FDTD simulation of the electromagnetic field surface states in 2D photonic crystals

Kirill I Zaytsev[1], Vladimir S Gorelik[1,2], Alexey M Khorokhorov[1] and Stanislav O Yurchenko[1]

[1] Bauman Moscow State Technical University, Moscow, Russia
[2] Lebedev Physical Institute of the Russian Academy of Sciences, Moscow, Russia

E-mail: kirzay@gmail.com

Abstract. FDTD simulation was applied to study an optical field structure near the $2D$ photonic crystal surface. An effect of the optical field intensity redistribution was demonstrated for the first time. Spatial distribution of light intensity contains sharp peaks, focused in a certain parts of the crystal structure. The intensity peaks' magnitude could be very high. In case the incident light wavelength corresponds to the photonic crystal bandgap, the light could penetrate in a small depth into the crystal, but magnitude of the intensity peaks becomes several times higher in comparison to magnitude of the light intensity in the equal but homogeneous medium. Observed effect could be used for the enhancement of the light-matter interactions efficiency, for instance, for effective nonlinear conversion of light with photonic crystals, for Raman spectroscopy of small particles injected in crystals and etc.

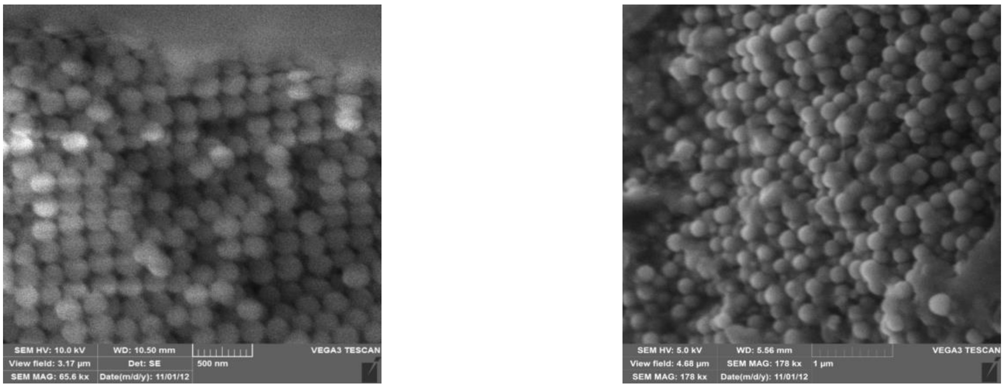
1. Introduction and background

Photonic crystal is the structure characterized by the periodic spatial distribution of optical properties. The period of the optical properties' fluctuations is comparable to the wavelength of electromagnetic field [1],[2]. Usually the photonic crystals are formed of nanoparticles or nanowires. An example of natural photonic crystal is opal. It consists of the spherical quartz globules, organizing the face-centered-cubic lattice [3]. The diameter of the globules varies from 200 to 500 nm, and the approximate size if interglobular cavities is $10\ nm$. The properties of photonic crystal could be modified by filling the cavities with liquids or solids (figure 1).

The periodicity of the photonic crystal structure leads to the specificity in dispersion relation for photonic crystal. The photonic crystal is characterized with the presence of the bandgaps in the dispersion curves [4]-[7]. The easiest way to describe the principles of the bandgaps appearance is to use the 1D equivalent of the 3D globular face-centered-cubic lattice photonic crystal [8]. In the figure 2a the equivalent 1D periodic structure of the photonic crystal is presented. According to the Bloch's theorem, the solution of the Helmholtz equation in the periodic optical structure has the following form:

$$\tilde{u}(z) = \tilde{u}_K(z)\, exp(-iK(\omega)z)\,, \quad (1)$$

where $\tilde{u}_K(z) = \tilde{u}_K(z + \Lambda)$ is a periodic complex function with the period Λ, and $K(\omega)$ is the dispersion relation of the 1D photonic structure. It is easy to find rigorous solution for $K(\omega)$ [8]:

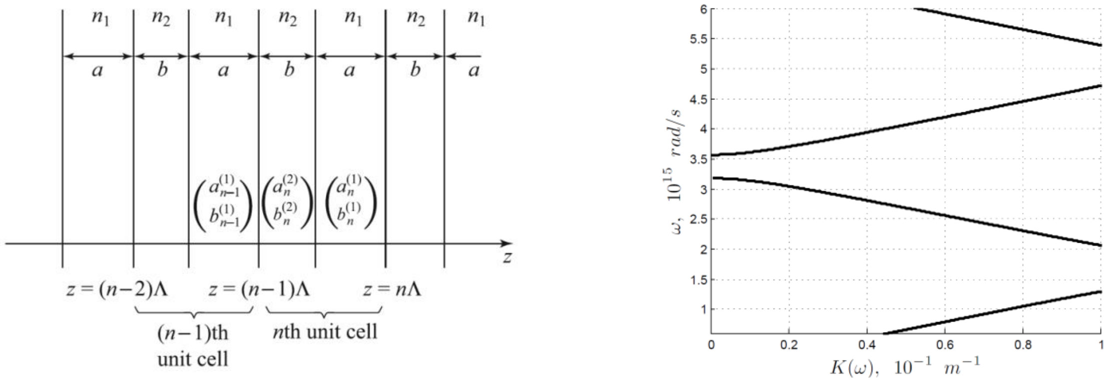


(a) **(b)**

Figure 1. Structure of $3D$ opal globular photonic crystal visualized with the atomic force microscopy: (a) is the initial opal matrix and (b) is the opal matrix filled with the $NaNO_2$.

$$\cos(K(\omega)\Lambda) = \cos(k_1 a)\cos(k_2 b) - \frac{1}{2}\left(\frac{n_2}{n_1} + \frac{n_1}{n_2}\right)\sin(k_1 a)\sin(k_2 b), \tag{2}$$

where a and b are the thicknesses of the layers, n_1 and n_2 are the refractive indexes of the media, k_1 and k_2 are the wavenumbers of the media. In the figure 2b the dispersion curve example is shown. The function $K(\omega)$ corresponds to the 1D photonic crystal structure with the following parameters: $a = 190\,nm$, $b = 60\,nm$, $n_1 = 4$, $n_2 = 3$. The dispersion relation contains several bandgaps, the region of the positive and negative group refractive indexes. The function $\tilde{u}_K(z)$ could be also found, for example, utilizing the perturbation theory.



(a) **(b)**

Figure 2. Equivalent 1D photonic crystal characteristics: (a) is a scheme of equivalent $1D$ structure, (b) is dispersion curves of the $1D$ structure with $a = 190\,nm$, $b = 60\,nm$, $n_1 = 4$, $n_2 = 3$.

One-dimensional model of the photonic crystal (figure 2) could be used to describe the light distribution in the volume of medium. One of the most important problems of the photonic crystal technology is the examination of the effects of light interactions with photonic crystals, which appear near the air/crystal interface. The present paper contains the results of the numerical simulation of the electromagnetic field structure near the air/crystal boundary.

2. Results

The FDTD simulation [9] was implemented to study the spatial distribution of light intensity near the interface between the air and the $2D$ photonic crystal. $2D$ photonic crystal model is presented in the figure 3a. The medium consists of cylinders with the diameter $d = 250nm$. The refractive index of the cylinder medium is $n = 2$. The matrix of cylinders is filled with the medium, which refractive index is $n = 3$. The plane electromagnetic wave reached the surface of the crystal from the left side. The crystal size in all directions is much bigger than the incident light wavelength. It helps to prevent the appearance of the numerical simulation errors.

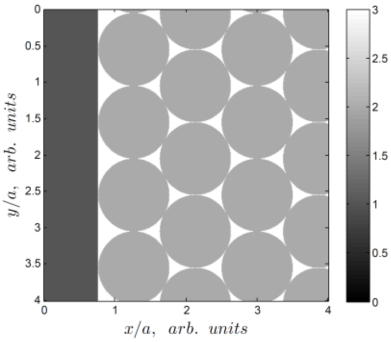
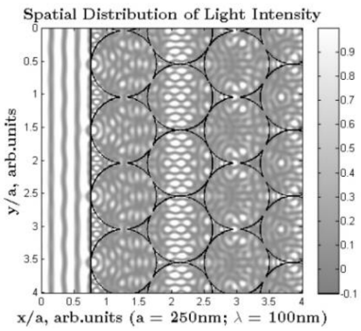


Figure 3. Spatial distribution of $2D$ photonic crystal refractive index.

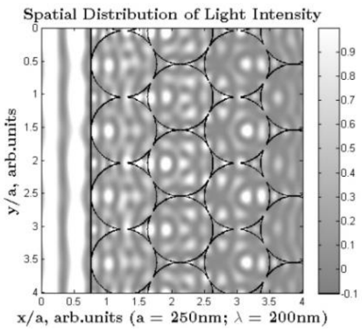
After the FDTD simulation the spatial distribution of the electromagnetic field magnitude time dependence $u_{sim}(x, y, t)$ was detected. The function $u_{sim}(x, y, t)$ was used for calculation of the light intensity spatial distribution:

$$I_{sim}(x, y) = \frac{1}{T}\int_0^T |u_{sim}(x, y, t)|^2 dt\,, \quad T \gg \lambda_t, \qquad (3)$$

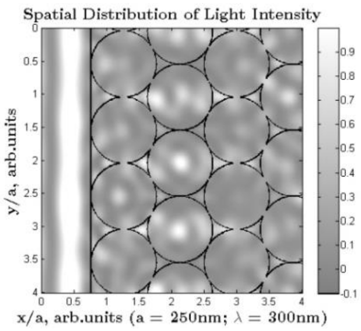
where T is an integration time, λ_t is a period of the electromagnetic field oscillations in each point of the modelling space. Figure 4 contains the results of numerical modelling for several light wavelength ranging from 100 to 600 nm.



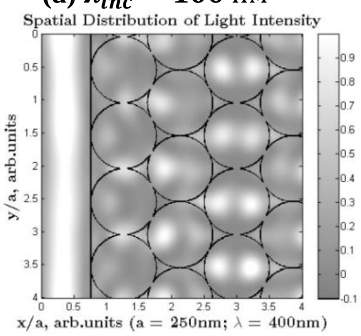
(a) $\lambda_{inc} = 100$ нм



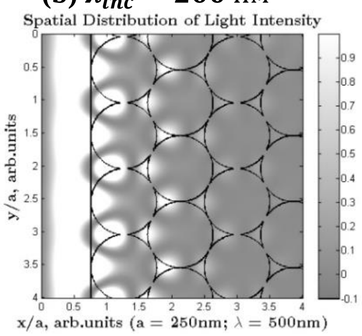
(b) $\lambda_{inc} = 200$ нм



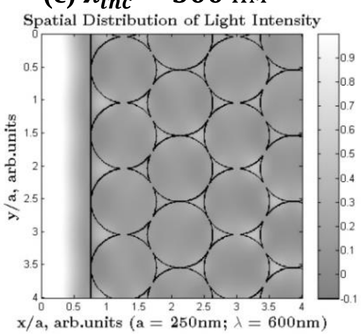
(c) $\lambda_{inc} = 300$ нм



(d) $\lambda_{inc} = 400$ нм



(e) $\lambda_{inc} = 500$ нм



(f) $\lambda_{inc} = 600$ нм

Figure 4. Spatial distribution of the electromagnetic field intensity near the interface between the air and the $2D$ photonic crystal.

In complete accordance with the Bloch's theorem (1) the function $I_{sim}(x, y)$ has a periodic character and decays with an increase of the crystal depth. All presented intensity distributions contain sharp peaks of light intensity. One could see, that the sharpest peaks and the highest decay of the field intensity corresponds to the wavelength $\lambda_{inc} = 500\ nm$ and it is equal to the wavelength of the crystal bandgap spectral position.

Conclusions

By means of the numerical FDTD simulation of the plane wave interaction with the air/2D-crystal interface, we have shown for the first time the effect of light intensity redistribution near the interface of photonic crystal. In case the incident light wavelength corresponds to bandgap of the photonic crystal, the peaks of the optical field intensity become several times higher than the intensity in equal homogeneous medium. The effect of the intensity redistribution is very important for a wide range of applications, in particular, for enhancement of nonlinear optical processes efficiency, for high efficient pumping of globular active structures, for increase of the Raman scattering on the particles injected in photonic crystals and others. It could become a basis for the creation of the new class of nonlinear optical media.

Acknowledgments

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