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Three-dimensional modeling of a photonic crystal spectra based on anodic aluminum oxide

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Three-dimensional optical modeling of a photonic crystal with cylindrical pores based on anodic aluminum oxide was carried out using the finite-difference time-domain method The influence of the pore radius and the angle of incidence of light on the position of the photonic band gap is shown. The calculation results are compared with the results of one-dimensional calculations using effective medium theory. Despite the fact that both theories showed good agreement with each other, one-dimensional calculation does not allow taking into account the influence of foreign materials on the spectral properties of the structure, which explains the need for the development of three-dimensional modeling.

Keywords: photonic crystal, aluminum oxide, porous material, photonic band gap, anodization, effective refractive index.

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In recent years, nanoporous materials gained great relevance in such areas as biotechnology and medical sciences [1], energetics [2]. The optical properties of said materials are of special interest as many of their applications are based on their interaction with photons, for example, for photovoltaic energy conversion [3,4]. So, ability to forecast the optic behaviour of the porous materials is the decisive factor for the design and optimization of the material structure for its application. Therefore, the numerical modeling of the optic properties of the materials [5] ensures the theoretical basis for analysis of their optic behaviour and characteristics of devices based on them.

The nanoporous materials can be manufactured using the electrochemical anodizing of materials such as silicon [6], titanium [7] and aluminium [8,9]. In particular, due to their physical and chemical properties the anodic aluminium oxide is a well platform for the devices associated with sensing, delivery of medicines and energy. Periodic change in anodizing conditions provides materials with periodic modulation of space refractive index. This results in occurrence of photon band gaps, i.e. spectral regions where photons distribution through the structure does not occur in one, in two or in all three directions. Such structures are called as photonic crystals (PhC). PhCs of anodic aluminium oxide are used as optical filters [10,11], sensors [12,13], lasers and luminescence amplifiers [14].

Optical modeling of PhC based on anodic aluminium oxide shall consider its different geometric characteristics. Such PhC is a self-ordered porous material with pores perpendicular to surface in hexagonal location, obtained by electrochemical etching of aluminum. The pores shape depends on the anodizing modes. Most frequently we observe PhCs with cylindrical [15] and branching pores [16]. Main geometric parameters, to be considered additionally to the refractive indices of the materials during the optic properties modeling, include pore spacing (a), pore radius (r), barrier layer thickness and pore length (L).

Two main approaches for the spectral properties modeling of such photonic crystal. The first approach is one-dimensional calculation using transfer-matrix method and based on PhC division to homogeneous layers. The refractive index of each layer is determined using effective medium theory. The first method disadvantage is impossibility to strictly consider the influence of foreign materials [17,18] on spectral properties of the structure. The second method is direct three-dimensional modeling, for example, finite-difference time-domain (FDTD) method — ensures properties consideration of all materials. In present paper both methods are used, and their results are compared.

Schematic image of studied PhC made of anodic aluminium oxide is given in Fig. 1.

The optic properties of the structure were calculated by FDTD method. The structure was illuminated from top by plane wave with normal incidence along the axis z and polarization direction along axis y. The reflectance was calculated in top part of the modeling window. On side faces of the modeling block the periodic boundary condition were applied, and on top and bottom sides the boundary conditions of ideally boundary conditions of a perfectly matched layer (PML) were used. An adaptive mesh was used to accurately reproduce the pore shape. Although FDTD method is a comprehensive method and a well-proven tool which

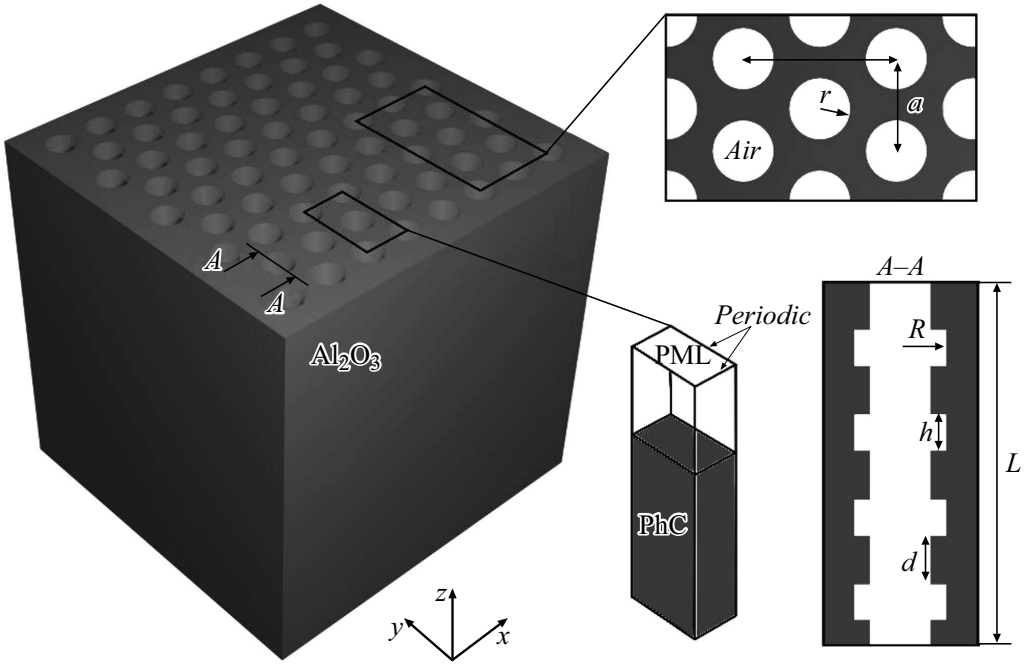

Figure 1. Schematic image of PhC made of anodic aluminium oxide. PhC is Al_2O_3 layer comprising a triangular lattice of air cylinders $L = 3.71\,\mu$m long with radius of $r = 40$ nm. Distance between pores is $a = 160$ nm. Along surface of cylinders at distance $d = 110$ nm 20 ring air thickenings with an outer radius $R = 60$ nm and height $h = 70$ nm are uniformly arranged. Refractive index is $n_{Al_2O_3} = 1.77$.

shows good compliance with the experimental results for PhC [19], the extensive tests were performed for each set of parameters to exclude unwanted refractions in PML.

Note that in addition to FDTD method for such structures a finite element method or Fourier modal method can be used. Anyway, the authors know studies where 3D-calculation is performed for spectra of photonic crystal based on anodic aluminium oxide.

PhC band gap is determined by the contrast of the refractive index of its layers. The higher the contrast is the larger band gap is. On porous PhC the refractive index of layers depends on bulk concentration of pores, their refractive index and matrix refractive index. In studied PhC made of anodic aluminium oxide the porosity of layers, and, hence, their refractive index depend on radiuses r, R and distance between pores (Fig. 1). These parameters control during anodizing ensures manufacturing of PhC with required band gap. For this effect demonstration we calculated dependence of PhC reflectance on wavelength of incident light and radius r at fixed radius of thickenings $R = 60$ nm and distance between pores $a = 160$ nm. The calculation results are presented in Fig. 2.

It is evident that if r increases the band gap decreases as the optical contrast between PhC layers becomes lower. So, at $r = 60$ nm the refractive indices of layer become equal, and, hence, the band gap disappears. Note that the refractive index decreasing of one PhC layer results not on;y in band gap decreasing, but also to change in its location. So, the band gap center upon radius r increasing from 40 to 50 nm shifts by 51.1 (from 541.1 to 490 nm).

Additionally to direct 3D-modeling the spectral properties of PhC based on anodic aluminium oxide can be calculated using 1D-method of transfer-matrix. The effective refractive indices of n_{eff} layers in PhC in this case will represent the combination of refractive indices of air n_{air} and aluminium oxide $n_{Al_2O_3}$. There are different effective medium approximations [9], which allow determining the optical properties of such media, including the Bruggeman, Maxwell Garnett, and Landau–Livshits/Luenga, Moneke, Lorenz–Lorenz approaches, and complex refractive index method. Each of the theories describes the effective dielectric permittivity of a heterogeneous two-component medium containing inclusions of various shapes and volume fractions of components. Inspite the fact that each model of the effective medium has its limits of applicability, it seems surprising that they all give similar values of refractive indices for the layers of PhC from Al_2O_3 [20].

Layers porosity of studied PhC is determined as

$$f_1 = \frac{2\pi}{\sqrt{3}}\left(\frac{r}{a}\right)^2, \qquad f_2 = \frac{2\pi}{\sqrt{3}}\left(\frac{R}{a}\right)^2. \tag{1}$$

In present paper we used Bruggeman approximation to determine the effective refractive indices of PhC layers

$$f\left(\frac{n_{air}^2 - n^2}{n_{air}^2 + 2n^2}\right) + (1-f)\left(\frac{n_{Al_2O_3}^2 - n^2}{n_{Al_2O_3}^2 + 2n^2}\right) = 0, \tag{2}$$

it assumes close concentrations of components.

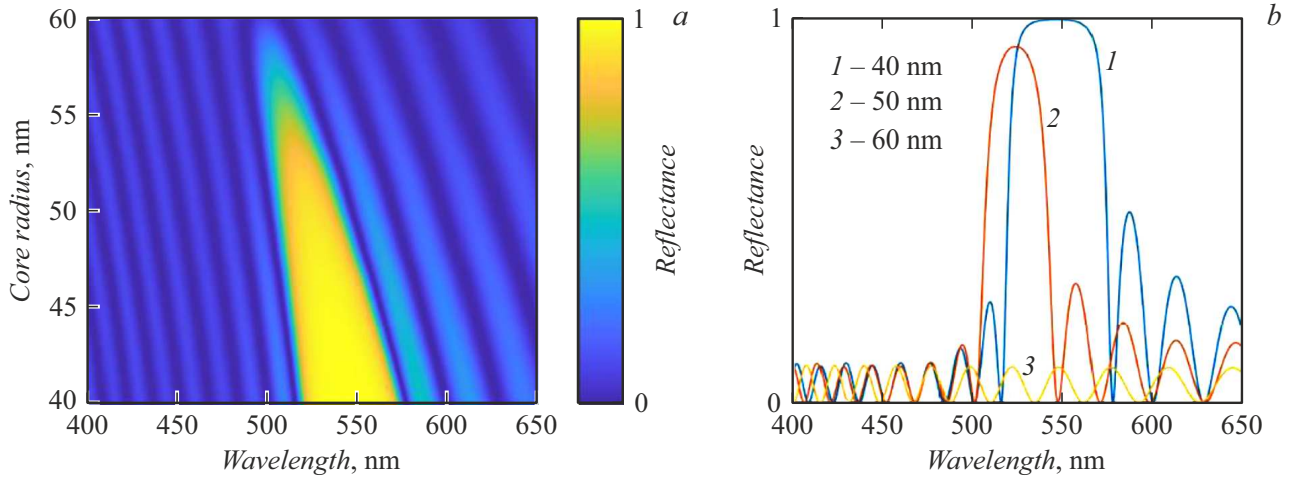

Figure 2. *a* — PhC reflectance spectra at different radiuses of air pores r. *b* — PhC reflectance spectra at $r = 40$ (*1*), 50 (*2*), 60 nm (*3*) and fixed other structure parameters.

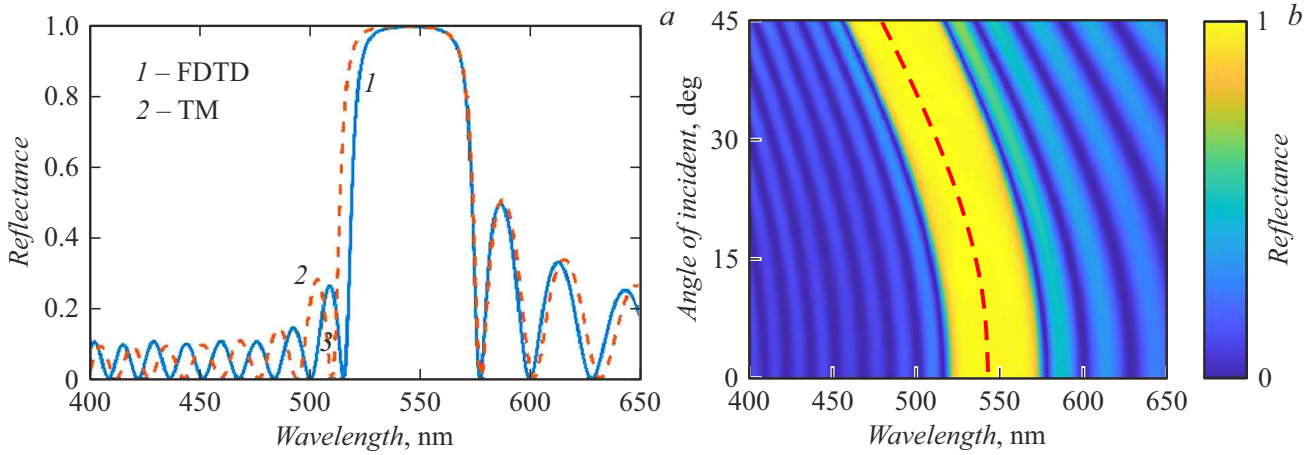

Figure 3. *a* — reflectance spectra of PhC made of anodic aluminium oxide calculated by FDTD method and transfer-matrix method considering Bruggeman effective medium model. Inaccuracy of the effective medium model resits in minor widening of band gap. *b* — angular dependence of the reflection spectrum of PhC for TE-polarized wave. Dashed line shows position of band gap center calculated using formula (3).

Thus, for structure showed in Fig. 1, the porosity of layers was $f_1 = 22.6\%$ and $f_2 = 51\%$, respectively. The refractive indices of PhC layers were calculated based on f_1, f_2 and formula (2): $n_1 = 1.59$ and $n_2 = 1.36$, respectively. By transfer-matrix method using thickness of layers d and h and refractive indices n_1 and n_2 the refraction spectra of PhC was calculated. Comparison of spectra calculated by FDTD method and by transfer-matrix method is given in Fig. 3, *a*. It is evident, that results obtained by two different methods are in good agreement.

When the refractive indices of the PhC $n_1 \approx n_2$ layers are close, the spectral position of PhC band gap satisfies the Bragg–Snell law, which can be written as [9]:

$$m\lambda = 2\Lambda\sqrt{n_{eff}^2 - n_{air}^2 \sin^2\theta}, \qquad (3)$$

where λ — wavelength of band gap center, m — band order, $\Lambda = d + h$ — structure period, θ — angle of incidence, n_{eff} — effective refractive index of PhC, n_{air} — refractive index of environment.

The effective refractive index of PhC and the refractive indices of the n_1 and n_2 layers are related to each other and the thicknesses of d and h layers a

$$n_{eff}^2 = \frac{d}{\Lambda}n_1^2 + \frac{h}{\Lambda}n_2^2. \qquad (4)$$

Fig. 3, *b* shows angular dependence of reflectance spectra of PhC made of anodic aluminium oxide, the dependence was calculated by FDTD method. Figure shows that the band gap of PhC shifts to blue region of the spectrum, as this is predicted by expression (3). Note that the results obtained using expression (3) are in good agreement with the results of direct numerical calculation.

So, paper presents the procedure of numerical 3D FDTD calculation of spectral properties of the photonic crystal based on anodic aluminium oxide. The method benefit is the possibility to consider spectral and structural features of the materials. The reflectance spectra were calculated upon varying of pore diameter, and angle of incidence of light. The results were compared with results of 1D-calculation by transfer-matrix method. For the refractive indices determination of crystal layers the theory of effective medium in Bruggeman approximation was used.

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Conflict of interest

The authors declare that they have no conflict of interest.

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