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DEFECTS AND STATISTICS OF METAMATERIALS

Spectral Properties of One-Dimensional Photonic Crystal with Anisotropic Defect Layer of Nanocomposite

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Abstract—The spectral properties of a one-dimensional photonic crystal with a structure defect—anisotropic nanocomposite layer incorporated between two multilayer dielectric mirrors—have been theoretically investigated. Some specific features are revealed in the transmission spectrum of a photonic crystal. They are primarily due to the resonant behavior of the effective permittivity of nanocomposite and the strong dependence of this parameter on the volume fraction of nanoparticles in the composite.

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1. INTRODUCTION

An important property of photonic crystals (PCs) is the localization of electromagnetic waves on structure defects. In this case, additional allowed levels arise in the PC bandgap, which correspond to localized defect modes. For a 1D PC, a defect layer incorporated between two multilayer mirrors is a Fabry–Perot microresonator, and the localized defect modes are microresonator eigenmodes. The position and transmission parameters of defect modes can be efficiently controlled by varying geometric and structural PC parameters. A study of PCs with defect modes made it possible to develop new types of PC waveguides, high-Q nanoresonators, and low-threshold lasers, as well as to propose some ways to increase the efficiency of nonlinear optical processes [1, 2].

New possibilities of light control arise when an isotropic [3, 4] or anisotropic [5] nanocomposite layer, consisting of metal nanoinclusions of spherical or orientationally ordered spheroidal shape, dispersed in a transparent matrix, is used as a defect layer in a 1D PC.

2. MODEL UNDER STUDY AND TRANSMISSION SPECTRUM

Calculations were performed for a PC structure in the form of a layered medium containing a resonant defect nanocomposite layer. The PC material parameters were chosen to be as follows: the defect nanocomposite layer with a thickness $W_\mathrm{d} = 130$ nm consists of silver nanoparticles in the form of ellipsoids of rotation, uniformly distributed in a dielectric matrix (transparent optical glass with a permittivity $\varepsilon_\mathrm{d} = 2.56$); the polar axis of nanospheroids is oriented parallel to the optical axis of the nanocomposite. The alternating layers constituting a PC unit cell were taken to be zirconium dioxide (ZrO_2) layer with a permittivity $\varepsilon_\mathrm{a} = 4.16$ and silicon dioxide (SiO_2) layer with a permittivity $\varepsilon_\mathrm{b} = 2.10$. The layer thicknesses were, respectively, $W_\mathrm{a} = 50$ nm and $W_\mathrm{b} = 74$ nm. The PC structure consists of $N = 19$ layers, including the defect layer in the center of symmetry of the structure; it is placed in a medium (air) with a permittivity equal to unity.

The effective permittivity of nanocomposite (possessing the properties of uniaxial material) in the main axes can be presented in the form of a diagonal tensor with the following components: $\varepsilon_{xx} = \varepsilon_\parallel$ and $\varepsilon_{yy} = \varepsilon_{zz} = \varepsilon_\perp$. Permittivities $\varepsilon_\perp$ and $\varepsilon_\parallel$ are determined by the Maxwell Garnett formula, which is widely used in consideration of matrix media containing dispersed isolated metallic inclusions with a small volume fraction [5]:

$$\varepsilon_{\perp,\parallel} = \varepsilon_\mathrm{d}\left[1 + \frac{f(\varepsilon_\mathrm{m} - \varepsilon_\mathrm{d})}{\varepsilon_\mathrm{d} + (1-f)(\varepsilon_\mathrm{m} - \varepsilon_\mathrm{d})L_{\perp,\parallel}}\right]. \quad (1)$$

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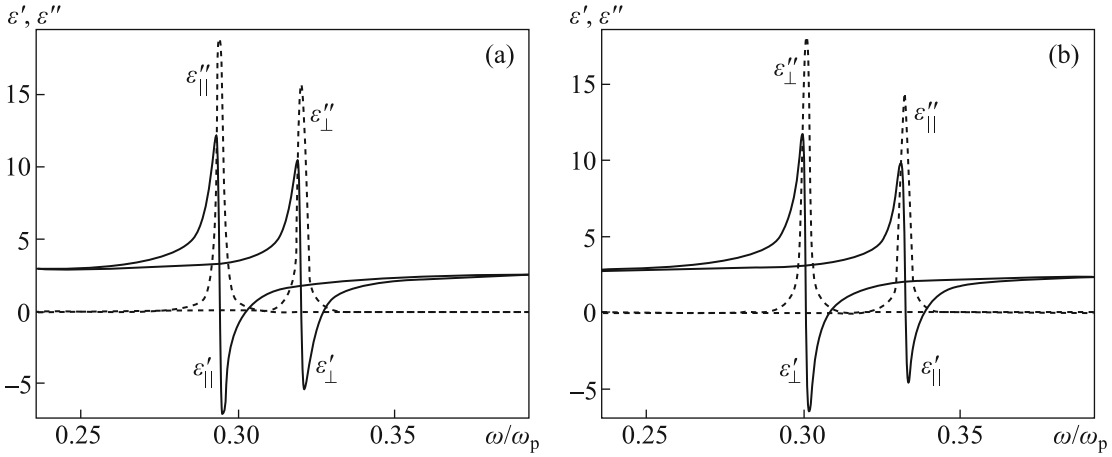

Fig. 1. Frequency dependences of the real ($\varepsilon'_{\parallel}$) and imaginary ($\varepsilon'_{\perp}$) parts of the effective permittivity of nanocomposite: $\xi = 1.2$ (a) and 0.8 (b); $f = 0.02$.

Here f is the filling factor (i.e., the fraction of nanoparticles in the matrix); $\varepsilon_{\rm d}$ and $\varepsilon_{\rm m}(\omega)$ are, respectively, the permittivities of the matrix and the material of nanoparticles (metal); and ω is the radiation frequency. The depolarization factors $L_{\perp,\parallel}$ in (1) depend on the ratio of the polar (c) and equatorial (a) semiaxes of the ellipsoid of rotation and on the field direction. For a field directed along the spheroid axis of revolution, factor $L_{\parallel}$ is given by the expression

$$L_{\parallel} = \frac{1}{1-\xi^2}\left(1 - \xi\frac{\arcsin\sqrt{1-\xi^2}}{\sqrt{1-\xi^2}}\right). \qquad (2)$$

For a field directed perpendicular to the spheroid axis of revolution,

$$L_{\perp} = \frac{1 - L_{\parallel}}{2}, \qquad (3)$$

where $\xi = c/a$. The cases $\xi < 1$ and $\xi > 1$ correspond to oblated and prolated spheroids, respectively. The condition $\xi = 1$ for which $L_{\perp} = L_{\parallel} = 1/3$ and $\varepsilon_{\perp} = \varepsilon_{\parallel}$ correspond to a sphere. The metal (nanoparticle material) permittivity can be found using the Drude approximation

$$\varepsilon_{\rm m}(\omega) = \varepsilon_0 - \frac{\omega_{\rm p}^2}{\omega(\omega + i\gamma)}, \qquad (4)$$

where ε_0 is a constant taking into account the contributions of interband transitions of bound electrons, $\omega_{\rm p}$ is the plasma frequency, and γ is a value inverse to the electron relaxation time. For silver, $\varepsilon_0 = 5$, $\omega_{\rm p} = 9$ eV, and $\gamma = 0.02$ eV.

Technologies for fabricating a nanocomposite (polarization glass) transparent in the visible or near-visible spectral ranges were described in [6, 7]. It was shown that nanocomposite samples are characterized by a high degree of orientational order of inclusions and their uniform distribution over the glass matrix. The orientational order of nanoparticles in the matrix turned out to be sufficiently high for observing pronounced polarization selectivity when measuring transmission [6] or optical density [7].

Figure 1 shows the results of calculating (using formula (1)) the resonant frequency dependences of the real and imaginary parts of the effective permittivities of anisotropic nanocomposite medium. It can be seen that the resonant frequencies depend on the electric field direction relative to the spheroid axis and the ratio of the polar and equatorial semiaxes of nanoparticles. Because of the difference in the resonant frequencies for permittivities $\varepsilon_{\perp}$ and $\varepsilon_{\parallel}$, the nanocomposite optical properties depend on the incident wave polarization.

To calculate the transmission of an s-polarized plane light wave with electromagnetic-field components (E_y, H_x, H_z), we used the transfer-matrix method [8]. The change in the light field of the wave passing through each layer of the structure is determined by the second-order transfer matrix, and the transfer matrix of the entire structure, which relates the amplitudes of the incident and outgoing waves, is determined by the product of these matrices:

$$M = T_{01}T_{12}...T_{N-1,N}T_{N,N+1}, \qquad (5)$$

where each transfer matrix has the form

$$T_{n-1,n} = \frac{1}{2}\begin{bmatrix} (1+h_n)\,e^{-i\alpha_n\gamma_n} & (1-h_n)\,e^{i\alpha_n\gamma_n} \\ (1-h_n)\,e^{-i\alpha_n\gamma_n} & (1+h_n)\,e^{i\alpha_n\gamma_n} \end{bmatrix}. \qquad (6)$$

Here $h_n = \sqrt{\varepsilon(n) - \sin^2\theta}/\sqrt{\varepsilon(n-1) - \sin^2\theta}$, $\varepsilon(n)$ is the permittivity of the nth isotropic layer; $\alpha_n = (\omega/c)\sqrt{\varepsilon(n) - \sin^2\theta}$; ω is the wave frequency; c is the speed of light; the layer thicknesses are $\gamma_n = z_n - z_{n-1}$, z_n is the coordinate of the boundary between

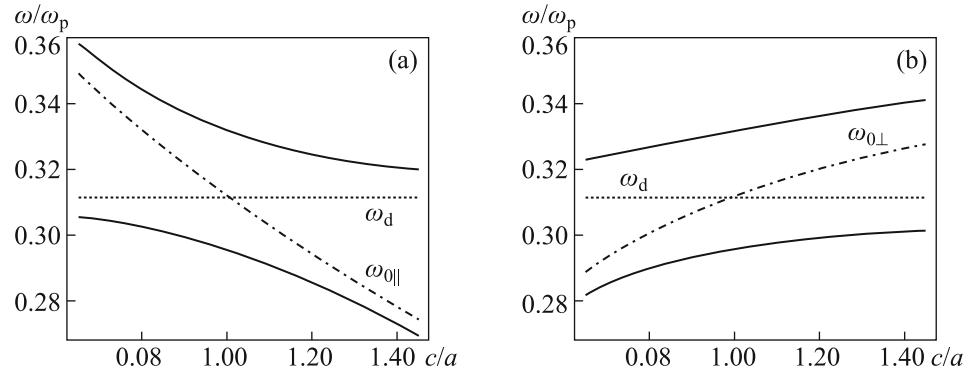

Fig. 2. Dependences of the positions of transmission peak maxima on the nanoparticle shape (solid lines). Dotted and dash-dotted lines correspond, respectively, to the PC defect-mode frequency (ω_d) and nanocomposite resonant frequency (ω_0). The polarization of light is (a) parallel and (b) perpendicular to the nanocomposite optical axis; $f = 0.02$ and $\theta = 0°$.

the nth layer and adjacent (from the right) $(n+1)$th layer, $\gamma_{N+1} = 0$, $n = 1, 2, ..., N$; and θ is the angle of incidence of light.

For the jth anisotropic layer, the h_j value in (6) has the form

$$h_j = \frac{\sqrt{\varepsilon_{yy}(j) - \sin^2\theta}}{\sqrt{\varepsilon(j-1) - \sin^2\theta}}, \qquad \alpha_j = \frac{\omega}{c}\sqrt{\varepsilon_{yy}(j) - \sin^2\theta}. \tag{7}$$

The transfer matrix for a p-polarized wave with electromagnetic-field components (E_x, E_z, H_y) is obtained by replacing h_j and α_j in (6) with the following expressions:

$$h_j = \frac{\varepsilon(j-1)\sqrt{\varepsilon_{zz}(j) - \sin^2\theta}}{\sqrt{\varepsilon_{xx}(j)\,\varepsilon_{zz}(j)[\varepsilon(j-1) - \sin^2\theta)]}}, \qquad \alpha_j = \frac{\omega}{c}\sqrt{\varepsilon_{xx}(j) - \frac{\sin^2\theta}{\varepsilon_{zz}(j)}}. \tag{8}$$

The wave transmittance is given by the expression

$$T(\omega) = 1/|M_{11}|^2, \tag{9}$$

where M_{11} is an element of matrix M.

3. CALCULATION RESULTS AND DISCUSSION

The structure under study exhibits defect-mode splitting in the bandgap, which is similar to the splitting of the frequency of two coupled oscillators and occurs when the defect-mode frequency is close to the resonant frequencies of nanocomposite [3].

Figure 2 shows how the positions of the transmission peaks related to the defect modes in the bandgap in the transmission spectrum of the structure under normal incidence of light depend on the nanoparticle shape. It can be seen that, when the defect-mode frequency is close to the resonant frequencies of nanocomposite, each of two orthogonal polarizations of the incident wave in the bandgap of the transmission spectrum is characterized by specific splitting of defect modes, which depends on parameter ξ. The degree of splitting increases with the degree of oblateness (prolation) of ellipsoidal nanoparticles. At a specified nanoparticle shape, the transmission spectrum and splitting depend strongly on the incident-wave polarization. The defect-mode splitting is minimal when the resonant frequencies of nanocomposite and PC have close values.

Splitting increases also with the concentration of spheroids in the nanocomposite for both polarizations of light; in particular, it reaches 100 nm for a nanoparticle volume fraction of 0.06. The splitting increases with concentration for both oblated and prolated particles.

Figure 3 shows a dependence of the positions of transmission peaks related to defect modes on the angle of incidence of s-polarized light. It can be seen that an increase in the angle of incidence causes shift of defect modes for both elongated (Fig. 3(a)) and flattened (Fig. 3(b)) nanoparticles. The defect modes in the bandgap of PC structure are blue-shifted. This behavior can be visually interpreted by presenting a defect mode as a standing wave induced by reflection from the mirrors of the resonator formed by the nanodefect with a thickness corresponding to the resonator eigenmode. Indeed, the resonance condition $\lambda = 2W_d\sqrt{n^2 - \sin^2\theta}$, where n is the refractive index of the defect layer and θ is the angle of incidence of light, shows that the defect-mode wavelength decreases with an increase in the angle of incidence; this behavior is in agreement with the results of numerical calculation. Note that the bandgap boundary is also blueshifted in correspondence with the Bragg condition. One can also see in Fig. 3 that the splitting is minimal when the nanocomposite and PC have close resonant frequencies.

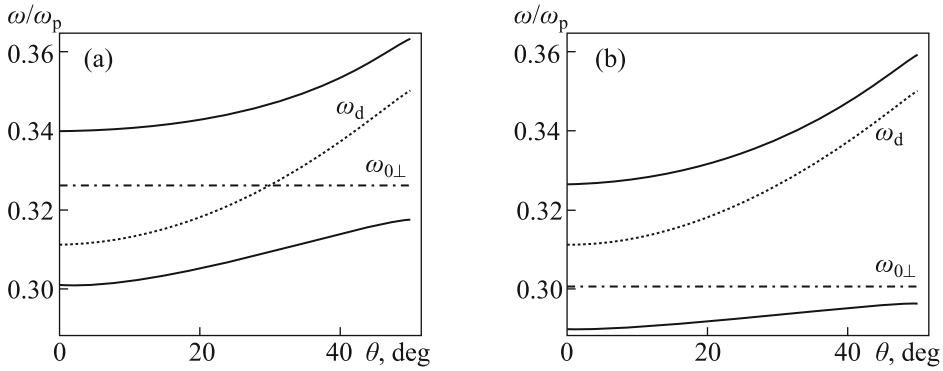

Fig. 3. Dependences of the positions of maxima of transmission peaks on the angle of incidence of s-polarized light (solid lines). Dotted and dash-dotted lines correspond, respectively, to the PC defect-mode frequency (ω_d) and the nanocomposite resonant frequency (ω_0); $\xi = 1.4$ (a) and 0.8 (b); $f = 0.02$.

The dependence of the transmission spectra of the structure under consideration on the incident-light wavelength, nanoparticle shape, the angle of incidence of light, and the concentration of nanospheroids in the nanocomposite can be is used to control and separate light waves with different wavelengths and polarizations. Each of two mutually orthogonal polarizations of light incident on such a structure is characterized by a specific defect-mode splitting; therefore, when an unpolarized white light beam is incident of this structure, one observes four narrow spectral bands of linearly polarized light at the wavelengths corresponding to the defect modes in the bandgap of the transmission spectrum. Thus, an ultrafine selective polarizer can be designed. In addition, doping a nanocomposite with atoms allowing for formation of inverse population of levels (which is necessary for lasing), one can develop a multimode laser based on this structure. Lasing will occur at frequencies corresponding to the defect modes in the transmission spectrum bandgap.

4. CONCLUSIONS

We numerically investigated the specific features of spectral properties of a 1D photonic crystal with a defect layer (resonantly absorbing, anisotropic nanocomposite layer), composed of orientationally ordered metal nanoparticles of spheroidal shape, suspended in a transparent matrix. The manifestation of the defect-mode splitting in the transmission spectrum bandgap was studied for this structure. It was shown that each of the two orthogonal polarizations of incident wave is characterized by specific defect-mode splitting, which is minimal when the nanocomposite and photonic crystal have similar resonant frequencies, and depends on the angle of incidence of light, the volume fraction of nanoparticles, and the structural parameters of photonic crystal. The angular and polarization sensitivity of the transmission spectra of the structure under consideration can be used to control and separate light waves with different wavelengths and polarizations.

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