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CONDENSED-MATTER  
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# Specific Features of the Spectral Properties of a Photonic Crystal with a Nanocomposite Defect with Allowance for the Size Effects

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**Abstract**—The spectral properties of a one-dimensional photonic crystal (PC) with a structure defect (a layer of isotropic nanocomposite inserted between two multilayer dielectric mirrors) have been investigated. The nanocomposite consists of spherical gold nanoparticles dispersed in a transparent matrix; it is characterized by effective resonant permittivity. The dependence of the transmission and absorption spectra on the size and concentration of nanoparticles is analyzed. It is shown that the transmission spectrum contains, along with the band gap caused by Bragg diffraction of light, an additional nontransmission band due to the nanocomposite absorption near the resonant frequency.

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## INTRODUCTION

Photonic crystals (PCs) are metamaterials with a refractive index periodically varying in space; the period value allows for Bragg diffraction of light. An important property of PCs is the localization of electromagnetic waves on structural defects. In this case, additional allowed levels arise in the PC band gap, which correspond to localized defect modes. In the case of one-dimensional PC, a defect layer inserted between two multilayer dielectric mirrors behaves as a structure of Fabry–Perot microcavity type, and the localized defect modes are microcavity eigenmodes. The position and transmittance of defect modes, as well as the band gap shape and size, can be efficiently controlled by varying the geometric and structural PC parameters. New types of PC waveguides, nanocavities with a high  $Q$  factor, and low-threshold lasers have been developed based on PCs with defect modes, and some new ways were proposed to increase the efficiency of nonlinear optical processes [1, 2].

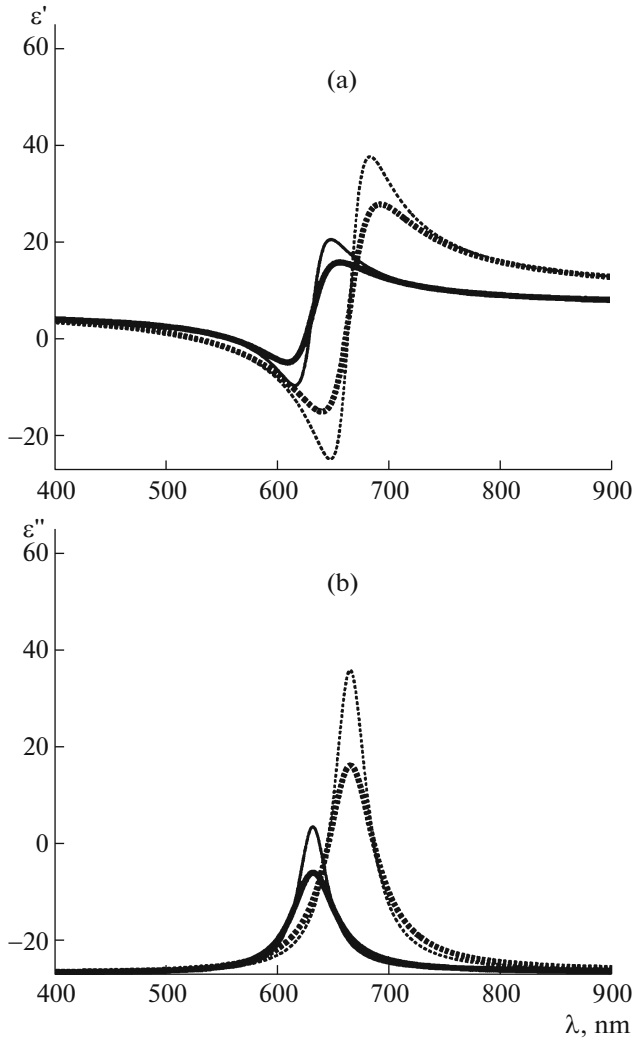
New techniques for controlling light can be implemented using a defect layer in a one-dimensional PC in the form of an isotropic nanocomposite layer consisting of spherical metal nanoparticles dispersed in a transparent matrix [3–6]. SiO<sub>2</sub>- and TiO<sub>2</sub>-based nanocomposite films containing spherical gold nanoparticles were fabricated and investigated (both experimentally and theoretically) in [7]. It was shown that these nanocomposites are characterized by effective resonant permittivity, described by the Maxwell–

Garnett formula [8]. Note that SiO<sub>2</sub> and TiO<sub>2</sub> films with gold nanoparticles dispersed in them are of great interest as photovoltaic materials [7, 9]. In this paper, we report the results of studying the spectral properties of a one-dimensional PC with a defect layer in the form of nanocomposite TiO<sub>2</sub>-based film [7], with allowance for the size effects in gold nanoparticles.

## DESCRIPTION OF THE MODEL

The PC structure under consideration is a layered medium with a resonant defect nanocomposite layer. The defect nanocomposite layer with thickness  $W_d$  consists of gold spherical nanoparticles uniformly distributed over a dielectric titanium dioxide (TiO<sub>2</sub>) matrix with permittivity  $\epsilon_d = 4.57$ . The nanoparticles in our study, as in [7], were assumed to be made of gold, which is one of the most widespread materials for plasmonics. The electron damping coefficient in the Drude–Sommerfeld model for gold differs from that for silver (used in [3–6]) by an order of magnitude.

The alternating layers forming a PC unit cell are a zirconia (ZrO<sub>2</sub>) layer with permittivity  $\epsilon_a = 4.16$  and a silicon dioxide (SiO<sub>2</sub>) layer with permittivity  $\epsilon_b = 2.10$ . The layer thicknesses are, respectively,  $W_a = 50$  nm and  $W_b = 74$  nm. The PC structure is placed in a medium with a permittivity equal to unity (air) and consists of  $N = 19$  layers, including the defect layer at the center of symmetry of the structure.



**Fig. 1.** (a) Real ( $\epsilon'$ ) and (b) imaginary ( $\epsilon''$ ) parts of the effective permittivity of nanocomposite at filling factors  $f=0.13$  and  $0.24$  (solid and dotted lines, respectively). Thin lines show the permittivity with the particle size disregarded and the bold lines describe the permittivity for particles with a radius  $r=20$  nm.

The effective permittivity of nanocomposite is determined by the Maxwell–Garnett formula, which is widely used in consideration of matrix media in the form of isolated metallic inclusions (with a small volume fraction) dispersed in the matrix material:

$$\epsilon = \epsilon_d \left[ 1 + \frac{3f(\epsilon_m - \epsilon_d)}{3\epsilon_d + (1-f)(\epsilon_m - \epsilon_d)} \right], \quad (1)$$

where  $f$  is the filling factor (i.e., the fraction of nanoparticles in the matrix) and  $\epsilon_d$  and  $\epsilon_m$  are, respectively, the permittivities of the matrix and metal (nanoparticle material). The Maxwell–Garnett model implies a quasi-static approximation. Its main features are that the nanocomposite layer is electro-dynamically isotropic, the nanocomposite inclusions in the

dielectric matrix are located at distances greatly exceeding their characteristic size, and this size is small in comparison with the light wavelength in the effective medium. The predictions of the Maxwell–Garnett model of an effective medium are reliable for a moderate fraction of inclusions with filling factor  $f \ll 1$  [10].

The permittivity of the nanoparticle metal will be found using the Drude–Sommerfeld approximation:

$$\epsilon_m(\omega) = \epsilon_0 - \frac{\omega_p^2}{\omega \left( \omega + i \left( \gamma + A \frac{v_F}{r} \right) \right)}, \quad (2)$$

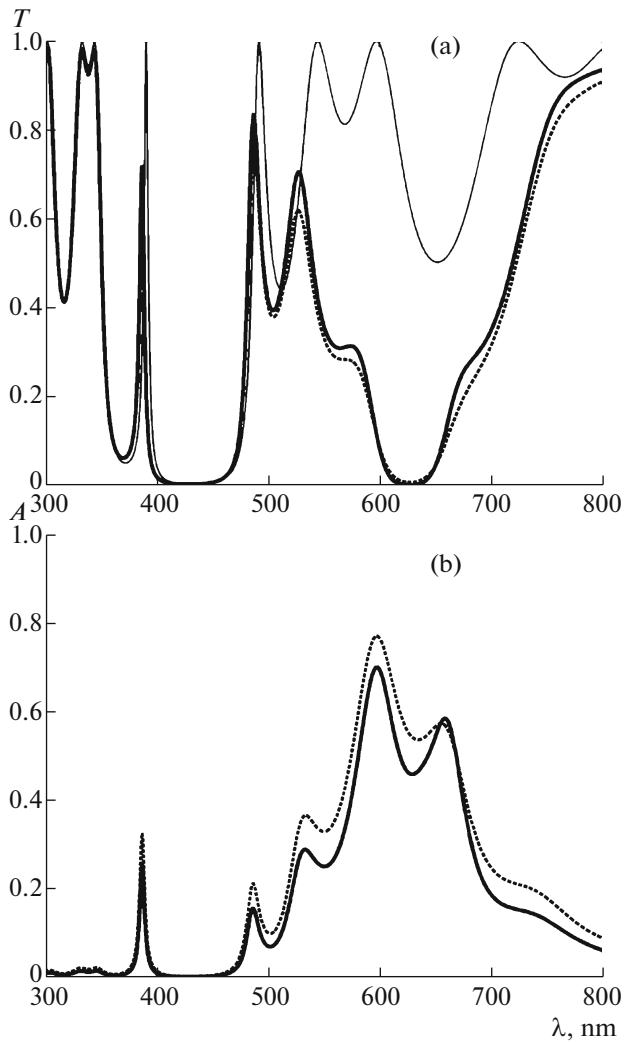
where  $\epsilon_0$  is a constant taking into account the contributions of the interband transitions of bound electrons,  $\omega_p$  is the plasma frequency,  $\gamma$  is the damping coefficient (a value inverse to the electron relaxation time),  $v_F$  is the Fermi velocity,  $r$  is the nanoparticle radius, and  $A$  is the effective parameter describing the degree of coherence loss at electron scattering from the surface. For gold,  $\epsilon_0 = 9.84$ ,  $\omega_p = 9$  eV,  $\gamma = 0.1$  eV,  $v_F = 1.4 \times 10^8$  cm/s, and  $A = 1$  [11, 12]. Figure 1 shows the real and imaginary parts of the effective permittivity of the nanocomposite calculated from formula (1) as functions of the incident light wavelength. The permittivity is given for two values of filling factor  $f$ . Thin lines show the permittivities calculated for particle radius  $r$  formally tending to infinity (approximation of unlimited material in the Drude–Sommerfeld formula (2)).

The data in Fig. 1 indicate that the real and imaginary parts of the nanocomposite permittivity, as well as the position of the resonant frequency, depend strongly on the real size and concentration of nanoparticles in the nanocomposite.

## CALCULATION RESULTS

The transmission and absorption spectra of the structure under consideration were calculated by the transfer-matrix method [13]. Figure 2 shows the transmission and absorption spectra for defect-layer thickness  $W_d = 70$  nm and filling factor  $f = 0.13$  [7]. The thin line presents the seed spectrum of a PC containing a defect titanium dioxide layer without nanoparticles.

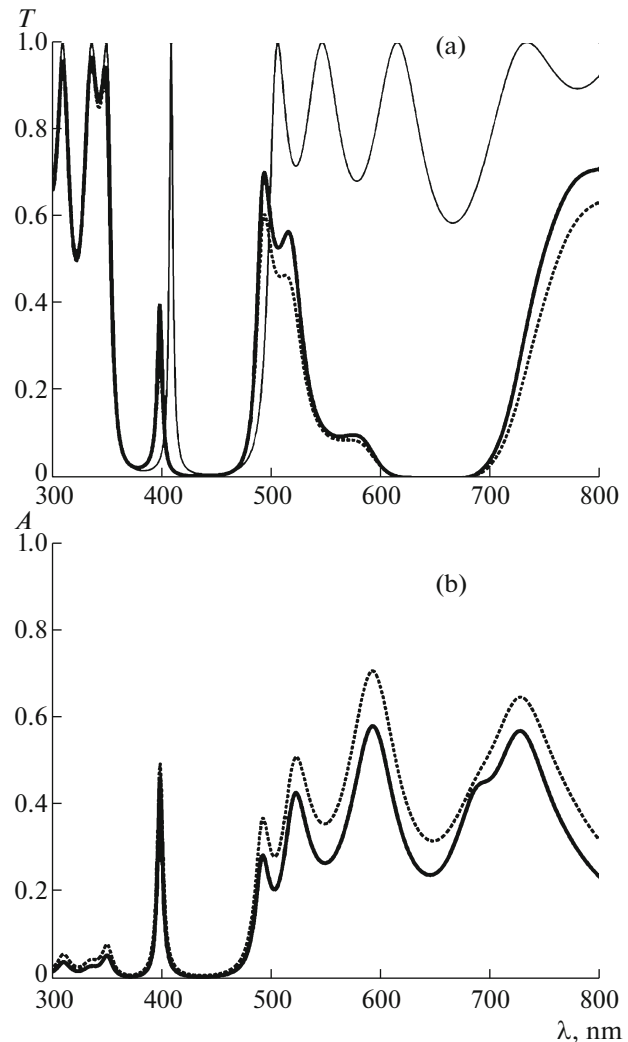
Figure 2a shows that an additional nontransmission band arises in the transmission spectrum at the wavelength corresponding to the resonant frequency of nanocomposite (Fig. 1). The reason for this is that gold has a large damping coefficient in the Drude–Sommerfeld model (2); therefore, this band is due to the absorption at the resonant plasmon frequency (Fig. 2b), in contrast to the initial band gap of the seed spectrum, which is related to the Bragg diffraction of light. Thus, the transmission spectrum contains, along with the band gap due to the Bragg diffraction of light, a nontransmission band related to the nanocomposite absorption near the resonant frequency. A decrease in



**Fig. 2.** Dependences of the (a) transmittance  $T$  and (b) absorption coefficient  $A$  of the system on the incident light wavelength. The defect thickness is  $W_d = 70$  nm. The parameters are as follows:  $f = 0$  (thin solid line);  $f = 0.13$ , with the particle size disregarded (bold solid line); and  $f = 0.13$  and  $r = 20$  nm (dotted line).

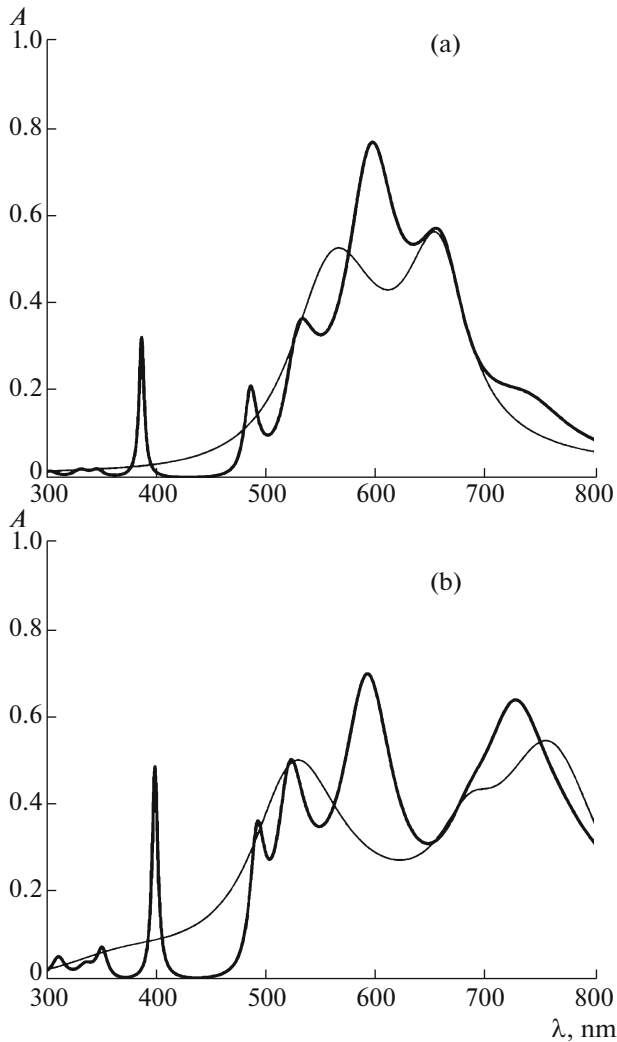
transmission is also observed, which is caused by absorption of the microcavity eigenmode energy, and a small frequency shift of the defect peak in the Bragg band gap as a result of introduction of nanoparticles into the nanocomposite. The transmission of the system decreases when the nanoparticle size is taken into account. The reason is that the nanocomposite permittivity decreases when size effects are taken into consideration (Fig. 1).

Figure 3 shows the transmission and absorption spectra of the system for defect-layer thickness  $W_d = 90$  nm and filling factor  $f = 0.24$  [7]. The thin line shows the seed spectrum of a PC containing a defect titanium dioxide layer without nanoparticles.



**Fig. 3.** Dependences of the (a) transmittance  $T$  and (b) absorption coefficient  $A$  of the system on the incident light wavelength. The defect thickness is  $W_d = 90$  nm. The parameters are as follows:  $f = 0$  (thin solid line);  $f = 0.24$ , with the particle size disregarded (bold solid line); and  $f = 0.24$  and  $r = 20$  nm (dotted line).

Figure 3a presents also a nontransmission band due to the absorption in nanocomposite at the resonant frequency of nanocomposite permittivity; the width of this band at a specified defect-layer thickness ( $W_d = 90$  nm) increased in comparison with the band in Fig. 2a. This increase was accompanied by a change in the transmission bandwidth between the Bragg band gap and the nontransmission band due to absorption. This effect can be used to design broadband light filters based on this structure. The decrease in transmission for the defect peak in the Bragg band gap and its frequency shift are more pronounced when the filling factor increases. Consideration of the nanoparticle size leads to a decrease in transmission, as in the case presented in Fig. 2a.



**Fig. 4.** Dependences of the absorption coefficient  $A$  of a nanocomposite film (thin line) and a PC with a nanocomposite defect (bold line) on the incident light wavelength. Film thickness  $W_d =$  (a) 70 and (b) 90 nm.

Figure 4 shows absorption spectra for an isolated nanocomposite film and for the same film incorporated into a PC structure.

It can be seen in Fig. 4 that introduction of nanocomposite into a PC leads to an increase in absorption in separate frequency ranges, a circumstance that can be useful for photovoltaics applications.

## CONCLUSIONS

We showed that the possibility exists of changing radically the spectral characteristics of a one-dimensional PC using a defect nanocomposite layer with

inserted gold nanoparticles. The transmission and absorption spectra depend strongly on the nanoparticle concentration in nanocomposite. This effect can be used to design broadband light filters based on these structures. It is noteworthy that the transmission spectrum contains, along with the Bragg band gap, a nontransmission band due to the nanocomposite absorption near the resonant frequency. When the particle size is taken into account, the spectrum is modified due to the dissipation effects: damping for the unlimited metal volume and the processes of electron scattering from the nanoparticle surface. The application of a PC cavity to increase absorption of light in such a nanocomposite is promising for photovoltaics.

## ACKNOWLEDGMENTS

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## REFERENCES

1. J. D. Joannopoulos, S. G. Johnson, J. N. Winn, and R. D. Meade, *Photonic Crystals: Molding the Flow of Light* (Princeton Univ. Press, Princeton, 2008).
2. B. I. Mantsyzov, *Coherent and Nonlinear Optics of Photonic Crystals* (Fizmatlit, Moscow, 2009) [in Russian].
3. S. Ya. Vetrov, A. Yu. Avdeeva, and I. V. Timofeev, *J. Exp. Theor. Phys.* **113** (5), 755 (2011).
4. S. Ya. Vetrov, R. G. Bikbaev, and I. V. Timofeev, *J. Exp. Theor. Phys.* **117** (6), 988 (2013).
5. S. G. Moiseev, V. A. Ostatochnikov, and D. I. Sementsov, *Kvantovaya Elektron.* **42** (6), 557 (2012).
6. S. G. Moiseev, V. A. Ostatochnikov, and D. I. Sementsov, *JETP Lett.* **100** (6), 371 (2014).
7. E. Pedrueza et al., *Adv. Funct. Mater.* **21**, 3502 (2011).
8. J. C. Maxwell-Garnett, *Philos. Trans. R. Soc. London* **203**, 385 (1904).
9. V. E. Ferry, J. N. Munday, and H. A. Atwater, *Adv. Funct. Mater.* **22**, 4794 (2010).
10. S. G. Moiseev, *Opt. Spectrosc.* **111** (2), 233 (2011).
11. V. V. Klimov, *Nanoplasmonics* (Fizmatlit, Moscow, 2009) [in Russian].
12. W. T. Doyle, *Phys. Rev. B* **39** (14), 9852 (1989).
13. P. Yeh, *J. Opt. Soc. Am.* **69** (5), 742 (1979).

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