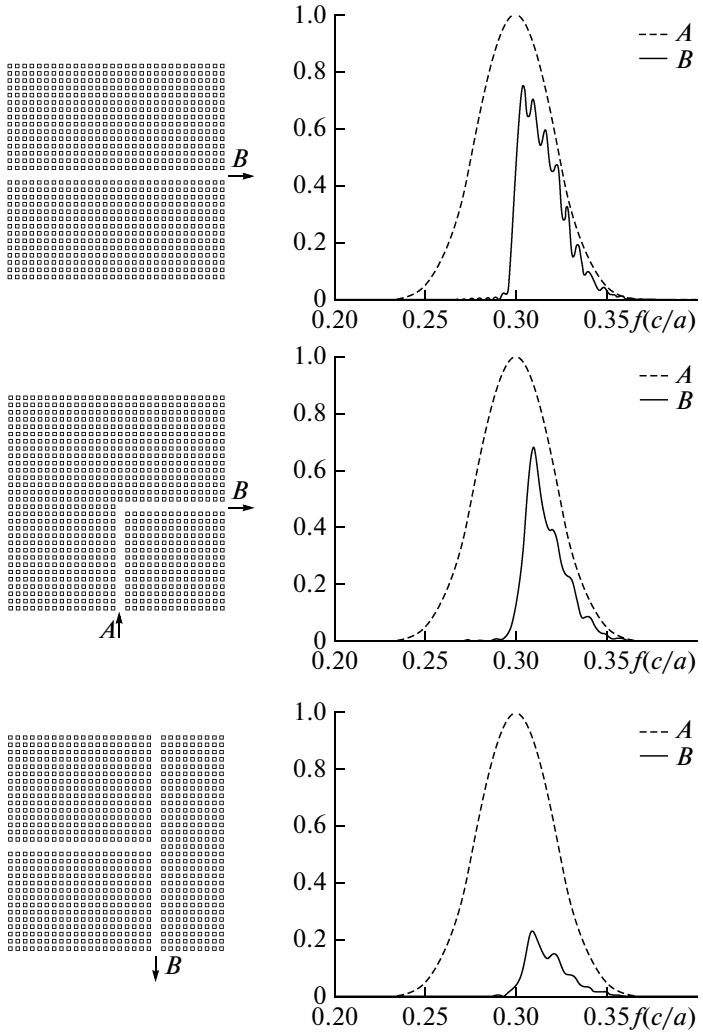

Fig. 5. Spectral characteristics of a photonic crystal waveguide, bend, and splitter.

the range of the bandgaps. The spectral characteristics of simple photonic crystal–based waveguide systems, namely, a waveguide, a bend, and a splitter are shown in Fig. 5.

The simulation of PCs in the form of H-fractals with the aid of the developed algorithm was also carried out in the context of the present study. The spectral characteristics of photonic crystals in the form of H-fractals are presented in Fig. 6.

3. THE COMPUTATION ALGORITHM FOR THREE-DIMENSIONAL SYSTEMS

The algorithm for the computation of a waveguide system in a three-dimensional domain is developed along similar lines as the algorithm for a two-dimensional domain described above. For a three-dimensional domain the problem is rather resource-consuming, therefore parallel programming is used in its solution.

The computations in the study were carried on a computer cluster belonging to the Research Computing Center of Moscow State University, on the SKIF MSU supercomputer Chebyshev. The programming technique most generally employed for parallel computers with distributed memory, the Message Passing Interface (MPI), was used.

The pattern for the parallelization of the computation is the following. The three-dimensional domain of computation is broken down into several identical parts sharing common boundary layers, depending on the number of processors involved in the computation, as shown in Fig. 7.

At every step with respect to time, the problem in each domain of computation is first solved independently on an individual processor and next the resulting solution for the points in boundary layers is passed to the processors that compute the neighboring domains. Thus, the computation of the electromagnetic field at every step with respect to time has two

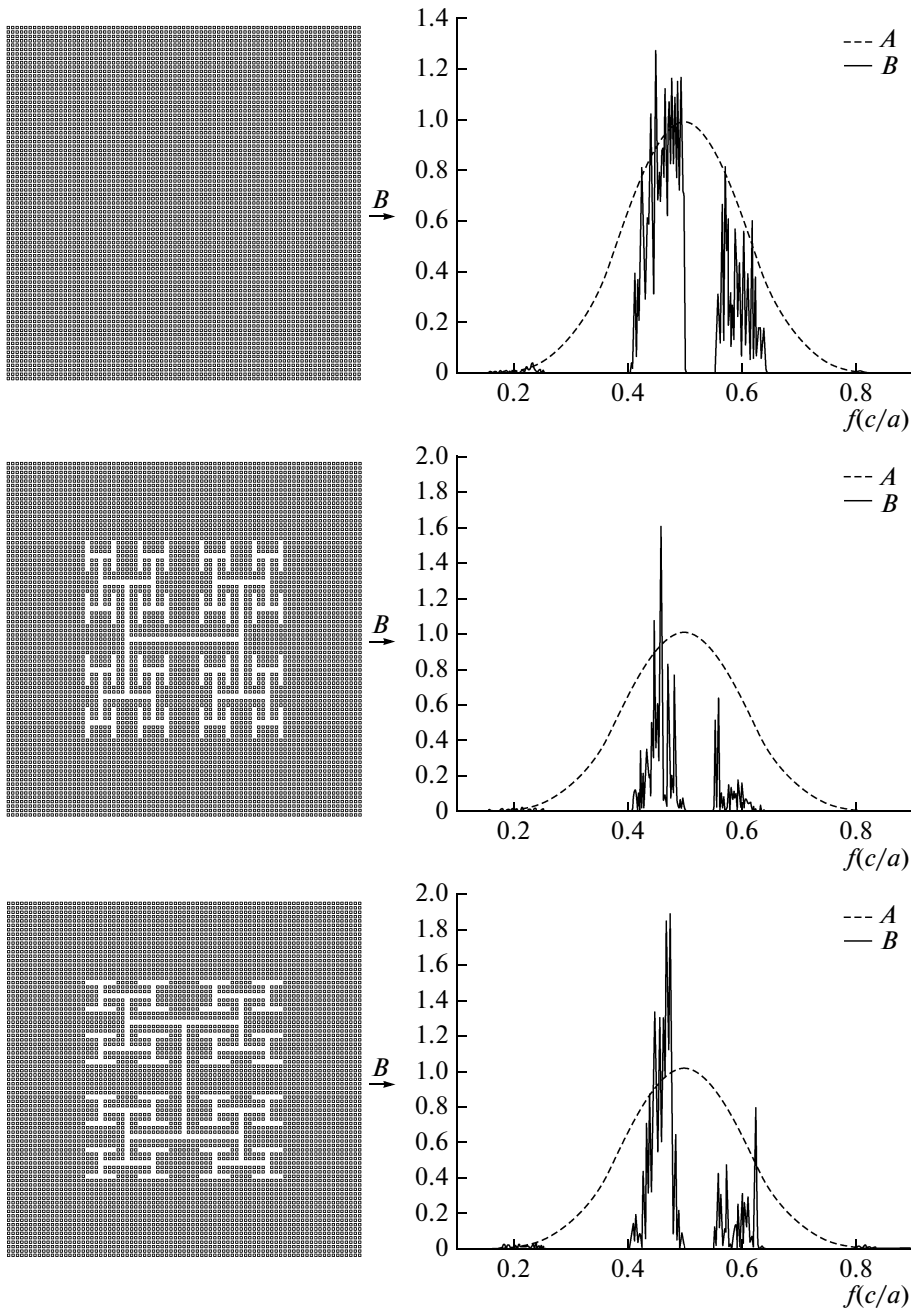

Fig. 6. The spectral characteristics of photonic crystals (a) of conventional structure and (b, c) in the form of H-fractals.

stages, the computation, which is carried out simultaneously in all domains, and the transmission of the data for the boundary layers, performed consecutively.

Such parallelization makes it possible to reduce the duration of the computation nearly as many times as the number of processors involved (without regard for the time spent on the transmission of data, which, as computations show, is small when the number of processors is not too great). The dependence of the duration of computation on the number of employed processors is shown in Fig. 8. This dependence aggress with Amdahl's law for acceleration:

$$S \le \frac{1}{f + \dfrac{1-f}{p}},$$

where f is the fraction of operations executed consecutively and p is the number of processors [10].

The computations in this study were carried out using from 20 to 32 processors, depending on the

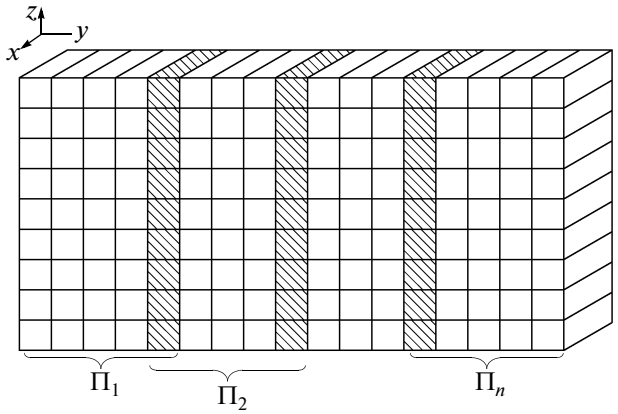

Fig. 7. The pattern for breaking the computation domain into several domains, depending on the number of employed processors (N). The boundary layers that are shared by neighboring domains are set off in grey.

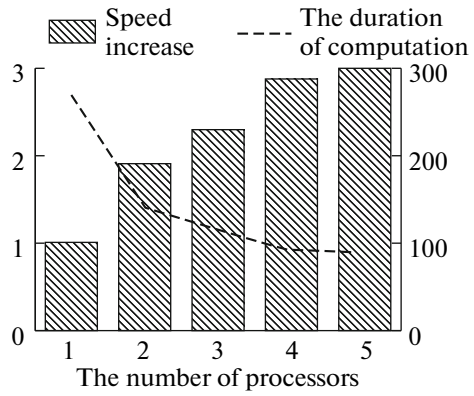

Fig. 8. The dependence of the duration of computation and speed increase on the number of processors.

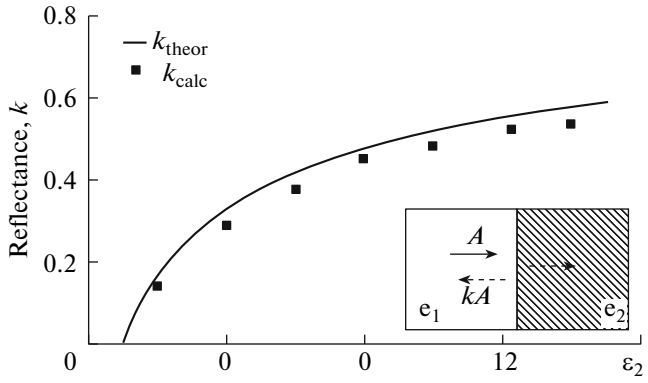

Fig. 9. Comparison of the computed and theoretical reflectance of the interface between two distinct dielectric mediums.

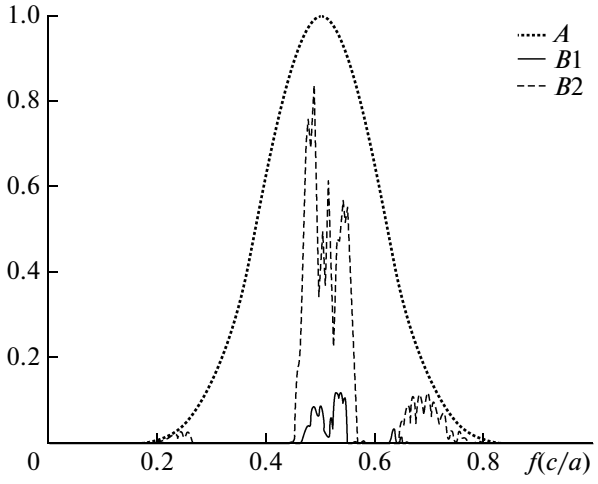

Fig. 10. The comparison of the spectra of the incident field A, scattered field $B2$ in the case of computation in a two-dimensional domain and the scattered field $B1$ in the case of a three-dimensional domain.

problem, with the domain of computation comprising up to $600 \times 800 \times 600$ points.

4. THE RESULTS OF COMPUTATION FOR THREE-DIMENSIONAL WAVEGUIDE SYSTEMS

As a test task for the program, we considered the problem of the reflection of a wave from the interface between two distinct dielectric mediums in a three-dimensional domain. The diagram of the computation domain and the plot of the dependence of the calculated reflectance on the insertion, as compared to the analytical solution, are given in Fig. 9. For the analytical solution we take the following well-known dependence:

$$k_{\text{theor}} = \frac{\sqrt{\varepsilon_2} - \sqrt{\varepsilon_1}}{\sqrt{\varepsilon_2} + \sqrt{\varepsilon_1}}.$$

Or, in view of the fact that in the computations $\varepsilon_1 = 1$,

$$k_{\text{theor}} = \frac{\sqrt{\varepsilon_2} - 1}{\sqrt{\varepsilon_2} + 1}.$$

The comparison shows good agreement between the result and the theoretical value.

In a three-dimensional domain we considered the problem of the passage of an electromagnetic pulse through a photonic crystal of a two-dimensional structure (see Fig. 2). The comparison of the result with a similar calculation for a two-dimensional domain is presented in Fig. 10. From the figure it can be seen that after the pulse traverses such a system, the scattering is much greater in the three-dimensional case, as compared to the similar computation for a two-dimensional case.

The results of the computations for a three-dimensional crystal are shown in Fig. 11. The structure of

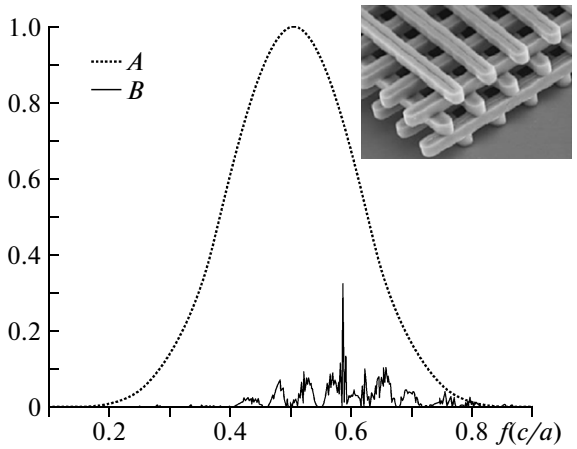

Fig. 11. The spectra of incident field *A* and of field *B* scattered by a three-dimensional photonic crystal. An example of the structure of such a crystal is displayed in the insertion at the right of the figure.

such a crystal is displayed at the right of the same figure. The following parameters were used in the computation: the dimensions of the rods that form the structure of the crystal were $3 \times 10^{-6} \times 3 \times 10^{-6} \times 90 \times 10^{-6}$ m, the number of layers was 30, and the dielectric constant of those layers was 12.25. The incident field impinged on the structure from above.

CONCLUSIONS

The investigations carried out in the present study showed that the developed algorithm can be effectively used for the computation of diverse waveguide systems, including those based on photonic crystals, in two- and three-dimensional domains.

The designed mathematical model provides a sufficiently full and adequate description of physical processes that take place in such waveguide systems. The program built upon the presented procedure is quite flexible and makes it possible to compute the spectral characteristics of devices based on photonic crystals of different structures. The combined application of the PML and TF/SF methods allows a substantial reduction of computation expenses through a decrease in the size of the computation domain. The parallelization of calculations also significantly lowers the computation time.

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