Photonic band structure of two-dimensional systems: The triangular lattice

M. Plihal and A. A. Maradudin
Department of Physics, University of California, Irvine, California 92717
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By the use of a position-dependent dielectric constant and the plane-wave method, we have calculated the photonic band structure for electromagnetic waves in a structure consisting of a periodic array of parallel dielectric rods of circular cross section, whose intersections with a perpendicular plane form a triangular lattice. The rods are embedded in a background medium with a different dielectric constant. The electromagnetic waves are assumed to propagate in a plane perpendicular to the rods, and two polarizations of the waves are considered. Absolute gaps in the resulting band structures are found for waves of both polarizations, and the dependence of the widths of these gaps on the ratio of the dielectric constants of the rods and of the background, and on the fraction of the total volume occupied by the rods, is investigated.

There has been a growing interest in recent years in the determination of the dispersion curves for electromagnetic waves propagating in three-dimensional, periodic, dielectric structures. The object of these investigations is finding out whether the band formed by the branches of these dispersion curves can be separated by absolute frequency gaps, which exist for all values of the wave vector in the corresponding Brillouin zone, and which give rise to gaps in the density of states of the waves propagating in these structures. These *photonic band structures* have now been calculated in a scalar wave approximation[1–5] and on the basis of Maxwell's equations.[6–8] They have also been investigated experimentally.[9,10]

There are several reasons for the interest in photonic band structures. It has been suggested that if a three-dimensional, periodic, dielectric structure is disordered in such a way that it remains periodic on average, it may be easier to observe in it the Anderson localization of light whose frequency is close to a band edge of the corresponding periodic structure than it would be in a disordered dielectric structure that is homogeneous on average.[11] In addition, since electromagnetic modes with frequencies in the absolute gaps are totally absent, spontaneous emission is forbidden in situations in which the band gap overlaps the electronic band edge. The suppression of spontaneous emission can improve the performance of many optical and electronic devices.[1,12] The absence of electromagnetic modes in a certain frequency range can also modify the basic properties of many atomic, molecular, and excitonic systems.[13]

In contrast with the several studies of the photonic band structures of three-dimensional, periodic, dielectric systems, to our knowledge there has been only one investigation of these band structures for two-dimensional, periodic, dielectric systems. In a recent paper[14] we have calculated the (photonic) band structure for a system that consists of an array of infinitely long, parallel, dielectric rods, each with a circular cross section of radius R and characterized by a dielectric constant ϵ_a, embedded in a background dielectric material characterized by a dielectric constant ϵ_b. The intersections of these rods with a perpendicular plane formed a square lattice. The electromagnetic waves were assumed to propagate in a plane perpendicular to the rods, and two polarizations of these waves were considered: the magnetic vector parallel to the rods (H polarization) and the electric vector parallel to the rods (E polarization). It was found that the band structure in each case displays an absolute gap, i.e., a gap that exists for all values of the two-dimensional wave vector $\mathbf{k}_\parallel$ characterizing these electromagnetic waves in the corresponding Brillouin zone, and gives rise to a gap in their density of states.

In this paper we present the results for the photonic band structures for electromagnetic waves of both H and E polarization in a structure consisting of a periodic array of parallel dielectric rods of circular cross section and dielectric constant ϵ_a whose intersections with a perpendicular plane form a triangular lattice. The dielectric rods are embedded in a background dielectric material whose dielectric constant is ϵ_b. This structure is of interest because dielectric structures of this symmetry are now being fabricated for experimental studies of photonic band structures.[15]

As in Ref. 14 we assume that the dielectric rods of dielectric constant ϵ_a are parallel to the x_3 axis. We further assume that the rods do not overlap. The intersections of the axes of these rods with the x_1x_2 plane form a two-dimensional Bravais lattice whose sites are given by the vectors

$$\mathbf{x}_\parallel(l)=l_1\mathbf{a}_1+l_2\mathbf{a}_2 \ . \tag{1}$$

Here $\mathbf{a}_1$ and $\mathbf{a}_2$ are the two noncollinear primitive translation vectors of the lattice, while l_1 and l_2 are any two integers, positive, negative, or zero, which we denote collectively by l. The area of the primitive unit cell of this lattice or, equivalently, of the corresponding Wigner-Seitz cell, is $a_c=|\mathbf{a}_1\times\mathbf{a}_2|$.

The dielectric constant of this composite system is position dependent, and will be denoted by $\epsilon(\mathbf{x}_\parallel)$. Here $\mathbf{x}_\parallel=\hat{\mathbf{x}}_1x_1+\hat{\mathbf{x}}_2x_2$, where $\hat{\mathbf{x}}_1$ and $\hat{\mathbf{x}}_2$ are unit vectors along the x_1 and x_2 axes, respectively, is a position vector in the x_1x_2 plane. $\epsilon(\mathbf{x}_\parallel)$ is a periodic function of $\mathbf{x}_\parallel$ and satisfies the relation $\epsilon(\mathbf{x}_\parallel+\mathbf{x}_\parallel(l))=\epsilon(\mathbf{x}_\parallel)$.

We now turn to a calculation of the photonic band structure for electromagentic waves propagating in this structure in a plane perpendicular to the dielectric rods. As in Ref. 14 we use the position-dependent dielectric constant together with the plane-wave method for this purpose. We consider electromagnetic waves of H and E polarization in turn.

In the case of H polarization we seek solutions of Maxwell's equations which have the forms

$$\mathbf{H}(\mathbf{x};t)=(0,0,H_3(x_1,x_2|\omega))\exp(-i\omega t)\ , \tag{2a}$$

$$\mathbf{E}(\mathbf{x};t)=(E_1(x_2,x_2|\omega),E_2(x_1,x_2|\omega),0)\exp(-i\omega t)\ . \tag{2b}$$

The Maxwell "curl" equations for the three nonzero field components are

$$\frac{\partial E_2}{\partial x_1}-\frac{\partial E_1}{\partial x_2}=\frac{i\omega}{c}H_3\ , \tag{3a}$$

$$\frac{\partial H_3}{\partial x_1}=\frac{i\omega}{c}D_2=\frac{i\omega}{c}\epsilon(\mathbf{x}_\parallel)E_2\ , \tag{3b}$$

$$\frac{\partial H_3}{\partial x_2}=-\frac{i\omega}{c}D_1=-\frac{i\omega}{c}\epsilon(\mathbf{x}_\parallel)E_1\ . \tag{3c}$$

When we eliminate E_1 and E_2 from these equations we obtain the equation satisfied by H_3, which we write in the form

$$\frac{\partial}{\partial x_1}\left[\frac{1}{\epsilon(\mathbf{x}_\parallel)}\frac{\partial H_3}{\partial x_1}\right]+\frac{\partial}{\partial x_2}\left[\frac{1}{\epsilon(\mathbf{x}_\parallel)}\frac{\partial H_3}{\partial x_2}\right]+\frac{\omega^2}{c^2}H_3=0\ . \tag{4}$$

To solve this equation we expand $\epsilon^{-1}(\mathbf{x}_\parallel)$ and $H_3(\mathbf{x}_\parallel|\omega)$ according to

$$\frac{1}{\epsilon(\mathbf{x}_\parallel)}=\sum_{\mathbf{G}_\parallel}\kappa(\mathbf{G}_\parallel)e^{i\mathbf{G}_\parallel\cdot\mathbf{x}_\parallel}\ , \tag{5}$$

$$H_3(\mathbf{x}_\parallel|\omega)=\sum_{\mathbf{G}_\parallel}A(\mathbf{k}_\parallel|\mathbf{G}_\parallel)e^{i(\mathbf{k}_\parallel+\mathbf{G}_\parallel)\cdot\mathbf{x}_\parallel}\ , \tag{6}$$

where $\mathbf{k}_\parallel=\hat{\mathbf{x}}_1k_2+\hat{\mathbf{x}}_2k_2$ is the two-dimensional wave vector of the wave and

$$\mathbf{G}_\parallel(h)=h_1\mathbf{b}_1+h_2\mathbf{b}_2 \tag{7}$$

is a vector of the lattice reciprocal to the one defined by the vectors $\{\mathbf{x}_\parallel(l)\}$. Here h_1 and h_2 are any two integers that we denote collectively by h, while the primitive translation vectors of this lattice are given by

$$\mathbf{b}_1=\frac{2\pi}{a_c}(a_2^{(2)},-a_1^{(2)})\ ,\qquad \mathbf{b}_2=\frac{2\pi}{a_c}(-a_2^{(1)},a_1^{(1)})\ , \tag{8}$$

where $a_j^{(i)}$ is the jth Cartesian component of $\mathbf{a}_i$. When these expansions are substituted into Eq. (4) we obtain as the equation for the coefficients $\{A(\mathbf{k}_\parallel|\mathbf{G}_\parallel)\}$

$$\sum_{\mathbf{G}'_\parallel}(\mathbf{k}_\parallel+\mathbf{G}_\parallel)\cdot(\mathbf{k}_\parallel+\mathbf{G}'_\parallel)\kappa(\mathbf{G}_\parallel-\mathbf{G}'_\parallel)A(\mathbf{k}_\parallel|\mathbf{G}'_\parallel)=\frac{\omega^2}{c^2}A(\mathbf{k}_\parallel|\mathbf{G}_\parallel)\ , \tag{9}$$

which has the form of a standard eigenvalue problem for a symmetric matrix.

In the case of E polarization we seek solutions of Maxwell's equations which have the forms

$$\mathbf{E}(\mathbf{x};t)=(0,0,E_3(x_1,x_2|\omega))\exp(-i\omega t)\ , \tag{10a}$$

$$\mathbf{H}(\mathbf{x};t)=(H_1(x_1,x_2|\omega),H_2(x_1,x_2|\omega),0)\exp(-i\omega t)\ . \tag{10b}$$

The Maxwell curl equations in this case are

$$\frac{\partial H_2}{\partial x_1}-\frac{\partial H_1}{\partial x_2}=-\frac{i\omega}{c}D_3=-i\frac{\omega}{c}\epsilon(\mathbf{x}_\parallel)E_3\ , \tag{11a}$$

$$\frac{\partial E_3}{\partial x_1}=-i\frac{\omega}{c}H_2\ , \tag{11b}$$

$$\frac{\partial E_3}{\partial x_2}=i\frac{\omega}{c}H_1\ . \tag{11c}$$

We eliminate H_1 and H_2 from these equations and obtain as the equation for E_3

$$\frac{1}{\epsilon(\mathbf{x}_\parallel)}\left[\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}\right]E_3+\frac{\omega^2}{c^2}E_3=0\ . \tag{12}$$

To solve Eq. (12) we again use the expansion (5) and write $E_3(\mathbf{x}_\parallel|\omega)$ in the form

$$E_3(\mathbf{x}_\parallel|\omega)=\sum_{\mathbf{G}_\parallel}B(\mathbf{k}_\parallel|\mathbf{G}_\parallel)e^{i(\mathbf{k}_\parallel+\mathbf{G}_\parallel)\cdot\mathbf{x}_\parallel}\ . \tag{13}$$

The equation satisfied by the coefficients $\{B(\mathbf{k}_\parallel|\mathbf{G}_\parallel)\}$ is

$$\sum_{\mathbf{G}'_\parallel}\kappa(\mathbf{G}_\parallel-\mathbf{G}'_\parallel)(\mathbf{k}_\parallel+\mathbf{G}'_\parallel)^2B(\mathbf{k}_\parallel|\mathbf{G}'_\parallel)=\frac{\omega^2}{c^2}B(\mathbf{k}_\parallel|\mathbf{G}_\parallel)\ , \tag{14}$$

which also has the form of a standard eigenvalue problem, albeit for a nonsymmetric matrix. However, the replacement

$$C(\mathbf{k}_\parallel|\mathbf{G}_\parallel)=|\mathbf{k}_\parallel+\mathbf{G}_\parallel|B(\mathbf{k}_\parallel|\mathbf{G}_\parallel) \tag{15}$$

yields an eigenvalue problem for a symmetric matrix:

$$\sum_{\mathbf{G}'_\parallel}|\mathbf{k}_\parallel+\mathbf{G}_\parallel|\kappa(\mathbf{G}_\parallel-\mathbf{G}'_\parallel)|\mathbf{k}_\parallel+\mathbf{G}'_\parallel|C(\mathbf{k}_\parallel|\mathbf{G}'_\parallel)=\frac{\omega^2}{c^2}C(\mathbf{k}_\parallel|\mathbf{G}_\parallel)\ . \tag{16}$$

The eigenvalue problems posed by Eqs. (9) and (16) are somewhat simpler than their counterparts in Ref. 14.

We see that Fourier coefficients $\{\kappa(\mathbf{G}_\parallel)\}$ of $\epsilon^{-1}(\mathbf{x}_\parallel)$ play a central role in the determination of the photonic band structures for both polarizations. To determine them we write $\epsilon^{-1}(\mathbf{x}_\parallel)$ in the form

$$\frac{1}{\epsilon(\mathbf{x}_\parallel)}=\frac{1}{\epsilon_b}+\left[\frac{1}{\epsilon_a}-\frac{1}{\epsilon_b}\right]\sum_l S(\mathbf{x}_\parallel-\mathbf{x}_\parallel(l)) \;, \tag{17}$$

with

$$S(\mathbf{x}_\parallel)=\begin{cases}1 & \text{for } \mathbf{x}_\parallel\in R\\ 0 & \text{for } \mathbf{x}_\parallel\notin R \;,\end{cases} \tag{18}$$

where R is the region of the x_1x_2 plane defined by the cross section of the rod whose axis intersects that plane at $\mathbf{x}_\parallel=\mathbf{0}$. The Fourier coefficient $\hat{\kappa}(\mathbf{G}_\parallel)$ is then given by

$$\begin{aligned}\hat{\kappa}(\mathbf{G}_\parallel)&=\frac{1}{a_c}\int_{a_c}d^2x_\parallel e^{-i\mathbf{G}_\parallel\cdot\mathbf{x}_\parallel}\frac{1}{\epsilon(\mathbf{x}_\parallel)}\\&=\frac{1}{\epsilon_b}\delta_{\mathbf{G}_\parallel,\mathbf{0}}+\left[\frac{1}{\epsilon_a}-\frac{1}{\epsilon_b}\right]\frac{1}{a_c}\int d^2x_\parallel e^{-i\mathbf{G}_\parallel\cdot\mathbf{x}_\parallel}S(\mathbf{x}_\parallel) \;,\end{aligned} \tag{19}$$

where the integration in the second line of this equation is over the entire x_1x_2 plane. When we take into account the definition of the function $S(\mathbf{x}_\parallel)$, Eq. (18), we obtain

$$\hat{\kappa}(\mathbf{G}_\parallel)=\begin{cases}\frac{1}{\epsilon_a}f+\frac{1}{\epsilon_b}(1-f), & \mathbf{G}_\parallel=\mathbf{0} \quad (20a)\\ \left[\frac{1}{\epsilon_a}-\frac{1}{\epsilon_b}\right]\frac{1}{a_c}\int_R d^2x_\parallel e^{-i\mathbf{G}_\parallel\cdot\mathbf{x}_\parallel}, & \mathbf{G}_\parallel\neq\mathbf{0} \;, \quad (20b)\end{cases}$$

where f is the filling fraction, i.e., the fraction of the total volume occupied by the rods. It is given by $f=a_R/a_c$, where a_R is the area of the domain R, i.e., the cross-sectional area of the rod.

We apply the preceding results to the case in which the intersections of the axes of the dielectric rods with the x_1x_2 plane form a triangular lattice, for which

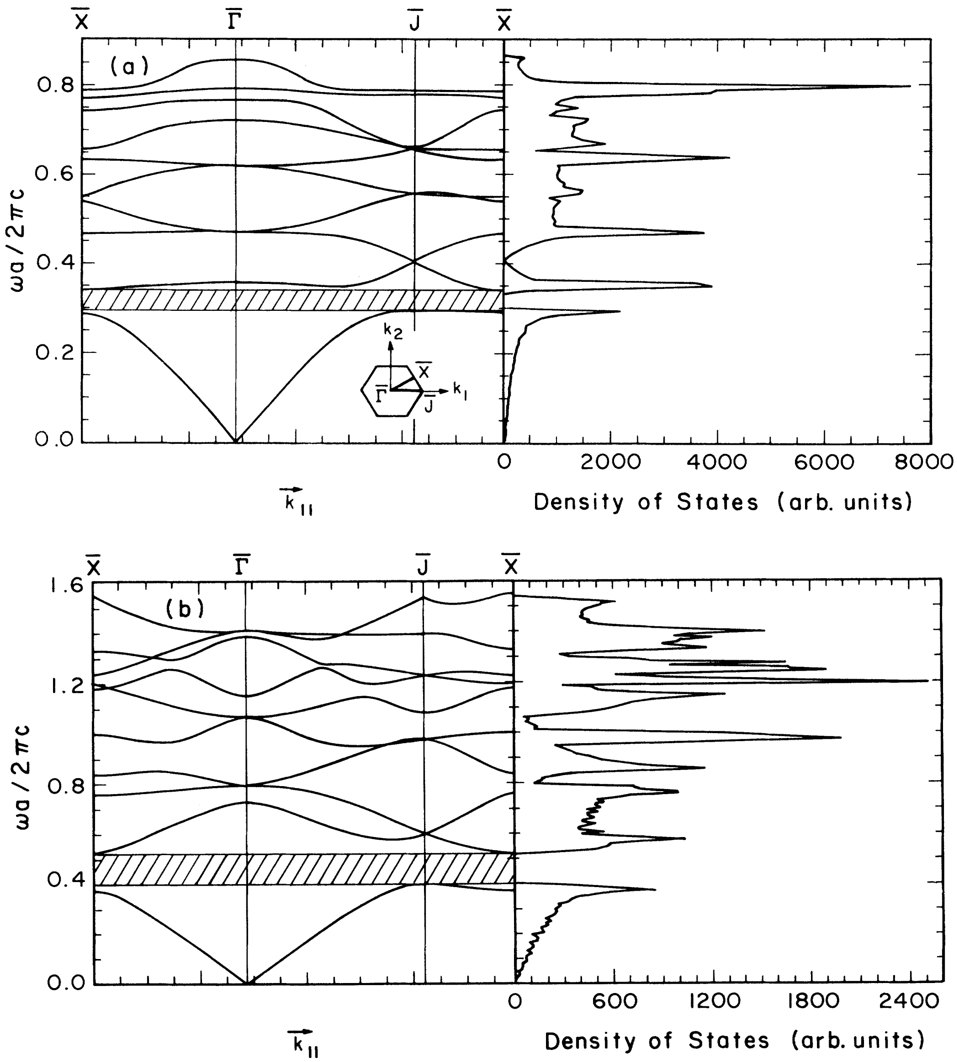

FIG. 1. The photonic band structure and density of states. (a) H polarization: $\epsilon_a=14$, $\epsilon_b=1$, $f=0.431$; (b) E polarization: $\epsilon_a=5$, $\epsilon_b=1$, $f=0.169$. The inset shows the first Brillouin zone for the periodic structure studied, with the symmetry points indicated.

$\mathbf{a}_1=a(1,0)$, $\mathbf{a}_2=a(\frac{1}{2},\frac{1}{2}\sqrt{3})$ and $\mathbf{b}_1=(2\pi/a)(1,-\frac{1}{3}\sqrt{3})$, $\mathbf{b}_2=(2\pi/a)(0,\frac{2}{3}\sqrt{3})$. The rods are assumed to have a circular cross section of radius R, and we find that for this case

$$\hat{\kappa}(\mathbf{G}_\parallel)=\begin{cases}\dfrac{1}{\epsilon_a}f+\dfrac{1}{\epsilon_b}(1-f), & \mathbf{G}_\parallel=0 \quad (21a)\\[2ex] \left[\dfrac{1}{\epsilon_a}-\dfrac{1}{\epsilon_b}\right]f\dfrac{2J_1(G_\parallel R)}{(G_\parallel R)}, & \mathbf{G}_\parallel\neq 0\ , \quad (21b)\end{cases}$$

where the filling fraction $f=(2\pi/\sqrt{3})R^2/a^2$, and $J_1(x)$ is a Bessel function.

In Fig. 1(a) we present the photonic band structure for the case of H polarization when $\epsilon_a=14$, $\epsilon_b=1$, and the filling fraction $f=0.431$. A total of 271 plane waves was used in obtaining this result. Along the right-hand margin of this figure we have plotted the density of photonic states in arbitrary units. This density of states was obtained by solving Eqs. (9) and (16) at each of 9600 uniformly spaced values of $\mathbf{k}_\parallel$ inside the first Brillouin zone for the triangular lattice studied here. In fact, the calculations were carried out for values of $\mathbf{k}_\parallel$ in the irreducible 1/12 of this Brillouin zone, outlined by the heavy lines in the inset to Fig. 1(a). This was possible because, due to the circular cross section of the dielectric cylinders, the frequency $\omega(\mathbf{k}_\parallel)$ in each band satisfies the relation $\omega(\underline{S}\mathbf{k}_\parallel)=\omega(\mathbf{k}_\parallel)$, where $\underline{S}$ is a 2×2 real, orthogonal matrix representative of any of the 12 operations of the point group C_{6v} of the triangular lattice. The plot of the density of states confirms what can be seen from the band structure itself, viz., that an absolute band gap exists in the band structure in the frequency range considered.

In Fig. 1(b) we present the photonic band structure and the corresponding photonic density of states for the case of E polarization when $\epsilon_a=5$, $\epsilon_b=1$, and $f=0.169$. A

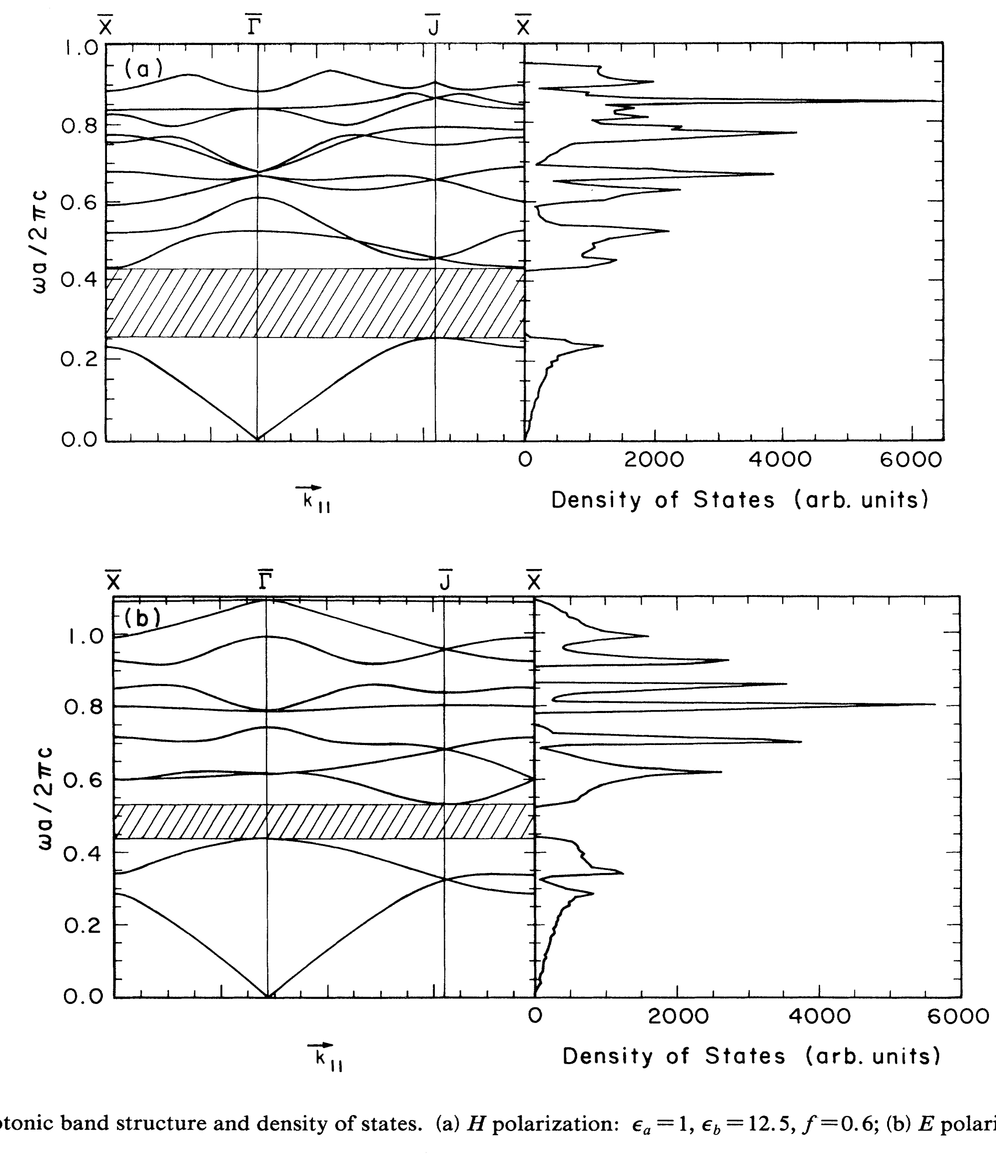

FIG. 2. The photonic band structure and density of states. (a) H polarization: $\epsilon_a=1$, $\epsilon_b=12.5$, $f=0.6$; (b) E polarization: $\epsilon_a=1$, $\epsilon_b=12.5$, $f=0.8$.

total of 271 plane waves was used in obtaining this result. An absolute band gap is also present in this band structure.

The results presented in Fig. 1 represent the photonic band structure for a periodic array of dielectric rods in vacuum. In Fig. 2 we present photonic band structures for a periodic array of cylindrical holes drilled in a dielectric matrix. In Fig. 2(a) we present the photonic band structure and the corresponding photonic density of states for the case of H polarization when $\epsilon_a = 1$, $\epsilon_b = 12.5$, and $f = 0.6$. A total of 271 plane waves was used in obtaining this result. Both the band structure and the density of states reveal the existence of an absolute band gap in the frequency range considered. In Fig. 2(b) the photonic band structure and density of states are presented for the case of E polarization when $\epsilon_a = 1$, $\epsilon_b = 12.5$, and $f = 0.8$. The number of plane waves used in obtaining this result was 469. Three absolute band gaps are present in this band structure in the frequency range considered, of which the lowest-frequency one is the broadest and the one explicitly indicated.

The filling fraction f employed in calculating the results presented in Figs. 1 and 2 was the optimal filling fraction for the contrast $\epsilon_> / \epsilon_<$ assumed. The optimal filling fraction is defined as the value of f that gives the largest width of the lowest-frequency band gap for a given value of $\epsilon_> / \epsilon_<$. In Fig. 3(a) we plot the optimal filling fraction as a function of ϵ_a when $\epsilon_b = 1$, for the case of H polarization. The optimal filling fraction was calculated on the basis of the variation with f of the width of the band gap in the photonic density of states for each value of $\epsilon_> / \epsilon_<$. The nonmonotonic dependence of the optimal filling fraction on the contrast in this case should be noted. In Fig. 3(b) we plot the optimal filling fraction as a function of ϵ_a for $\epsilon_b = 1$, for the case of E polarization.

In Fig. 4(a) the optimal filling fraction is plotted as a function of ϵ_b when $\epsilon_a = 1$, for the case of H polarization. In Fig. 4(b) it is plotted as a function of ϵ_b when $\epsilon_a = 1$, for the case of E polarization.

Finally, in Figs. 5 and 6 we present the dependence of the width of the absolute band gap on the contrast $\epsilon_> / \epsilon_<$, when the filling fraction at each contrast has the optimal value. In Figs. 5(a) and 5(b) this dependence is plotted as a function of ϵ_a when $\epsilon_b = 1$, for the cases of H and E polarization, respectively. Similarly, in Figs. 6(a) and 6(b) this dependence is plotted as a function of ϵ_b when $\epsilon_a = 1$, for the cases of H and E polarization, respectively. In all four cases plotted in Figs. 5 and 6 the width of the absolute band gap increases with increasing contrast.

In this paper we have presented an approach to the calculation of the photonic band structures for electromagnetic waves of H and E polarization propagating in the plane perpendicular to a two-dimensional, periodic array of identical, nonoverlapping dielectric cylinders of arbi-

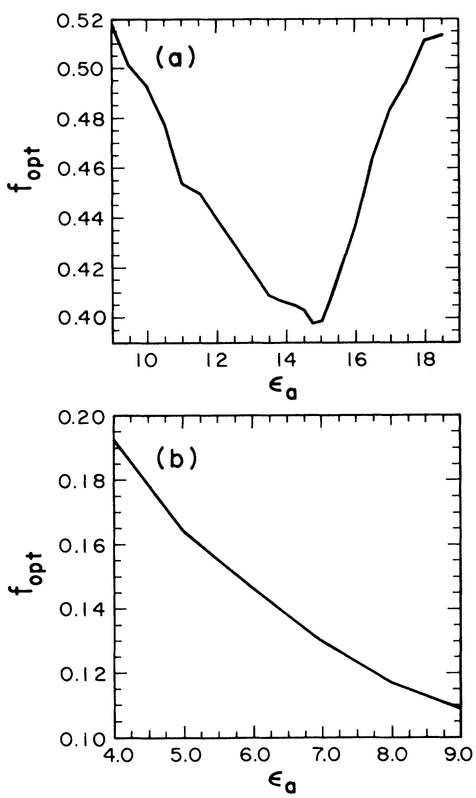

FIG. 3. The optimal filling fraction. (a) H polarization, $\epsilon_b = 1$; (b) E polarization, $\epsilon_b = 1$.

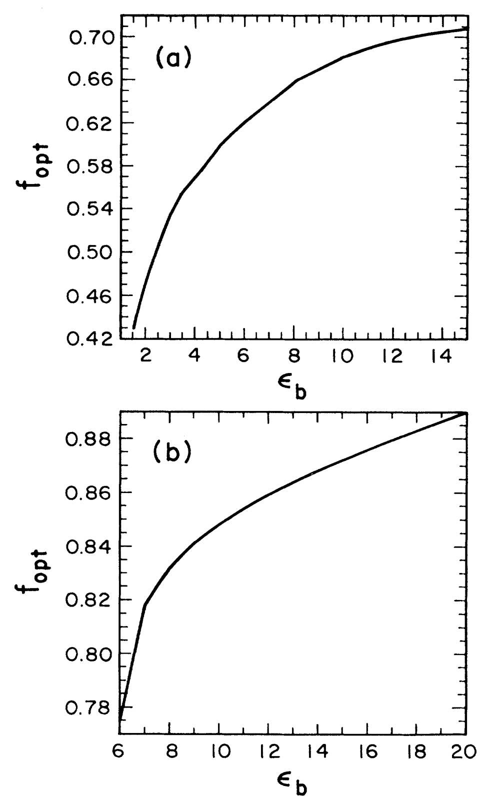

FIG. 4. The optimal filling fraction. (a) H polarization, $\epsilon_a = 1$; (b) E polarization, $\epsilon_a = 1$.

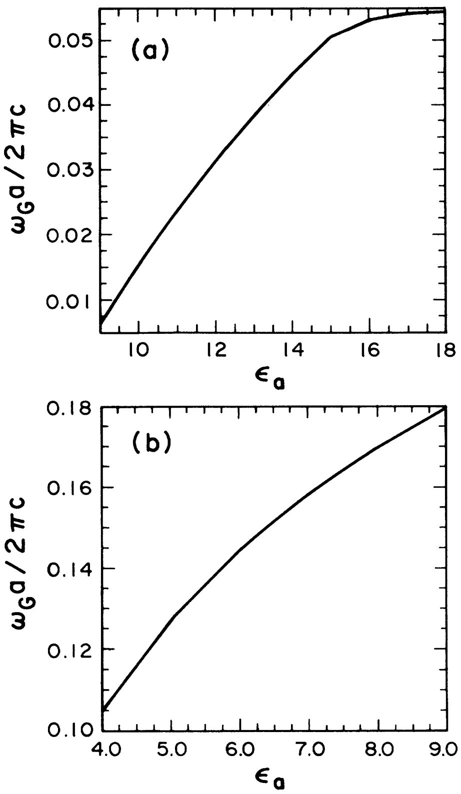

FIG. 5. The width of the absolute band gap as a function of contrast at the optimal filling fraction for that contrast. (a) H polarization, $\epsilon_b = 1$; E polarization, $\epsilon_b = 1$.

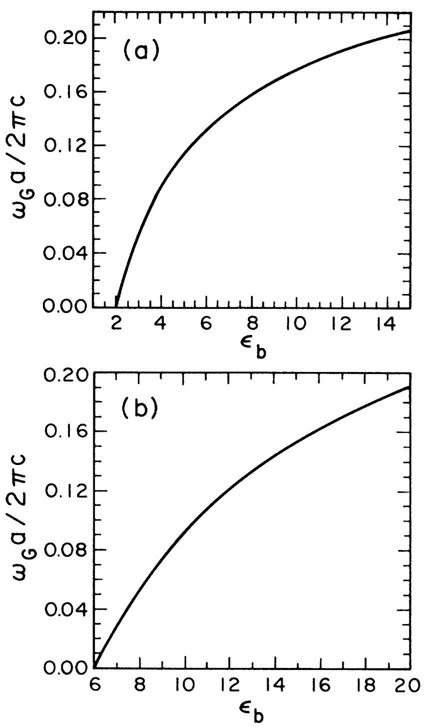

FIG. 6. The width of the absolute band gap as a function of contrast at the optimal filling fraction for that contrast. (a) H polarization, $\epsilon_a = 1$; (b) E polarization, $\epsilon_a = 1$.

trary cross section embedded in a dielectric matrix whose dielectric constant differs from that of the cylinders. This approach, which is based on the use of a position-dependent dielectric constant and an expansion of the electromagnetic field components in plane waves, results in a standard eigenvalue problem for a symmetric matrix for determining the dispersion curves (band structure) of the electromagnetic waves propagating in the system being studied. We have applied it here to obtain the photonic band structures of an infinite array of dielectric cylinders of circular cross section, whose intersections with a perpendicular plane form a triangular lattice. In this case the matrices to be diagonalized become real symmetric matrices.

In all four cases considered, viz., waves of H and E polarization in structures of dielectric cylinders in vacuum and of cylindrical holes in a dielectric matrix, an absolute band gap has been found, i.e., a frequency range in which no electromagnetic waves of either polarization can propagate in a plane perpendicular to the cylinders. The dependence of the optimal filling fraction on the contrast in these systems has been studied together with the dependence of the width of the absolute band gap on the contrast at the optimal filling fraction.

The frequencies of these absolute band gaps fall into an experimentally accessible range for reasonable values of the cylinder radius R and lattice constant a. Thus, for example, the width of the absolute band gap depicted in Fig. 1(b) is 1.62 GHz, and is centered at a frequency of 5.99 GHz, when $R = 5$ mm and $a = 2.32$ cm. It is hoped that experimental determinations of the photonic band structures for the systems investigated in this paper will be available in the near future for comparison with the theoretical results presented here.

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