Photonic band structures of a two-dimensional ionic dielectric medium

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(Received 23 April 1996)

The photonic band structures of the two-dimensional square lattice of air cylinders embedded in an ionic crystal are calculated using the plane-wave method. The dielectric function of the ionic crystal is taken as $\epsilon(\omega)=\epsilon(\infty)(\omega_{\rm LO}^2-\omega^2)/(\omega_{\rm TO}^2-\omega^2)$, with $\epsilon(\infty)$, $\omega_{\rm TO}$, and $\omega_{\rm LO}$ denoting the high-frequency dielectric constant and 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. Both E and H polarizations are considered. Our calculation shows that the low-frequency photonic bands resemble the bands of a frequency-independent dielectric medium, while the bands near the transverse-optical-phonon frequency $\omega_{\rm TO}$ are strongly flattened. Our study also suggests that while the plane-wave method gives reliable photonic bands for the frequency below $\omega_{\rm TO}$, a better method has to be used for the photonic bands very near or above $\omega_{\rm TO}$. [S0163-1829(96)05140-5]

Since the pioneering works by Yablonovitch and co-workers[1–3] on the propogation of electromagnetic waves in periodic dielectric media, the study of photonic band structures of photonic materials has been attracting a great deal of attention both theoretically and experimentally. Various dielectric structures have been investigated, and particular attention is paid to the dielectric structure possessing the photonic band gaps. The existence of the photonic band gap is of great interest for both basic research and potential technological applications. This is so since Yablonovitch and co-workers[1–3] suggested that the overlap of the photonic gap and electronic band edge suppresses the spontaneous emission of light and favors the population reverse, which can improve the performance of many optical and electronic devices. An earlier study by John[4] also demonstrated that the Anderson localization of light in the band gap is easier to observe 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, an early frequently adopted technique was plane-wave expansion with its scale wave approximation.[5–7] However, discrepancies between theories and experimental observations indicate that the vector nature of the electromagnetic waves is important. Subsequent calculations using the vector wave approximation[8–12] do agree with experimental results.[13,14] At the same time, research on the photonic band-gap materials has also been carried out in two-dimensional cases.[15,16] These studies show that various periodic structures do possess the 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 in a certain order, and this may cause a 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 to calculate the transmission spectra of photonic band-gap materials.[17]

In the last several years, the effort to search for photonic band-gap materials has been extended to systems with restricted geometry, and to frequency-dependent dielectric media.[18–24] A study carried out by Maradudin and McGurn[18] for a two-dimensional periodic array of dielectric rods between two metal plates shows that nearly dispersionless photonic bands exist when the thickness between the two plates becomes very thin. In the case of a frequency-dependent dielectric function, photonic band structures have been calculated for the metallic or semiconductor arrays[17,19–22] and for superconductor arrays.[23] These studies suggest that nearly dispersionless bands also appear below the plasma frequency. For photonic gap materials composed of ionic crystals, for which transmission spectra have already been obtained by Sigalas *et al.*[24] for the finite-slab two-dimensional dielectric medium, photonic band structures have not been studied yet.

With this motivation in our mind, we studied the photonic band structure of the ionic dielectric media with a two-dimensional periodic array of parallel air cylinders in it. The electromagnetic waves are assumed to propagate in the plane, and two polarization orientations are considered where either the electric field $\vec{E}$ or magnetic field $\vec{H}$ is normal to the plane. Our detailed calculations show that 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 frequency-independent dielectric media. In particular, this coupling is so strong near the long-wavelength transverse-optical-phonon frequency $\omega_{\rm TO}$ that makes the photons almost localized for certain volume filling of the air cylinders.

In this paper, periodic dielectric media are taken into account using the method of a position-dependent dielectric function, which has been shown to be effective in the earlier calculations of these types of frequency-independent dielectric media.[15,16] Dielectric functions for ionic dielectric media are frequency dependent due to the interaction between the transverse-optical-phonons and photons; they are generally given in terms of the high-frequency dielectric constant $\epsilon(\infty)$, transverse-optical-phonon frequency $\omega_{\rm TO}$, and longitudinal-optical-phonon frequency $\omega_{\rm LO}$. $\epsilon(\omega)=\epsilon(\infty)(\omega_{\rm LO}^2-\omega^2)/(\omega_{\rm TO}^2-\omega^2)$ and the high-frequency dielectric constant $\epsilon(\infty)$ and static dielectric constant $\epsilon(0)$ satisfy the Lyddane-Sachs-Teller (LST) relation $\epsilon(\infty)\omega_{\rm LO}^2=\epsilon(0)\omega_{\rm TO}^2$. The "eigen" equation which determines the photonic band structure for periodically modulated ionic dielectric media can be derived in the same way as that given by McGurn and Maradudin.[19]

In the case when the magnetic field is perpendicular to the two-dimensional plane, the nonvanishing component of the magnetic field $\vec{H}$ satisfies the following equation:[19]

$$\sum_{\vec{G}'}[\kappa(\vec{G}-\vec{G}',\omega)(\vec{G}+\vec{k})\cdot(\vec{G}'+\vec{k})]H_{\vec{k}}(\vec{G}',\omega)=\frac{\omega^2}{c^2}H_{\vec{k}}(\vec{G},\omega),\tag{1}$$

where $\vec{k}$ and $\vec{G}$ are the wave vector and the reciprocal-lattice vector, respectively. $\kappa(\vec{G},\omega)$ is the Fourier transformation of the inverse dielectric function. In the case when the electric field is normal to the two-dimensional plane, the equation satisfied by the nonvanishing component of the electric field $\vec{E}$ can be similarly obtained,

$$\sum_{\vec{G}'}[|\vec{G}+\vec{k}|\kappa(\vec{G}-\vec{G}',\omega)|\vec{G}'+\vec{k}|]\widetilde{E}_{\vec{k}}(\vec{G}',\omega)=\frac{\omega^2}{c^2}\widetilde{E}_{\vec{k}}(\vec{G},\omega).\tag{2}$$

Here $\widetilde{E}_{\vec{k}}(\vec{G},\omega)=|\vec{G}+\vec{k}|E_{\vec{k}}(\vec{G},\omega)$. Thus to obtain the photonic band structure of electromagnetic waves propagating in periodically modulated dielectric media, one has to solve the matrix solutions of Eqs. (1) and (2). However, Eqs. (1) and (2) are not eigenequations for the ionic dielectric media since κ also depends on the frequency. Instead of solving the eigenequation for frequency-independent dielectric media, the calculations of the photonic band structure for ionic dielectric media are numerically more complex and time consuming.

The above derivation is suitable for all periodic arrays of parallel dielectric rods of arbitrary cross sections, and applicable to any of the five Bravais lattices in two dimensions. For numerical calculations, we concentrate on the square lattice. The two fundamental translation vectors are $\vec{a_1}=a(1,0)$ and $\vec{a_2}=a(0,1)$, with a as the lattice constant; the corresponding fundamental translation vectors in reciprocal space are $\vec{b_1}=(2\pi/a)(1,0)$ and $\vec{b_2}=(2\pi/a)(0,1)$. In the case of rods with circular cross sections of radius R, we have

$$\kappa(\vec{G},\omega)=\begin{cases}\dfrac{f}{\epsilon_a(\omega)}+\dfrac{1-f}{\epsilon_b(\omega)} & \text{if } \vec{G}=0\\[2ex] \left(\dfrac{1}{\epsilon_a(\omega)}-\dfrac{1}{\epsilon_b(\omega)}\right)f\dfrac{2J_1(GR)}{GR} & \text{if } \vec{G}\neq 0,\end{cases}\tag{3}$$

where $\epsilon_a(\omega)$ and $\epsilon_b(\omega)$ are dielectric functions of the rods and the background, respectively. $\vec{G}=n_1\vec{b_1}+n_2\vec{b_2}$ with integers n_1 and n_2 and $G=|\vec{G}|$. $f=\pi R^2/a^2$ is the filling fraction, and $J_1(GR)$ is the first-rank Bessel function. We assume that the background dielectric function is of ionic type, and takes the form $\epsilon_b(\omega)=\epsilon_b(0)[\omega_{\rm TO}^2(\omega_{\rm LO}^2-\omega^2)]/[\omega_{\rm LO}^2(\omega_{\rm TO}^2-\omega^2)]$, the dielectric function for the rods is taken as a constant $\epsilon_a(\omega)=\epsilon_a$.

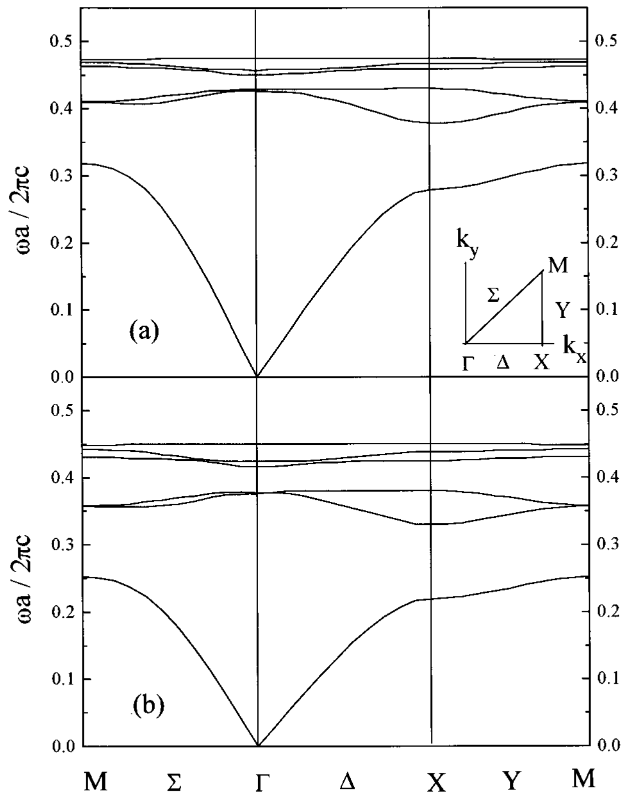

FIG. 1. The photonic band structure with the electric field normal to the plane. The values of the parameters are $\omega_{\rm TO}a/2\pi c=0.5$, $\omega_{\rm LO}a/2\pi c=1.0$, and $\epsilon_a=1$, and the filling fraction $f=0.78$. (a) $\epsilon_b(0)=5$. (b) $\epsilon_b(0)=10$. The inset shows the first Brillouin zone for the periodic dielectric structure studied, with the symmetry points and directions indicated.

The nonlinear matrix equations (1) and (2) are solved for various combinations of parameter sets $\epsilon_a,\epsilon_b(0),\omega_{\rm TO}$, $\omega_{\rm LO}$, and f, and for different polarizations of electromagnetic waves. The detailed numerical procedure is as follows: we take a large number of mesh points of $\omega a/2\pi c$ for a given $\vec{k}$; 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 the region where the determinants of the neighboring mesh points change sign. Thus the accuracy of the solutions for a given number of plane wave is 0.001. We have taken 361 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 361 plane waves, is within 3% for bands not too near to the transverse-optical-phonon frequency $\omega_{\rm TO}$. For photonic bands above $\omega_{\rm TO}$, the plane-wave expansion does not give reliable results because of the rapid change of the electromagnetic wave in the system. Thus in the following we only present bands below $\omega_{\rm TO}$.

In Fig. 1, we show the lowest six photonic bands for the electric field normal to the two-dimensional plane. The x

axis refers to the wave vector $\vec{k}$ as indicated in the inset. The y axis refers to the frequency scaled by $2\pi c/a$. The parameter values are $\omega_{\mathrm{TO}}a/2\pi c=0.5$, $\omega_{\mathrm{LO}}a/2\pi c=1.0$, and $\epsilon_a=1$ for Fig. 1(a), and $\epsilon_b(0)=5$ and $\epsilon_b(0)=10$ for Fig. 1(b), respectively. The filling fraction $f=0.78$ is chosen to maximize the size of photonic band gaps. Two absolute band gaps are observed in the frequency range; this is one more than that of the corresponding frequency-independent dielectric media for the same lattice type.[15] One also sees that a larger $\epsilon_b(0)$ results in larger photonic gaps. What differentiates this band structure most from its counterpart in the frequency-independent case is the appearance of very flat bands near the edge of the transverse optical-phonon frequency $\omega_{\mathrm{TO}}a/2\pi c=0.5$. In particular, the sixth band is essentially dispersionless.

The interesting feature of the flattened bands does not depend on the polarization orientations of electromagnetic waves, since they also appear in the band structure when the magnetic field is perpendicular to the two-dimensional plane, as shown in Fig. 2. The values of the parameter sets are the same as in Fig. 1, except that the filling fraction $f=0.57$. The bands with the smallest dispersion in this configuration are bands 5 and 7. Three absolute band gaps are observed in the low-frequency range, which is again one more than the frequency-independent case.[15] Thus the strong photon-phonon coupling generally reduces the band dispersion and favors the opening up of the photonic band gap.

Since the transmission spectra calculated by Sigalas *et al.*[24] is for the finite-slab two-dimensional geometry, their dielectric functions for the filling cylinders and background are just the opposite of ours; a direct comparison between their results and ours is not feasible. However, we found that the small peak just below the polariton gap in their Fig. 2 is very similar to our flattened bands at the same position. This suggests that flattened bands are a common feature in systems with frequency-dependent dielectric functions. We would also like to mention that the flattened bands found for the metallic cylinders[17,19–22] all occur below a plasma frequency where the dielectric function is negative, while our flattened bands occur at a frequency where the dielectric function is still positive.

As is well known from studies of localization problems, the flattened bands indicate massive particles which are difficult to propagate in the materials. The observation of flattened bands near the transverse-optical-phonon frequency suggests that strong photon-phonon coupling tends to make the photon more difficult to move in space, just as strong electron-phonon couplings or strong electronic correlations do for the electron. A recent study by John and Quang[25] shows that when two-level atoms placed within the photonic band-gap materials have resonance frequencies at the band

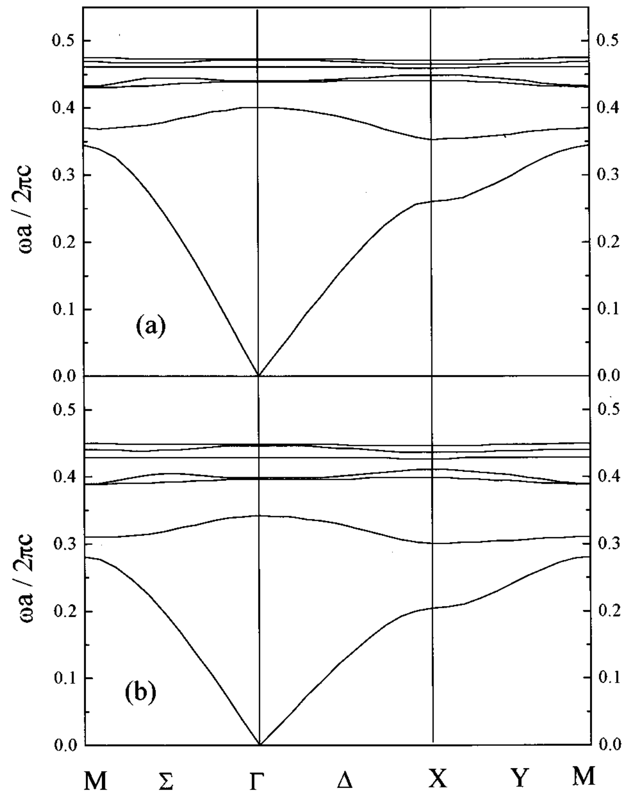

FIG. 2. The photonic band structure with the magnetic field normal to the plane. The values of the parameters are $\omega_{\mathrm{TO}}a/2\pi c=0.5$, $\omega_{\mathrm{LO}}a/2\pi c=1.0$, and $\epsilon_a=1$, and the filling fraction $f=0.57$. (a) $\epsilon_b(0)=5$. (b) $\epsilon_b(0)=10$.

edge, superradiant emission remains localized in the vicinity of the atoms. We speculate that the long-wavelength optical phonons may function in the same way, and thus cause the flattened bands near its resonance frequency.

In summary, in this paper we studied 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 the effect is most significant near the transverse-optical-phonon frequency. This property does not depend on the lattice type, and seems to be a universal feature.

One of the authors (W.Z.) would like to acknowledge partial financial support from the Education Commission of China and from the Keli Foundation. This work was supported in part by a grant for a key research project in a climbing program from the National Science and Technology Commission of China.

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