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The photonic band structure of the two-dimensional hexagonal lattice of ionic dielectric media

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Abstract. The photonic band structure of a two-dimensional hexagonal lattice of air cylinders embedded in an ionic crystal is calculated using the plane-wave method. The dielectric function of the ionic crystal is taken as $\epsilon(\omega) = \epsilon(\infty)(\omega_{LO}^2 - \omega^2)/(\omega_{TO}^2 - \omega^2)$, with $\epsilon(\infty), \omega_{TO}$, and ω_{LO} denoting the high-frequency dielectric constant, and the transverse and longitudinal optical phonon frequencies, respectively. The frequencies of the electromagnetic modes are determined from the zeros of the determinants of the matrix equation. Due to the strong coupling between the photon and transverse optical phonon, the photonic band dispersions are suppressed and photonic band gaps are easier to open up in comparison with those of non-ionic media. Our study also suggests that the plane-wave method gives reliable photonic bands only for frequency below ω_{TO}.

1. Introduction

The periodical spatial variation of certain physical properties affects the propagating behaviours of the corresponding Bloch waves; the strongest influence occurs near the Brillouin boundaries where the travelling waves are transformed into standing waves, and this results in an energy gap which splits the dispersion relation into infinite bands. The best-known example is that of the electronic band structures in all crystals due to the periodic potential experienced by the electrons. For electromagnetic wave propagation in bulk dielectric media, because the wavelength of the electromagnetic waves is much larger than the lattice constant, photons experience only a constant dielectric function, and thus there is no band gap. To make the propagation of electromagnetic waves parallel to the electron propagation in a periodic potential, one can however introduce artificial periodic structure in a dielectric function whose lattice constant is comparable to the wavelength of the electromagnetic waves so that the Bloch theorem can be applied again.

This was proposed several years ago in the pioneering work by Yablonovitch *et al* [1–3] on the electromagnetic waves propagating in periodic dielectric media. Since the studies of photonic band structures in these materials are of fundamental physical interest and since there are potential applications in numerous laser-related semiconductor devices, this new research field has been attracting a great deal of attention recently [4–16]. Various numerical methods have been employed and particular attention is focused on the search for dielectric structure possessing photonic band gaps. This has been the case since Yablonovitch *et al* [1–3] suggested that the overlap of the photonic gap and electronic band edge suppresses the spontaneous emission of light and favours a population reverse which can improve the performance of many optical and electronic devices. It is also suggested [16] that the

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Anderson localization of light in the band gap can be more easily observed if the periodic structure of the dielectric is disordered than if the atomic structure of the dielectric is disordered.

Among the numerical methods used for calculating the photonic band structures, the most frequently adopted technique is the plane-wave expansion with its scale wave and vector wave approximations. The search for photonic-band-gap materials has been carried out for both three-dimensional dielectric media [4–10] and two-dimensional ones [11–13]. These studies show that various periodic structures do possess photonic gaps, and thus have potential for future applications. They also suggest that the plane-wave expansion method is a straightforward method and easy to implement; it gives reliable results in most circumstances. However, in the plane-wave method, one has to truncate the expansion series at a certain order; this may cause slow convergence of the solution in the presence of a very rapid change of electromagnetic waves in the system. To overcome this difficulty, the transfer-matrix method has also been in wide use recently for calculating the transmission spectra of photonic-band-gap materials [14].

In the last few years, the search for photonic-band-gap materials has extended to systems with restricted geometry and to frequency-dependent dielectric media [17–22]. The study carried out by Maradudin and McGurn [17] for the truncated, two-dimensional periodic dielectric medium shows that nearly dispersionless photonic bands exist for very thin plates due to the quantization conditions. For the frequency-dependent dielectric function, the photonic band structures have been calculated for metallic and semiconductor arrays [14, 18–20] and for superconductor arrays [21]. These studies suggest that nearly dispersionless bands also appear below the plasma frequency. For the photonic-band-gap materials composed of ionic crystal, while the transmission spectra have already been obtained by Sigalas *et al* [22] for the finite-slab square-lattice dielectric medium, the photonic band structures have not been studied yet.

Therefore, we have studied the photonic band structure for the ionic dielectric media consisting of two-dimensional periodic arrays of parallel dielectric rods with circular cross sections, where the rods are embedded in a background medium with a different dielectric function. The electromagnetic waves are assumed to propagate in the plane, and two polarization orientations are considered where either the electric field $\boldsymbol{E}$ or the magnetic field $\boldsymbol{H}$ is normal to the plane. Our detailed calculations show that the photonic band structures in ionic dielectric media are generally quite different from their counterparts in non-ionic dielectric media. The strong photon–phonon coupling makes the photonic gaps easier to open up since it reduces the dispersion of the photonic bands in comparison with that of the non-ionic dielectric media. In particular, this coupling is so strong near the long-wavelength transverse optical phonon frequency ω_{TO} that it makes the photons almost localized for a certain volume filling of the dielectric rods. This result is of great physical interest since it offers an alternative mechanism for the photon localization and it suggests that strong photon–phonon interaction plays the same role in photon localization as the strong electronic correlations play in the electron localization.

The rest of the paper is organized as follows. In section 2, we derive the basic equation sets which govern the behaviour of the electromagnetic waves using the plane-wave expansion method. The frequencies of the electromagnetic modes are determined from the zeros of the determinants of the matrix equation. The numerical results for the photonic band structures are presented and discussed in section 3 for different filling fractions, dielectric constants, and characteristic frequencies. Section 4 gives our conclusions.

2. The ionic dielectric model and the numerical method

In this paper, the periodic dielectric media are taken into account using a method based on a position-dependent dielectric function, which has been shown to be effective in earlier calculations of this type for non-ionic dielectric media [4–13]. The dielectric function for ionic dielectric media is frequency dependent due to the interaction between the transverse optical phonons and photons; it is generally given in terms of the high-frequency dielectric constant $\epsilon(\infty)$, transverse optical phonon frequency ω_{TO}, and longitudinal optical phonon frequency ω_{LO}: $\epsilon(\omega) = \epsilon(\infty)(\omega_{LO}^2 - \omega^2)/(\omega_{TO}^2 - \omega^2)$, and the high-frequency dielectric constant $\epsilon(\infty)$ and static dielectric constant $\epsilon(0)$ satisfy the Lyddane–Sachs–Teller (LST) relation $\epsilon(\infty)\omega_{LO}^2 = \epsilon(0)\omega_{TO}^2$. The 'eigen'-equation which determines the photonic band structure for the periodically modulated ionic dielectric media can be derived in a similar way to that given by McGurn and Maradudin [18].

(1) $\boldsymbol{H}$*-polarization.* When the magnetic field is perpendicular to the two-dimensional plane, the non-vanishing components of the magnetic field $\boldsymbol{H}$ and electric field $\boldsymbol{E}$ are

$$\boldsymbol{H}(x_1, x_2, t) = [0, 0, H_3(x_1, x_2, \omega)]\mathrm{e}^{-\mathrm{i}\omega t} \tag{1a}$$

$$\boldsymbol{E}(x_1, x_2, t) = [E_1(x_1, x_2, \omega), E_2(x_1, x_2, \omega), 0]\mathrm{e}^{-\mathrm{i}\omega t}. \tag{1b}$$

Here, x_1 and x_2 are the two coordinates in the two-dimensional plane and t is the time. After eliminating E_1 and E_2 in terms of H_3, the magnetic field is described by a second-order partial differential equation:

$$\frac{\partial}{\partial x_1}\left[\frac{1}{\epsilon(\boldsymbol{x}, \omega)}\frac{\partial H_3}{\partial x_1}\right] + \frac{\partial}{\partial x_2}\left[\frac{1}{\epsilon(\boldsymbol{x}, \omega)}\frac{\partial H_3}{\partial x_2}\right] = -\frac{\omega^2}{c^2}H_3. \tag{2}$$

Since the dielectric function $\epsilon(\boldsymbol{x}, \omega)$ is a periodic function in real space, the magnetic field H_3 satisfies the Bloch theorem. Thus the dielectric function and the magnetic field can be expanded in the reciprocal space as follows:

$$\frac{1}{\epsilon(\boldsymbol{x}, \omega)} = \sum_{\boldsymbol{G}} \kappa(\boldsymbol{G}, \omega)\mathrm{e}^{\mathrm{i}\boldsymbol{G}\cdot\boldsymbol{x}} \tag{3}$$

$$H_3(\boldsymbol{x}, \omega) = \sum_{\boldsymbol{G}} H_{\boldsymbol{k}}(\boldsymbol{G}, \omega)\mathrm{e}^{\mathrm{i}(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{x}} \tag{4}$$

where $\boldsymbol{k}$ and $\boldsymbol{G}$ are the wave vector and the reciprocal-lattice vector, respectively. When these expansions are substituted into equation (2), we obtain the following equation for the coefficient $H_{\boldsymbol{k}}(\boldsymbol{G}, \omega)$:

$$\sum_{\boldsymbol{G}'}\left[\kappa(\boldsymbol{G} - \boldsymbol{G}', \omega)(\boldsymbol{G} + \boldsymbol{k}) \cdot (\boldsymbol{G}' + \boldsymbol{k})\right] H_{\boldsymbol{k}}(\boldsymbol{G}', \omega) = \frac{\omega^2}{c^2}H_{\boldsymbol{k}}(\boldsymbol{G}, \omega). \tag{5}$$

(2) $\boldsymbol{E}$*-polarization.* In the case where the electric field is normal to the two-dimensional plane, the non-vanishing components of the electric field $\boldsymbol{E}$ and magnetic field $\boldsymbol{H}$ are

$$\boldsymbol{E}(x_1, x_2, t) = [0, 0, E_3(x_1, x_2, \omega)]\mathrm{e}^{-\mathrm{i}\omega t} \tag{6a}$$

$$\boldsymbol{H}(x_1, x_2, t) = [H_1(x_1, x_2, \omega), H_2(x_1, x_2, \omega), 0]\mathrm{e}^{-\mathrm{i}\omega t}. \tag{6b}$$

H_1 and H_2 can be expressed in terms of E_3, and the Maxwell equation for the electric field is reduced to

$$\frac{1}{\epsilon(\boldsymbol{x}, \omega)}\left[\frac{\partial^2 E_3}{\partial x_1^2} + \frac{\partial^2 E_3}{\partial x_2^2}\right] = -\frac{\omega^2}{c^2}E_3. \tag{7}$$

After expanding the electric fields in the reciprocal space

$$E_3(\boldsymbol{x}, \omega) = \sum_{\boldsymbol{G}} E_{\boldsymbol{k}}(\boldsymbol{G}, \omega) \mathrm{e}^{\mathrm{i}(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{x}} \tag{8}$$

one obtains the equation satisfied by the coefficient $E_{\boldsymbol{k}}(\boldsymbol{G}, \omega)$:

$$\sum_{\boldsymbol{G}'} \left[\kappa(\boldsymbol{G}-\boldsymbol{G}', \omega)(\boldsymbol{G}'+\boldsymbol{k})^2\right] E_{\boldsymbol{k}}(\boldsymbol{G}', \omega) = \frac{\omega^2}{c^2} E_{\boldsymbol{k}}(\boldsymbol{G}, \omega). \tag{9}$$

This equation can be made symmetrical with respect to $\boldsymbol{G}$ and $\boldsymbol{G}'$ if one introduces a set of new coefficients $\tilde{E}_{\boldsymbol{k}}(\boldsymbol{G}, \omega) = |\boldsymbol{G}+\boldsymbol{k}| E_{\boldsymbol{k}}(\boldsymbol{G}, \omega)$. Then the matrix equation, for the new coefficients, becomes

$$\sum_{\boldsymbol{G}'} \left[|\boldsymbol{G}+\boldsymbol{k}| \kappa(\boldsymbol{G}-\boldsymbol{G}', \omega) |\boldsymbol{G}'+\boldsymbol{k}|\right] \tilde{E}_{\boldsymbol{k}}(\boldsymbol{G}', \omega) = \frac{\omega^2}{c^2} \tilde{E}_{\boldsymbol{k}}(\boldsymbol{G}, \omega). \tag{10}$$

Thus to obtain the photonic band structure for electromagnetic waves propagating in periodically modulated dielectric media, one has to obtain solutions of the matrix equation (5) and equation (10). However, equation (5) and equation (10) are not linear equations for ionic dielectric media since κ depends also on the frequency.

The above derivation is suitable for all periodic arrays of parallel dielectric rods of arbitrary cross section and applicable to any of the five Bravais lattices in two dimensions. In this paper, we concentrate on the hexagonal lattice. The two fundamental translation vectors for hexagonal lattice are $\boldsymbol{a}_1 = a(\sqrt{3}/2, 1/2)$ and $\boldsymbol{a}_2 = a(-\sqrt{3}/2, 1/2)$ in real space and $\boldsymbol{b}_1 = (4\pi/\sqrt{3}a)(1/2, \sqrt{3}/2)$ and $\boldsymbol{b}_2 = (4\pi/\sqrt{3}a)(-1/2, \sqrt{3}/2)$ in reciprocal space. a is the lattice constant. In the case of rods with circular cross section of radius R, we have

$$\kappa(\boldsymbol{G}, \omega) = \begin{cases} \dfrac{f}{\epsilon_a(\omega)} + \dfrac{1-f}{\epsilon_b(\omega)} & \text{if } \boldsymbol{G} = 0 \\ \left(\dfrac{1}{\epsilon_a(\omega)} - \dfrac{1}{\epsilon_b(\omega)}\right) f \dfrac{2J_1(GR)}{GR} & \text{if } \boldsymbol{G} \neq 0 \end{cases} \tag{11}$$

where $\epsilon_a(\omega)$ and $\epsilon_b(\omega)$ are the dielectric functions of the rods and the background, respectively. $\boldsymbol{G} = n_1\boldsymbol{b}_1 + n_2\boldsymbol{b}_2$ with integers n_1 and n_2 and $G = |\boldsymbol{G}|$. $J_1(GR)$ is the first-rank Bessel function. The filling fractions f are given by $f = 2\pi R^2/\sqrt{3}a^2$ for the hexagonal lattice. We assume that the background dielectric function is of ionic type and takes the form $\epsilon_b(\omega) = \epsilon_b(0)[\omega_{TO}^2(\omega_{LO}^2 - \omega^2)]/[\omega_{LO}^2(\omega_{TO}^2 - \omega^2)]$. The dielectric function for the rods is taken as a constant, $\epsilon_a(\omega) = \epsilon_a$.

3. Results and discussion

The non-linear matrix equations (5) and (10) are solved for various combinations of parameter sets ϵ_a, $\epsilon_b(0)$, ω_{TO}, ω_{LO}, f, and for different polarizations of electromagnetic waves. The detailed numerical procedure is as follows: we take a large number of mesh points $\omega a/2\pi c$ for a given $\boldsymbol{k}$—this number is 1000 in our case for $0 < \omega a/2\pi c < 1$. We calculate the determinants of the matrix equation at these mesh points and find out the region where the determinants of the neighbouring mesh points change sign. Thus the accuracy of the solutions for a given number of plane waves is 0.001. We have taken 331 plane waves in calculating the photonic band structures. Our results are checked for different numbers of plane waves and the accuracy of the photonic band structures using 331 plane waves is within 3% for the bands that are not too near to the transverse optical phonon

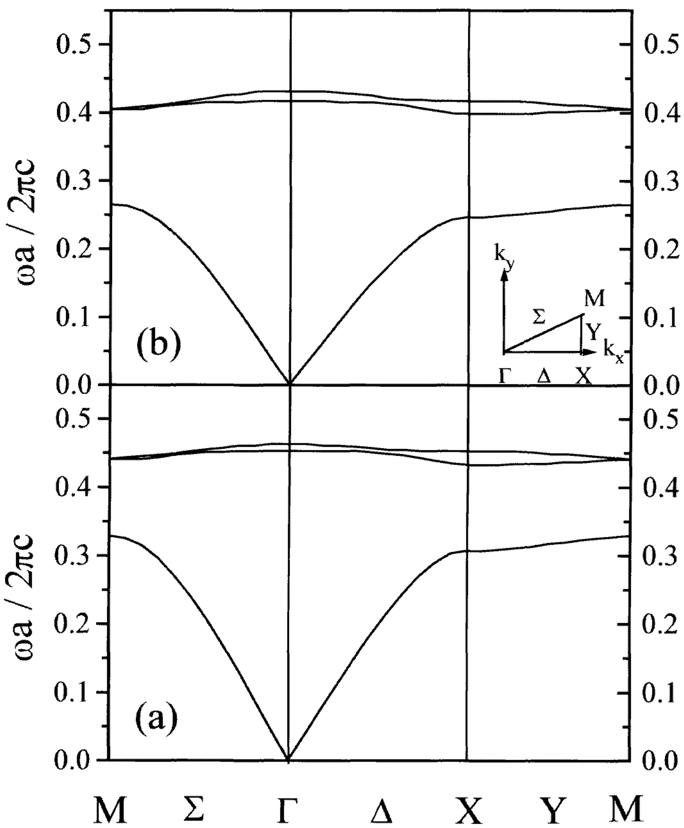

Figure 1. The photonic band structure with the magnetic field normal to the plane. The values of the parameters are $\omega_{TO}a/2\pi c = 0.5$, $\omega_{LO}a/2\pi c = 1.0$, $\epsilon_a = 1$, and the filling fraction $f = 0.64$. (a) $\epsilon_b(0) = 5$ and (b) $\epsilon_b(0) = 10$. The inset shows the first Brillouin zone for the hexagonal lattice, with the symmetry points and directions indicated.

frequency ω_{TO}. For the photonic bands above ω_{TO} the plane-wave expansion does not give reliable results because of the existence of the exponentially decaying solution. Thus, in the following we only present the bands below ω_{TO} and discuss the effect of $\epsilon_b(0)$, the polarization orientation, and the phonon frequencies, separately.

In figure 1, we show the three lowest photonic bands below ω_{TO} for the case of $\boldsymbol{H}$-polarization. The abscissa refers to the wave vector $\boldsymbol{k}$ as indicated in the inset, and the ordinate refers to the frequency scaled by $2\pi c/a$. The parameter values are taken as $\omega_{TO}a/2\pi c = 0.5$, $\omega_{LO}a/2\pi c = 1.0$, $\epsilon_a = 1$, and $\epsilon_b(0) = 5$ and $\epsilon_b(0) = 10$ for figure 1(a) and figure 1(b), respectively. The filling fraction $f = 0.64$ was chosen to maximize the size of the photonic band gaps. The lowest first band has large dispersion which is similar to that in the case of a non-ionic situation [10]; it is separated by a relatively large gap from other bands. One absolute band gap is observed in the frequency range. Comparing figure 1(a) and figure 1(b), one also sees that a larger $\epsilon_b(0)$ leads to a larger photonic gap; this is achieved by reducing the dispersion of the low bands. The main feature of the photonic band structure of the ionic medium is the appearance of very flat bands near the edge of the transverse optical phonon frequency $\omega_{TO}a/2\pi c = 0.5$.

It would be of interest to see whether the narrow dispersion features of some photonic

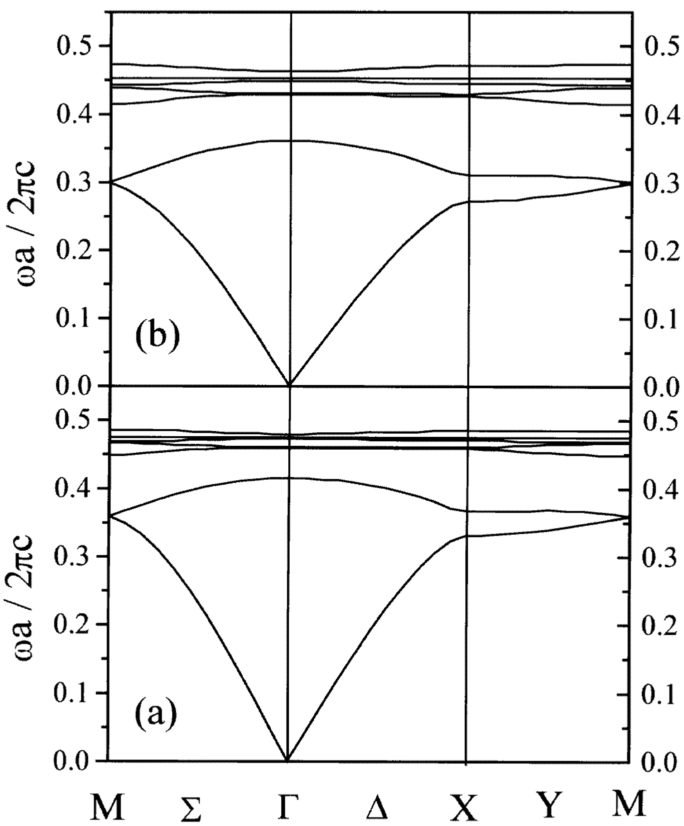

Figure 2. The photonic band structure with the electric field normal to the plane. The values of the parameters are $\omega_{TO}a/2\pi c = 0.5$, $\omega_{LO}a/2\pi c = 1.0$, $\epsilon_a = 1$, and the filling fraction $f = 0.78$. (a) $\epsilon_b(0) = 5$ and (b) $\epsilon_b(0) = 10$.

bands are peculiar to certain polarization orientations. Our study suggests that this property is quite general, and that the flattening of the band does not depend on the polarization orientations of the electromagnetic waves, since it also occurs in the band structure when the electric field is perpendicular to the two-dimensional plane, as shown in figure 2. The values of the parameter sets are the same as in figure 1 except that the filling fraction $f = 0.78$. One absolute band gap is observed in the low-frequency range, and the size of the lowest photonic gap is smaller than those in figure 1. The effect of the background dielectric constant $\epsilon_b(0)$ is the same as before: a larger $\epsilon_b(0)$ enhances the photonic gap by pushing the lower bands downwards. Note that the bands near $\omega_{TO}a/2\pi c = 0.5$ all have very narrow dispersion.

To see how the phonon frequency affects the propagation behaviour of the electromagnetic waves, we have also calculated the photonic band structures for $\omega_{TO}a/2\pi c = 1.0$ and $\omega_{LO}a/2\pi c = 2.0$, which are shown in figure 3. The magnetic field is taken to be normal to the two-dimensional plane. The other parameter values are taken as $f = 0.64$, $\epsilon_a = 1$, and $\epsilon_b(0) = 5$ and $\epsilon_b(0) = 10$ for figure 3(a) and figure 3(b), respectively. As in figure 1, one absolute photonic band gap is observed in the nine lowest bands below ω_{TO}, but the size of the photonic band gap is slightly larger than in figure 1. Due to the increase of the transverse and longitudinal optical phonon frequencies, the narrow bands are also

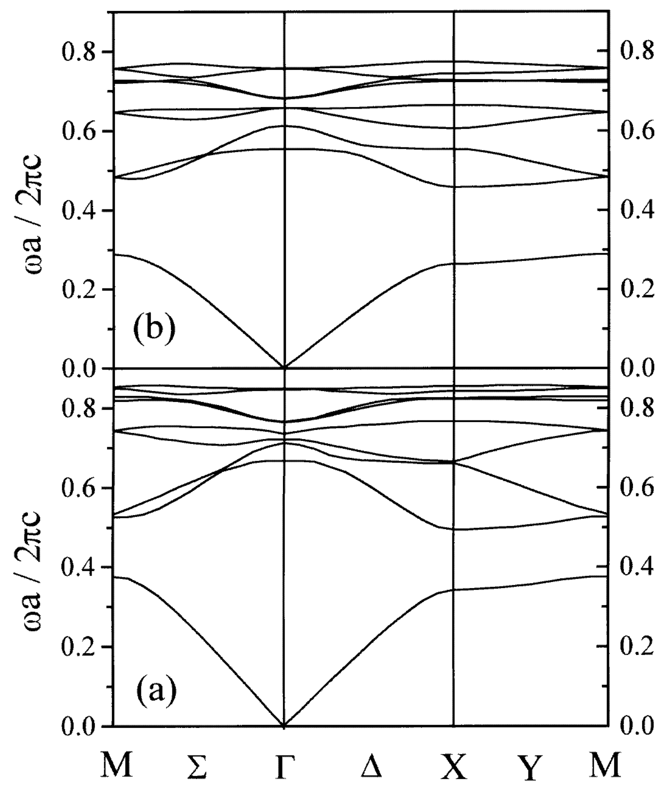

Figure 3. The photonic band structure with the magnetic field normal to the plane. The values of the parameters are $\omega_{TO}a/2\pi c = 1.0$, $\omega_{LO}a/2\pi c = 2.0$, $\epsilon_a = 1$, and the filling fraction $f = 0.64$. (a) $\epsilon_b(0) = 5$ and (b) $\epsilon_b(0) = 10$.

shifted upwards towards $\omega_{TO}a/2\pi c = 1.0$. The influence of the dielectric constant is the same as before.

The photonic band structure with the electric field perpendicular to the two-dimensional plane is illustrated in figure 4; other parameters are exactly the same as in figure 3. Unlike in figure 3 where the size of the lowest photonic band gap increases as the phonon frequencies increase, the size change of the photonic band gap with the electric field normal to the two-dimensional plane is more subtle and depends on the value of $\epsilon_b(0)$: the size of the gap increases with the phonon frequency for $\epsilon_b(0) = 10$ and decreases for $\epsilon_b(0) = 5$. From the above discussion, we found that the introduction of the photon–phonon coupling generally narrows the band dispersion and makes the photonic band gap easier to open up; this coupling has the strongest effect near the transverse optical phonon frequency.

4. Conclusion

In summary, we have studied in this paper the effect of strong photon–phonon coupling on the photonic band structure. We found that strong photon–phonon coupling flattens the photonic bands, and that photonic band gaps are generally enhanced in comparison with those of non-ionic media.

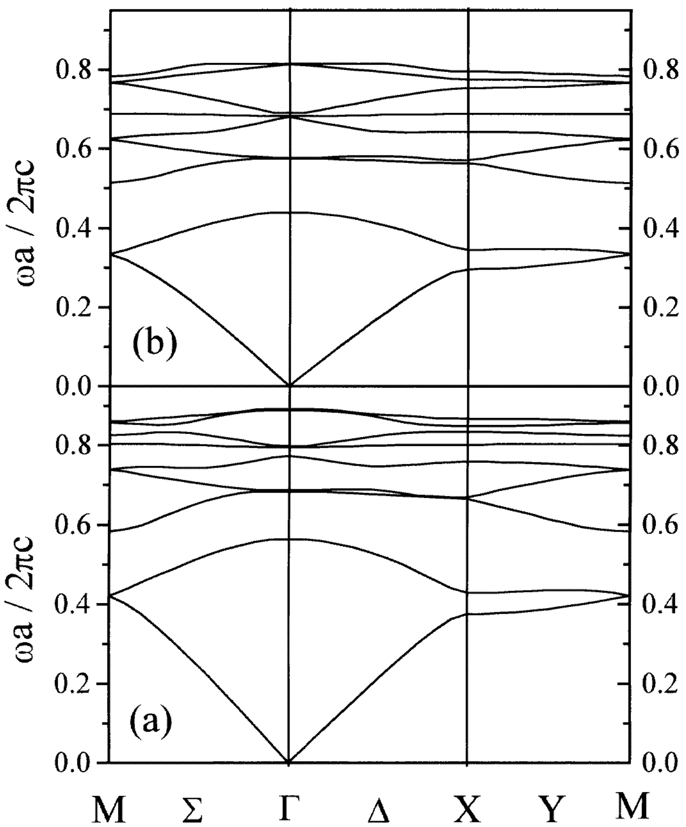

Figure 4. The photonic band structure with the electric field normal to the plane. The values of the parameters are $\omega_{TO}a/2\pi c = 1.0$, $\omega_{LO}a/2\pi c = 2.0$, $\epsilon_a = 1$, and the filling fraction $f = 0.78$. (a) $\epsilon_b(0) = 5$ and (b) $\epsilon_b(0) = 10$.

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