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OPTICAL PROPERTIES

Band Structure of a Two-Dimensional Resonant Photonic Crystal

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Abstract—The band structure of two-dimensional resonant photonic crystals of two types has been calculated using the expansion of eigenfunctions in plane waves. Crystals of one type consist of infinite dielectric cylinders forming a square lattice filled with a resonant gas, and crystals of the other type consist of infinite cylindrical holes filled with a resonant gas and forming a square lattice in a dielectric matrix. It has been shown that, in both cases, the dispersion of a resonant gas in combination with the dispersion of a two-dimensional structure with a photonic band gap leads to the appearance of an additional narrow transmission band near the edge of the band gap or an additional band gap in the continuous spectrum of the photonic crystal. The calculations performed have demonstrated that new dispersion properties substantially depend on the density of the resonant gas, the position of the resonant frequency with respect to the edge of the band gap, and the direction of propagation of electromagnetic waves.

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1. INTRODUCTION

Photonic crystals, as a rule, are artificial structures with a permittivity periodically varying in space. Owing to the spatial periodicity, electromagnetic waves in photonic crystals have a band-type spectrum, much as the space-periodic potential leads to the electron band spectrum.

The existence of photonic band gaps and regions of an anomalous increase in the density of photon states in photonic crystals due to the periodicity makes it possible to implement a number of interesting modes of propagation of electromagnetic waves [1–3]. For example, complete band gaps can exist in three-dimensional photonic crystals. This means that, in the forbidden spectral range, light of any polarization cannot enter a photonic crystal in any direction. In the region of the complete photonic band gap, spontaneous emission is impossible when the frequency of a quantum transition lies in the range of forbidden photon energies. Another important property of photonic crystals is the high degree of localization of electromagnetic waves at lattice defects. The presence of defects in the crystal lattice leads to the appearance of defect energy levels in band gaps of the photonic crystals. Photonic crystal materials differ from other optical systems in that the light localization in photonic crystals is combined with the possibility of controlling the atomic lifetime. Photonic materials have attracted the particular attention of researchers as new optical materials exhibiting unique properties.

Based on photonic crystal materials, it has become possible to create new types of waveguides [4, 5], to devise methods for increasing the efficiency of nonlinear-optical processes [6–8], and to implement ideas on the development of optoelectronic hardware and information technologies [9].

The spectral properties of photonic crystals can also be changed significantly by placing resonant media (atomic or molecular gases) inside a periodic structure. However, these changes manifest themselves only in a narrow frequency range near the resonant frequency; consequently, this type of a photonic structure is referred to as a "resonant photonic crystal." The simplest one-dimensional resonant photonic crystals are layered structures that consist of alternating layers of two materials, one of which is a resonant gas [10]. The spectral properties of such resonant photonic crystals with inclusion of damping were studied in [11, 12]. It was found that the dispersion of a resonant gas in combination with the dispersion of a photonic crystal structure leads to qualitative changes in spectra of the photonic crystals; more specifically, narrow transmission bands appear in the photonic band gap, and additional band gaps arise in the transmission spectrum of the photonic crystal structure. Such structures with a combined dispersion are promising materials for use in the design of spectral prisms with an increased dispersion and narrow-band filters with controlled performance characteristics.

In this paper, the spectrum of electromagnetic excitations of two-dimensional photonic band-gap

structures filled with a resonant gas has been studied using the expansion of eigenfunctions in plane waves.

2. DESCRIPTION OF THE MODEL AND THE PLANE WAVE METHOD

Let us consider two types of resonant photonic crystals: (a) elements of the crystal are identical dielectric cylinders of infinite length that form a square lattice filled with a resonant gas, and (b) elements of the crystal are hollow cylinders of infinite length that are filled with a resonant gas and form a square lattice in a dielectric matrix.

In the former case, the structure is characterized by the permittivity of rods ε_1 and the permittivity of the resonant gas $\varepsilon_2(\omega)$. The permittivity of the gas in the Lorentz model is given by the expression [13]

$$\varepsilon_2(\omega) = 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 + i\gamma\omega}, \quad (1)$$

where $\omega_p^2 = 4\pi NFe^2/m$, e is the elementary charge, m is the electron mass, N is the density of resonant atoms, F is the oscillator strength, γ is the linewidth, ω_0 is the central resonant frequency, and ω is the radiation frequency.

It is assumed that the cylinder axis is perpendicular to the xy plane and parallel to the z axis. The centers of the cylinder cross sections form a square Bravais lattice in the xy plane. The vector of an arbitrary site of the square Bravais lattice can be written as

$$\mathbf{r}_\perp(l) = l_1\mathbf{a}_1 + l_2\mathbf{a}_2, \quad (2)$$

where l_1 and l_2 are integer numbers, and the vectors of elementary translations are given by

$$\mathbf{a}_1 = a(1, 0), \quad \mathbf{a}_2 = a(0, 1). \quad (3)$$

Here, a is the lattice parameter. The reciprocal lattice vector is written as

$$\mathbf{G} \equiv \mathbf{G}_\perp(h) = h_1\mathbf{b}_1 + h_2\mathbf{b}_2, \quad (4)$$

where h_1 and h_2 are integer numbers, and the vectors of elementary translations of the reciprocal lattice are given by

$$\mathbf{b}_1 = \frac{2\pi}{a}(1, 0), \quad \mathbf{b}_2 = \frac{2\pi}{a}(0, 1). \quad (5)$$

The dispersion pattern of the resonant photonic crystal under consideration will be calculated by the plane wave method [14–16] for the electromagnetic waves propagating in the xy plane perpendicular to the rods so that the electric field vector is directed along the z axis (s polarization).

For the s-polarized electromagnetic waves propagating in the resonant photonic crystal, the wave equation is reduced to the scalar equation for the z component of the electric field, $E_z(\mathbf{r}) = E(\mathbf{r})$,

$$\left(\frac{\partial}{\partial x^2} + \frac{\partial}{\partial y^2}\right)E(\mathbf{r}_\perp) + \frac{\omega^2}{c^2}\varepsilon(\mathbf{r}_\perp)E(\mathbf{r}_\perp) = 0, \quad (6)$$

where $\mathbf{r} \equiv \mathbf{r}_\perp = (x, y)$ is the two-dimensional radius vector and $\varepsilon(\mathbf{r}_\perp)$ is the permittivity.

Equation (6) is a differential equation with periodic coefficients; therefore, the field $E(\mathbf{r}_\perp)$ can be represented in the form of a Bloch wave. As a result, the Fourier expansion for the electric field has the form

$$E(\mathbf{r}_\perp) = \sum_{\mathbf{G}_\perp} E_{\mathbf{k}_\perp}(\mathbf{G}_\perp)e^{i(\mathbf{G}_\perp + \mathbf{k}_\perp)\mathbf{r}_\perp}, \quad (7)$$

where summation is performed over all vectors of the reciprocal lattice and $\mathbf{k} \equiv \mathbf{k}_\perp = (k_1, k_2, 0)$ is the two-dimensional wave vector.

Since $\varepsilon(\mathbf{r}_\perp)$ is a periodic function with the period of the Bravais lattice,

$$\varepsilon(\mathbf{r}_\perp + \mathbf{r}_\perp(l)) = \varepsilon(\mathbf{r}_\perp), \quad (8)$$

it can be expanded in the Fourier series

$$\varepsilon(\mathbf{r}_\perp) = \sum_{\mathbf{G}_\perp} \hat{\varepsilon}(\mathbf{G}_\perp)e^{i\mathbf{G}_\perp\mathbf{r}_\perp}. \quad (9)$$

The permittivity of a resonant photonic crystal of the a type can be written as

$$\varepsilon(\mathbf{r}_\perp) = \varepsilon_2(\omega) + (\varepsilon_1 - \varepsilon_2(\omega))\sum_l \Theta(\mathbf{r}_\perp - \mathbf{r}_\perp(l)), \quad (10)$$

where ε_1 and $\varepsilon_2(\omega)$ are the permittivities of the cylinder and the resonant gas in the Lorentz model, respectively; the function $\Theta(\mathbf{r}_\perp) = 1$ inside the cylinder cross section; and $\Theta(\mathbf{r}_\perp) = 0$ outside it. For the model of a resonant photonic crystal of the b type, the permittivity is derived from expression (10) with the changes $\varepsilon_2(\omega) \longrightarrow \varepsilon_1$ and $\varepsilon_1 \longrightarrow \varepsilon_2(\omega)$. The Fourier coefficients in expression (9) for the permittivity $\varepsilon(\mathbf{r}_\perp)$ defined in the form of expression (10) are determined from the expression

$$\hat{\varepsilon}(\mathbf{G}_\perp) = \varepsilon_2\delta_{\mathbf{G}_\perp 0} + (\varepsilon_1 - \varepsilon_2(\omega))M_{\mathbf{G}_\perp 0}, \quad (11)$$

where

$$M_{\mathbf{G}_\perp 0} = \frac{1}{S}\int_S d^2\mathbf{r}_\perp \Theta(\mathbf{r}_\perp)e^{-i\mathbf{G}_\perp\mathbf{r}_\perp} = 2f\frac{J_1(|\mathbf{G}_\perp|r)}{|\mathbf{G}_\perp|r}. \quad (12)$$

Here, $J_1(z)$ is the Bessel function of the first kind; r is the cylinder radius; and $f = \pi r^2/a^2$ is the filling factor, i.e., the fraction of the dielectric material or the resonant gas in the photonic crystal for models of the a and b types, respectively.

After substituting expressions (7) and (9) into the Maxwell equation (6), we obtain

$$(\mathbf{k}_\perp + \mathbf{G}_\perp)^2 E_{\mathbf{k}_\perp}(\mathbf{G}_\perp) = \frac{\omega^2}{c^2}\sum_{\mathbf{G}'_\perp}\hat{\varepsilon}(\mathbf{G}_\perp - \mathbf{G}'_\perp)E_{\mathbf{k}_\perp}(\mathbf{G}'_\perp). \quad (13)$$

Substituting expression (11) for the permittivity into Eq. (13) and taking into account expression (1), we derive the equation for a two-dimensional resonant photonic crystal:

$$\left[(\mathbf{k}_\perp + \mathbf{G}_\perp)^2\delta_{\mathbf{G}_\perp\mathbf{G}'_\perp} - \frac{\omega^2}{c^2}\left(1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 + i\gamma\omega}\right)\delta_{\mathbf{G}_\perp\mathbf{G}'_\perp} - \frac{\omega^2}{c^2}\left(\varepsilon_1 - 1 - \frac{\omega_p^2}{\omega_0^2 - \omega^2 + i\gamma\omega}\right)M_{\mathbf{G}_\perp\mathbf{G}'_\perp}\right]E_{\mathbf{k}_\perp}(\mathbf{G}'_\perp) = 0. \quad (14)$$

The further transformation of Eq. (14) will be performed using the technique described in [15, 16]. We will restrict our analysis to a finite number of terms in the Fourier expansion for an electromagnetic field. In this case, Eq. (14) takes the form of the matrix equation, which is reduced to the polynomial in the eigenvalues ω; that is,

$$\omega^4 I - \omega^3 i\gamma I - \omega^2(I\omega_0^2 + KT^{-1} + (I - M)T^{-1}\omega_p^2) + \omega i\gamma KT^{-1} + \omega_0^2 KT^{-1} = 0. \quad (15)$$

Here, we introduced the following notation for the matrices:

$$I = \delta_{\mathbf{G}_\perp\mathbf{G}'_\perp}, \quad M = M_{\mathbf{G}_\perp\mathbf{G}'_\perp}, \quad K = (\mathbf{k}_\perp + \mathbf{G}_\perp)^2\delta_{\mathbf{G}_\perp\mathbf{G}'_\perp}, \quad T = I + (\varepsilon_1 - 1)M. \quad (16)$$

The polynomial eigenvalue equation is equivalent to the linear eigenvalue equation,

$$Wu = \omega u, \quad (17)$$

with the Frobenius normal form W composed of the coefficients of polynomial (15),

$$W = \begin{pmatrix} 0 & I & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & 0 & 0 & I \\ D & C & B & A \end{pmatrix}, \quad (18)$$

where the coefficients are given by the expressions

$$A = i\gamma I,$$
$$B = I\omega_0^2 + KT^{-1} + (I - M)T^{-1}\omega_p^2,$$
$$C = -i\gamma KT^{-1},$$
$$D = -\omega_0^2 KT^{-1}.$$

For a given wave vector $\mathbf{k}_\perp$ in the Brillouin zone, Eq. (17) allows one to determine the eigenfrequencies ω, so that their real part gives the eigenfrequency of the electromagnetic field and their imaginary part characterizes the mode damping. Redundant solutions to Eq. (17), which correspond to electromagnetic field modes undamping with time, are likewise possible. Therefore, in order to obtain the dispersion curves, it is necessary to choose physically correct solutions according to the condition $\mathrm{Im}(\omega) \geq 0$.

For the model of a resonant photonic crystal of the *b* type, the permittivity is given by the expression

$$\varepsilon(\bar{r}_\perp) = \varepsilon_1 + (\varepsilon_2(\omega) - \varepsilon_1)\sum_l \Theta(\mathbf{r}_\perp - \mathbf{r}_\perp(l)), \quad (19)$$

where ε_1 is the permittivity of the dielectric matrix and $\varepsilon_2(\omega)$ is the permittivity of the resonant gas filling the hollow cylinders. The expression for the Fourier coefficients $\hat{\varepsilon}(\mathbf{G}_\perp)$ has the form

$$\hat{\varepsilon}(\mathbf{G}_\perp) = \varepsilon_1\delta_{\mathbf{G}_\perp 0} + (\varepsilon_2(\omega) - \varepsilon_1)M_{\mathbf{G}_\perp 0}, \quad (20)$$

$$M_{\mathbf{G}_\perp 0} = \frac{1}{S}\int_S d^2\mathbf{r}_\perp \Theta(\mathbf{r}_\perp)e^{-i\mathbf{G}_\perp\mathbf{r}_\perp} = 2f\frac{J_1(|\mathbf{G}_\perp|r)}{|\mathbf{G}_\perp|r}. \quad (21)$$

Equation (17) has the same structure of the matrix W as that in Eq. (18), with the coefficients

$$A = i\gamma I,$$
$$B = I\omega_0^2 + KT^{-1} + MT^{-1}\omega_p^2,$$
$$C = -i\gamma KT^{-1},$$
$$D = -\omega_0^2 KT^{-1}, \quad (22)$$

where

$$I = \delta_{\mathbf{G}_\perp\mathbf{G}'_\perp}, \quad M = M_{\mathbf{G}_\perp\mathbf{G}'_\perp}, \quad K = (\mathbf{k}_\perp + \mathbf{G}_\perp)^2\delta_{\mathbf{G}_\perp\mathbf{G}'_\perp}, \quad T = \varepsilon_1\delta_{\mathbf{G}_\perp\mathbf{G}'_\perp} + (1 - \varepsilon_1)M. \quad (23)$$

3. RESULTS OF THE CALCULATION

First, we consider the results obtained from the calculation of the band structure of the spectrum for the sample of a resonant photonic crystal of the *a* type, which consists of elements in the form of dielectric cylinders forming a square lattice filled with a resonant gas. The calculations are performed for a resonant photonic crystal with the permittivity of the cylinders $\varepsilon_1 = 3.24$ and the period of the structure $a = 152$ nm. The filling factor is $f = 24\%$. The linewidth and the plasma frequency of the resonant gas are close to those

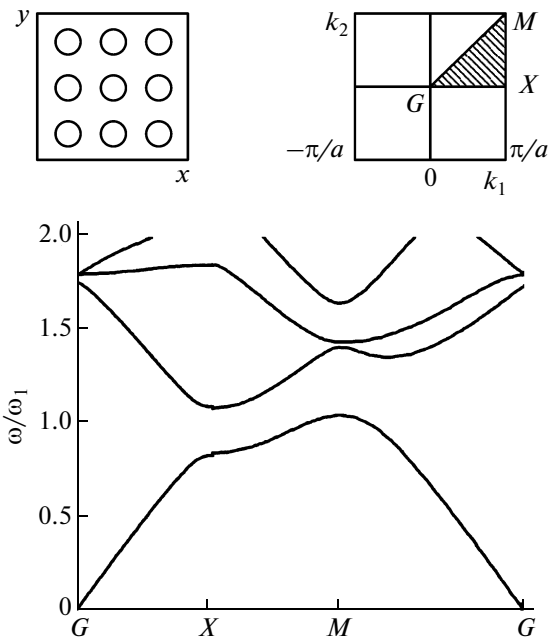

Fig. 1. Band structure of the square lattice of dielectric cylinders in vacuum for *s*-polarized waves. The insets show the square lattice and the corresponding Brillouin zone (the irreducible zone is cross-hatched). The number of plane waves in the expansion is $M = 121$, and the filling factor is $f = 24\%$.

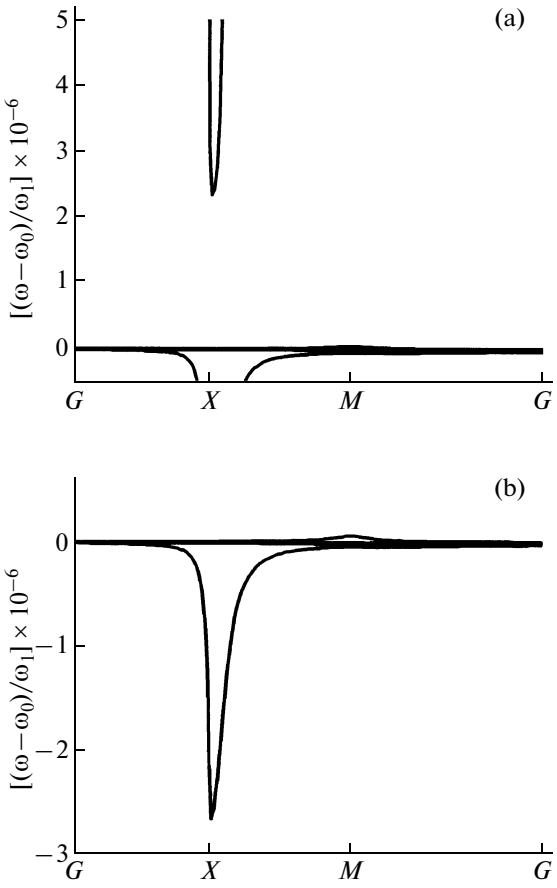

Fig. 2. A fragment of the band structure corresponding to Fig. 1: (a) the resonant frequency at the edge of the continuous spectrum is $\omega_0/\omega_1 = 1.089$, and (b) the resonant frequency in the band gap is $\omega_0/\omega_1 = 1.079$ (the density of resonant atoms is 4×10^{14} cm^{-3}). The other parameters are the same as in Fig. 1.

used in [10] for mercury vapors; i.e., $\gamma = 5 \times 10^{-7}\omega_1$ and $\omega_p^2 = 7 \times 10^{-8}\omega_1^2$, where $\omega_1 = \pi c n_1/a$ is the characteristic frequency in the photonic band gap and $n_1 = \sqrt{\varepsilon_1}f + (1-f)$ is the averaged refractive index of the medium. The linewidth at the frequency $\gamma = 1.2$ GHz corresponds to the resonance of mercury atoms at the wavelength $\lambda_0 = 253.7$ nm.

Figure 1 shows the seed band structure of the photonic crystal with the permittivity of the dielectric cylinders $\varepsilon_1 = 3.24$ and the permittivity of free space $\varepsilon_2 = 1$. For the filling factor $f = 24\%$, this photonic crystal has the maximum width of the first complete band gap. In this case, the photonic band gap in the X direction of the Brillouin zone lies in the frequency range ω/ω_1 from 0.843 to 1.084.

The dispersion of the photonic crystal structure in combination with the dispersion of the resonant gas, which is described by expression (1), leads to the appearance of additional band gaps in the continuous spectrum of the seed photonic crystal and additional narrow transmission bands in the band gap of the photonic crystal, which are imperceptible on the scale of Fig. 1. These effects are illustrated in Fig. 2. It can be seen from Fig. 2a that the presented fragment of the band structure of the spectrum exhibits an additional band gap with the width $\Delta\omega = \omega - \omega_0$. This width exceeds the width of the resonance line γ by an order of magnitude when the frequency of the resonant gas $\omega_0 = 1.089\omega_1$ lies in the continuous spectrum near the high-frequency edge of the first band gap.

A different situation arises when the resonant frequency $\omega_0 = 1.079\omega_1$ lies in the band gap of the photonic crystal (Fig. 2b). In this case, a narrow transmission band with the width exceeding the width of the resonance line γ by an order of magnitude appears in the band gap.

The widths of the additional transmission band and the band gap can be controlled by varying the gas pressure. For example, when the density of the resonant gas increases by a factor of 3, the damping of the resonance linewidth γ also increases by a factor of 3 in the case of the impact mechanism of the broadening. Incidentally, a comparison of Figs. 2 and 3 shows that the width of the additional band gap or the width of the additional transmission band increases by the same factor.

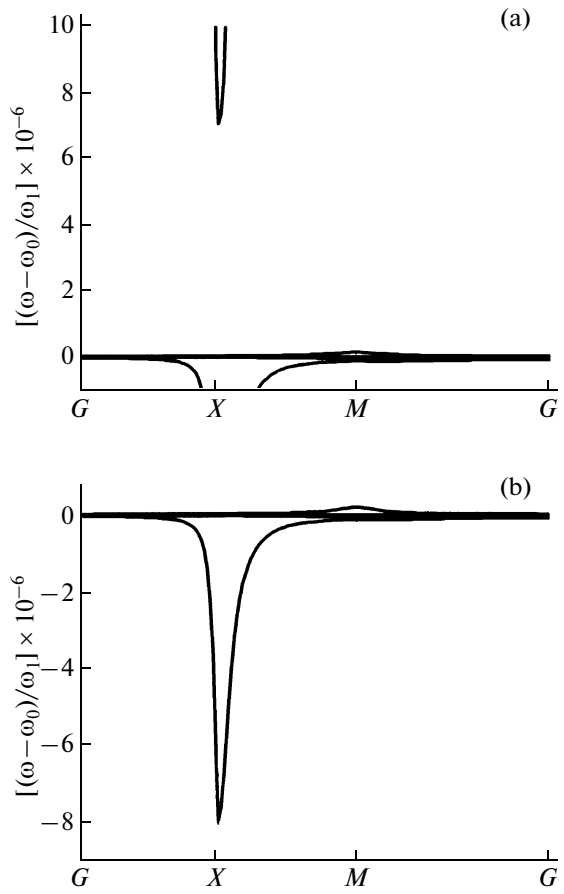

Fig. 3. A fragment of the band structure. The density of resonant atoms is 1.2×10^{15} cm^{-3}, the linewidth is $\gamma = 1.5 \times 10^{-6}\omega_1$, and the other parameters are the same as in Fig. 2 for the resonant frequencies ω_0/ω_1 = (a) 1.089 and (b) 1.079.

Let us turn to the analysis of the results obtained from the calculation of the band structure of the spectrum for the sample of a resonant photonic crystal of the *b* type, which consists of elements in the form of infinite hollow cylinders that are filled with a resonant gas and form a square lattice in a dielectric matrix. Figure 4 shows the seed band structure for the *b*-type photonic crystal sample with the parameters $\omega_2 = \pi c n_2/a$, where $n_2 = f + \sqrt{\varepsilon_1}(1-f)$, $\varepsilon_2 = 1$, and $\varepsilon_1 = 3.24$. For the filling factor $f = 79.5\%$, this photonic crystal has the maximum width of the complete band gap. In this case, the photonic band gap in the *X* direction of the Brillouin zone lies in the frequency range ω/ω_2 from 0.854 to 1.076. A comparison of Figs. 4 and 1 shows that the spectra of seed photonic crystals of both types have a similar structure. This is obviously explained by the fact that these crystals have close factors of filling with the dielectric material.

Figure 5 illustrates the variations in the dispersion properties of the resonant photonic crystal under consideration due to the dispersion of the resonant gas, which is described by expression (1). A specific feature of the band structure of the spectrum is the appearance

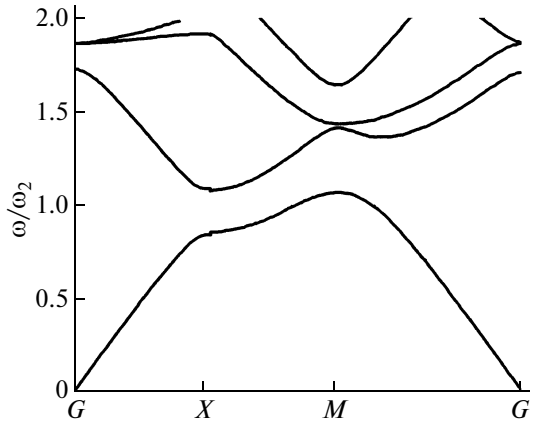

Fig. 4. Band structure of the square lattice of hollow dielectric cylinders in the dielectric matrix for *s*-polarized waves. The number of plane waves in the expansion is $M = 121$, and the filling factor is $f = 79.5\%$.

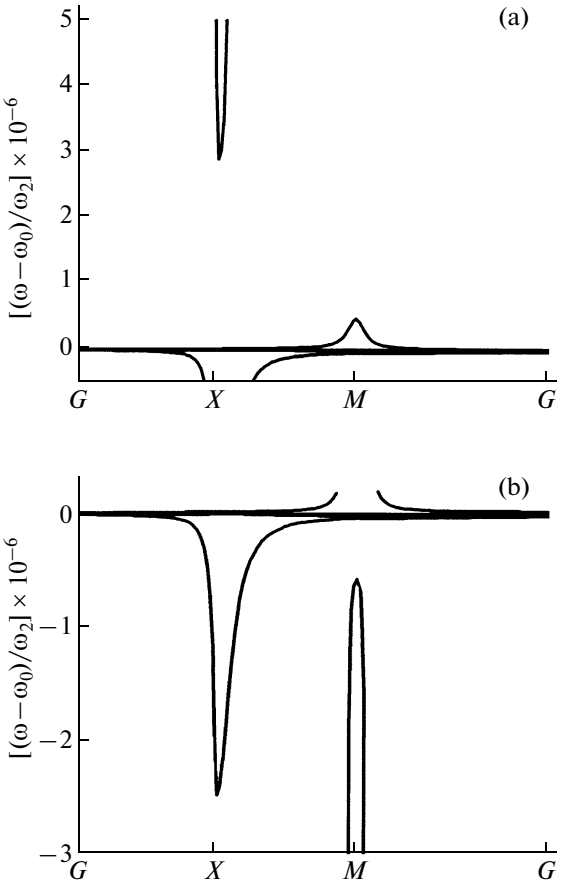

Fig. 5. A fragment of the band structure corresponding to Fig. 4 for different ratios of the resonant frequency and parameters of the photonic crystal structure. ω_0/ω_2 = (a) 1.081 and (b) 1.071.

of additional transmission bands and an additional band gap at the X and M points of the Brillouin zone, respectively (Fig. 5a). Therefore, the dispersion properties of the resonant photonic crystal depend on the direction of propagation of electromagnetic waves. We also note that the width of the additional transmission band or the band gap increases when the resonant frequency approaches the edge of the band gap with variations in the parameters of the photonic crystal structure.

4. CONCLUSIONS

Thus, the photonic band structure for s-polarized electromagnetic waves propagating in a system consisting of infinite dielectric cylinders forming a square lattice filled with a resonant gas has been studied using the plane wave method. The band structure has also been calculated for s-polarized waves propagating in a resonant photonic crystal consisting of infinite cylindrical holes that are filled with a resonant gas and form a square lattice in a dielectric matrix. It has been shown that the dispersion of two-dimensional seed photonic crystal structures in combination with the dispersion of a resonant gas leads to qualitative changes in the band structure of the spectrum of intrinsic electromagnetic excitations of the resonant photonic crystal; more specifically, additional band gaps arise in the continuous spectrum of the crystal and a transmission band appears in the photonic band gap. Since the transmission band appears in the band gap in which radiation cannot propagate, it has become possible to achieve a high contrast of the filtering of optical radiation.

In practical applications, such resonant photonic crystals are promising materials for use in the design of narrow-band filters, spectral prisms with an increased dispersion, and new types of optical devices.

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