Photonic band structures of two-dimensional systems containing metallic components

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By use of the plane-wave method, we calculate the photonic band structure for electromagnetic waves of E and H polarization propagating in a system consisting of an infinite array of identical, infinitely long, parallel, metal cylinders of circular cross section, embedded in vacuum, whose intersection with a perpendicular plane forms a simple square or triangular lattice. The dielectric function of the metal from which the cylinders are formed has the simple, free-electron form $\epsilon(\omega)=1-(\omega_p^2/\omega^2)$, where ω_p is the plasma frequency of the conduction electrons. For electromagnetic waves of both polarizations, the problem of obtaining the photonic band structure is reduced to the solution of a standard eigenvalue problem despite the frequency dependence of the dielectric constant of the two-dimensional, periodic system. For electromagnetic waves of E polarization the photonic band structure at low filling fractions of the metallic cylinders is a slightly perturbed version of the dispersion curves of electromagnetic waves in vacuum, except for the appearance of a band gap below the lowest frequency band, whose width increases with increasing filling fraction. A band gap between the first and second bands is present in the photonic band structure of the square lattice, but no band gap is found in the band structure of the triangular lattice. In the case of electromagnetic waves of H polarization the photonic band structure at low filling fractions of the metallic cylinders is also, for the most part, a slightly perturbed version of the dispersion curves of electromagnetic waves in vacuum, but possesses additional, nearly dispersionless, bands in the frequency range $\omega<\omega_p$. A possible origin of these flat bands is described.

I. INTRODUCTION

There has been a growing interest in recent years in the calculation of dispersion curves of electromagnetic waves propagating in two-dimensional, periodic, dielectric structures—the so-called photonic band structures of these systems.[1–22] They have also been the objects of experimental study.[4,10,23–29] A major reason for performing such calculations is the fact that periodic dielectric structures offer the possibility of eliminating propagating electromagnetic waves throughout a band of frequencies—the photonic band gap. The absence of electromagnetic modes in a certain frequency range can modify the basic properties of many atomic, molecular, and excitonic systems.[30]

As we have noted, all of the theoretical and experimental studies of the photonic band structures of two-dimensional, periodic structures cited above have been carried out for dielectric systems whose components are characterized by dielectric constants that are real, positive, and frequency independent. It is, therefore, of interest to explore the consequences for photonic band structures of including in the systems for which they are being calculated components that are not purely dielectric media, but instead are metallic, and are characterized by dielectric functions that are frequency dependent and can be negative in some frequency range. In a recent article by McGurn and one of the present authors,[31] we calculated the photonic band structure of a system consisting of an infinite array of identical, infinitely long, parallel, metal cylinders of circular cross section, embedded in vacuum, whose intersections with a perpendicular plane formed a simple square lattice. The dielectric function of the metal from which the cylinders were formed was assumed to have the simple, free-electron form

$$\epsilon(\omega)=1-(\omega_p^2/\omega^2)\ , \tag{1.1}$$

where ω_p is the plasma frequency of the conduction electrons. The electromagnetic field in this system was assumed to propagate in the plane perpendicular to the rods, and only the case (H polarization) in which the magnetic vector of the field was parallel to the rods was investigated. The single, nonzero component of this field was expanded in plane waves, and a homogeneous matrix equation for the coefficients in the expansion was obtained. Because the dielectric function of the metallic rods was frequency dependent, the matrix elements in the equation for the expansion coefficients were also frequency dependent. Consequently, the dispersion curves of the H-polarized electromagnetic waves propagating in this system—the photonic band structure—were obtained not by diagonalizing a matrix, but by finding the frequencies at which the determinant of the matrix in the equation for the expansion coefficients vanished for each value of the two-dimensional wave vector $\mathbf{k}_\parallel$ of the electromagnetic waves. This is a laborious computational procedure. In addition, there is always the concern that some zeros may be missed if the increment in frequency is insufficiently small. Finally, the band structure obtained was found to converge slowly as the number of plane waves retained in the expansion of the component of the magnetic field parallel to the cylinders was increased. This had the consequence that useful results could be obtained only for very small values of the filling fraction, i.e., the fraction of the total volume of the system occupied by the metal cylinders.

A striking feature of the photonic band structure obtained in this way was the presence, in the frequency range $0<\omega<\omega_p$ in which $\epsilon(\omega)$ is negative, of several very flat, nearly dispersionless, bands that are superimposed on dispersion curves, which otherwise are slightly perturbed versions of the dispersion curves for electromagnetic waves in vacuum. The number of these flat bands increased with increasing filling fraction. (Similar flat bands were also found in this frequency range in the photonic band structure of metal spheres arrayed in an fcc lattice[31] and in a simple cubic lattice.[32])

In this paper we exploit the special form of the dielectric function (1.1) to obtain a standard eigenvalue problem for determining the photonic band structure of electromagnetic waves of both E and H polarization for an arbitrary, periodic, two-dimensional system. The computational problem of obtaining the photonic band structure is greatly simplified thereby, and band structures for larger filling fractions can be calculated accurately.

We begin by formulating the problem of obtaining the photonic band structure of a periodic, two-dimensional system of parallel metal cylinders for the case in which the intersections of their axes with a perpendicular plane form an arbitrary two-dimensional Bravais lattice. The extension to more general two-dimensional structures is straightforward.

Thus, we assume that the axes of the cylinders are parallel to the x_3 axis, and that their intersections with the $x_1 x_2$ plane form one of the five two-dimensional Bravais lattices. The translation vectors of this Bravais lattice are

$$\mathbf{x}_\parallel(l)=l_1\mathbf{a}_1+l_2\mathbf{a}_2 , \tag{1.2}$$

where $\mathbf{a}_1$ and $\mathbf{a}_2$ are the two, noncollinear, primitive translation vectors of the lattice, while l_1 and l_2 are arbitrary integers that we denote collectively by l. The area a_c of a primitive unit cell of this lattice is given by

$$a_c=|\mathbf{a}_1\times\mathbf{a}_2| . \tag{1.3}$$

The lattice reciprocal to the direct lattice whose points are defined by Eq. (1.2) is defined by the translation vectors

$$\mathbf{G}_\parallel(h)=h_1\mathbf{b}_1+h_2\mathbf{b}_2 . \tag{1.4}$$

The primitive translation vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ of the reciprocal lattice are the solutions of the equations

$$\mathbf{a}_1\cdot\mathbf{b}_j=2\pi\delta_{ij} , \quad i,j=1,2 , \tag{1.5}$$

and h_1 and h_2 are arbitrary integers that we denote collectively by h.

The dielectric constant of this system is now position dependent, $\epsilon(\mathbf{x}_\parallel)$, where $\mathbf{x}_\parallel=(x_1,x_2)$ is a position vector in the x_1x_2 plane. It is in fact a periodic function of $\mathbf{x}_\parallel$ with the periodicity of the Bravais lattice defined by Eq. (1.2),

$$\epsilon[\mathbf{x}_\parallel+\mathbf{x}_\parallel(l)]=\epsilon(\mathbf{x}_\parallel) . \tag{1.6}$$

It can, therefore, be expanded in a two-dimensional Fourier series according to

$$\epsilon(\mathbf{x}_\parallel)=\sum_{\mathbf{G}_\parallel}\hat{\epsilon}(\mathbf{G}_\parallel)e^{i\mathbf{G}_\parallel\cdot\mathbf{x}_\parallel} , \tag{1.7}$$

where the Fourier coefficient $\hat{\epsilon}(\mathbf{G}_\parallel)$ is given by

$$\hat{\epsilon}(\mathbf{G}_\parallel)=\frac{1}{a_c}\int_{a_c}d^2x_\parallel\epsilon(\mathbf{x}_\parallel)e^{-i\mathbf{G}_\parallel\cdot\mathbf{x}_\parallel} . \tag{1.8}$$

The dielectric constant of the system being studied can be written explicitly in the form

$$\epsilon(\mathbf{x}_\parallel)=1+[\epsilon(\omega)-1]\sum_l S[\mathbf{x}_\parallel-\mathbf{x}_\parallel(l)] , \tag{1.9}$$

where the function $S(\mathbf{x}_\parallel)=1$ if $\mathbf{x}_\parallel$ is inside the cross section of the cylinder centered at the origin of coordinates and $S(\mathbf{x}_\parallel)=0$ if $\mathbf{x}_\parallel$ is outside this cross section. Thus, on substituting Eq. (1.9) into Eq. (1.8), we obtain for $\hat{\epsilon}(\mathbf{G}_\parallel)$

$$\hat{\epsilon}(\mathbf{G}_\parallel)=\delta_{\mathbf{G}_\parallel 0}+[\epsilon(\omega)-1]\frac{1}{a_c}\int d^2x_\parallel S(\mathbf{x}_\parallel)e^{-i\mathbf{G}_\parallel\cdot\mathbf{x}_\parallel} , \tag{1.10}$$

where the integral is now over the entire x_1x_2 plane. If we recall the definitions of $\epsilon(\omega)$ and $S(\mathbf{x}_\parallel)$, Eq. (1.10) can be rewritten in the form

$$\hat{\epsilon}(\mathbf{G}_\parallel)=1-f\frac{\omega_p^2}{\omega^2} , \quad \mathbf{G}_\parallel=\mathbf{0} , \tag{1.11a}$$

$$\hat{\epsilon}(\mathbf{G}_\parallel)=-\frac{\omega_p^2}{\omega^2}\frac{1}{a_c}\int d^2x_\parallel S(\mathbf{x}_\parallel)e^{-i\mathbf{G}_\parallel\cdot\mathbf{x}_\parallel} , \quad \mathbf{G}_\parallel\neq\mathbf{0} , \tag{1.11b}$$

where

$$f=\frac{1}{a_c}\int d^2x_\parallel S(\mathbf{x}_\parallel) \tag{1.12}$$

is the filling fraction. In the particular case of metallic cylinders whose cross section is a circle of radius R, $S(\mathbf{x}_\parallel)=\theta(R-\mathbf{x}_\parallel|)$, where $\theta(x)$ is the Heaviside unit step function, and we obtain for $\hat{\epsilon}(\mathbf{G}_\parallel)$

$$\hat{\epsilon}(\mathbf{G}_\parallel)=1-f\frac{\omega_p^2}{\omega^2} , \quad \mathbf{G}_\parallel=\mathbf{0} , \tag{1.13a}$$

$$\hat{\epsilon}(\mathbf{G}_\parallel)=-f\frac{\omega_p^2}{\omega^2}\frac{2J_1(G_\parallel R)}{G_\parallel R} , \quad \mathbf{G}_\parallel\neq\mathbf{0} , \tag{1.13b}$$

where $J_1(x)$ is a Bessel function.

We now apply these results to the determination of the photonic band structures of E- and H-polarized electromagnetic waves in the system described by this dielectric constant.

II. E POLARIZATION

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

$$\mathbf{E}(\mathbf{x};t)=[0,0,E_3(\mathbf{x}_\parallel|\omega)]\exp(-i\omega t) , \tag{2.1a}$$

$$\mathbf{H}(\mathbf{x};t)=[H_1(\mathbf{x}_\parallel|\omega),H_2(\mathbf{x}_\parallel|\omega),0]\exp(-i\omega t) . \tag{2.1b}$$

The Maxwell curl equations for the three nonzero field components are

$$\frac{\partial H_2}{\partial x_1}-\frac{\partial H_1}{\partial x_2}=-i\frac{\omega}{c}D_3=-i\frac{\omega}{c}\epsilon(\mathbf{x}_\parallel)E_3 , \tag{2.2a}$$

$$\frac{\partial E_3}{\partial x_1}=-i\frac{\omega}{c}H_2 , \tag{2.2b}$$

$$\frac{\partial E_3}{\partial x_2}=i\frac{\omega}{c}H_1 . \tag{2.2c}$$

When we eliminate H_1 and H_2 from these equations, we obtain as the equation satisfied by E_3

$$\left[\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}+\epsilon(\mathbf{x}_\parallel)\frac{\omega^2}{c^2}\right]E_3=0 . \tag{2.3}$$

To solve Eq. (2.3) we use the expansion (1.7) and write $E_3(\mathbf{x}_\parallel|\omega)$in the form

$$E_3(\mathbf{x}_\parallel|\omega)=\sum_{\mathbf{G}_\parallel}B(\mathbf{k}_\parallel|\mathbf{G}_\parallel)e^{i(\mathbf{k}_\parallel+\mathbf{G}_\parallel)\cdot\mathbf{x}_\parallel} , \tag{2.4}$$

where $\mathbf{k}_\parallel=(k_1k_2,0)$ is the two-dimensional wave vector of the wave. When these expansions are substituted in Eq. (2.3), we obtain as the equation satisfied by the coefficients $\{B(\mathbf{k}_\parallel|\mathbf{G}_\parallel)\}$

$$\begin{aligned}(\mathbf{k}_\parallel+\mathbf{G}_\parallel)^2B(\mathbf{k}_\parallel|\mathbf{G}_\parallel)&=\frac{\omega^2}{c^2}\sum_{G'_\parallel}\hat{\epsilon}(\mathbf{G}_\parallel-\mathbf{G}'_\parallel)B(\mathbf{k}_\parallel|\mathbf{G}'_\parallel)\\&=\frac{\omega^2}{c^2}\hat{\epsilon}(\mathbf{0})B(\mathbf{k}_\parallel|\mathbf{G}_\parallel)\\&\quad+\frac{\omega^2}{c^2}\sum_{\mathbf{G}'_\parallel}{}'\hat{\epsilon}(\mathbf{G}_\parallel-\mathbf{G}'_\parallel)B(\mathbf{k}_\parallel|\mathbf{G}'_\parallel) ,\end{aligned} \tag{2.5}$$

where the prime on the sum over $\mathbf{G}'_\parallel$ indicates that the term with $\mathbf{G}'_\parallel=\mathbf{G}_\parallel$ is omitted. The use of the result for $\hat{\epsilon}(\mathbf{G}_\parallel)$ given by Eq. (1.13) in Eq. (2.5) transforms the latter into

$$\sum_{\mathbf{G}'_\parallel}\left\{(\mathbf{k}_\parallel+\mathbf{G}_\parallel)^2\delta_{\mathbf{G}_\parallel,\mathbf{G}'_\parallel}+f\frac{\omega_p^2}{c^2}\frac{2J_1(|\mathbf{G}_\parallel-\mathbf{G}'_\parallel|R)}{(|\mathbf{G}_\parallel-\mathbf{G}'_\parallel|R)}\right\}\times B(\mathbf{k}_\parallel|\mathbf{G}'_\parallel)=\frac{\omega^2}{c^2}B(\mathbf{k}_\parallel|\mathbf{G}_\parallel) , \tag{2.6}$$

which has the form of a standard eigenvalue problem for a real, symmetric matrix. In solving Eq. (2.6), it should be kept in mind that $2J_1(x)/x$ equals unity at $x=0$.

III. *H* POLARIZATION

In our first approach to the case of H polarization, we seek solutions of Maxwell's equations that have the forms

$$\mathbf{H}(\mathbf{x};t)=[0,0,H_3(\mathbf{x}_\parallel|\omega)]\exp(-i\omega t) , \tag{3.1a}$$

$$\mathbf{E}(\mathbf{x};t)=[E_1(\mathbf{x}_\parallel|\omega),E_2(\mathbf{x}_\parallel|\omega),0]\exp(-i\omega t) . \tag{3.1b}$$

The Maxwell curl equations in this case are

$$\frac{\partial E_2}{\partial x_1}-\frac{\partial E_1}{\partial x_2}=i\frac{\omega}{c}H_3 , \tag{3.2a}$$

$$\frac{\partial H_3}{\partial x_1}=i\frac{\omega}{c}D_2=i\frac{\omega}{c}\epsilon(\mathbf{x}_\parallel)E_2 , \tag{3.2b}$$

$$\frac{\partial H_3}{\partial x_2}=-i\frac{\omega}{c}D_1=-i\frac{\omega}{c}\epsilon(\mathbf{x}_\parallel)E_1 . \tag{3.2c}$$

In this case it is convenient to eliminate H_3 from Eqs. (3.2) to obtain a pair of coupled equations for E_1 and E_2;

$$-\frac{\partial^2E_1}{\partial x_2^2}+\frac{\partial^2E_2}{\partial x_1\partial x_2}=\epsilon(\mathbf{x}_\parallel)\frac{\omega^2}{c^2}E_1 , \tag{3.3a}$$

$$\frac{\partial^2E_1}{\partial x_1\partial x_2}-\frac{\partial^2E_2}{\partial x_1^2}=\epsilon(\mathbf{x}_\parallel)\frac{\omega^2}{c^2}E_2 . \tag{3.3b}$$

We expand $E_1(\mathbf{x}_\parallel|\omega)$ and $E_2(\mathbf{x}_\parallel|\omega)$ according to

$$E_\alpha(\mathbf{x}_\parallel|\omega)=\sum_{\mathbf{G}_\parallel}A_\alpha(\mathbf{k}_\parallel|\mathbf{G}_\parallel)e^{i(\mathbf{k}_\parallel+\mathbf{G}_\parallel)\cdot\mathbf{x}_\parallel} , \quad \alpha=1,2 . \tag{3.4}$$

When we substitute Eq. (3.4) together with Eq. (1.7) into Eqs. (3.3), we obtain as the equations for the coefficients $\{A_{1,2}(\mathbf{k}_\parallel|\mathbf{G}_\parallel)\}$,

$$\begin{aligned}(k_2+G_2)^2A_1(\mathbf{k}_\parallel|\mathbf{G}_\parallel)-(k_1+G_1)(k_2+G_2)A_2(\mathbf{k}_\parallel|\mathbf{G}_\parallel)&=\frac{\omega^2}{c^2}\sum_{\mathbf{G}_\parallel}\hat{\epsilon}(\mathbf{G}_\parallel-\mathbf{G}'_\parallel)A_1(\mathbf{k}_\parallel|\mathbf{G}'_\parallel) ,\end{aligned} \tag{3.5a}$$

$$\begin{aligned}-(k_1+G_1)(k_2+G_2)A_1(\mathbf{k}_\parallel|\mathbf{G}_\parallel)+(k_1+G_1)^2A_2(\mathbf{k}_\parallel|\mathbf{G}_\parallel)&=\frac{\omega^2}{c^2}\sum_{\mathbf{G}'_\parallel}\hat{\epsilon}(\mathbf{G}_\parallel-\mathbf{G}'_\parallel)A_2(\mathbf{k}_\parallel|\mathbf{G}'_\parallel) .\end{aligned} \tag{3.5b}$$

The use of the result (1.13) for $\hat{\epsilon}(\mathbf{G}_\parallel)$ in Eqs. (3.5) yields the pair of equations

$$\sum_{\mathbf{G}'_\parallel}\left\{\left[(k_2+G_2)^2\delta_{\mathbf{G}_\parallel,\mathbf{G}'_\parallel}+f\frac{\omega_p^2}{c^2}\frac{2J_1(|\mathbf{G}_\parallel-\mathbf{G}'_\parallel|R)}{(|\mathbf{G}_\parallel-\mathbf{G}'_\parallel|R)}\right]A_1(\mathbf{k}_\parallel|\mathbf{G}'_\parallel)-(k_1+G_1)(k_2+G_2)\delta_{\mathbf{G}_\parallel,\mathbf{G}'_\parallel}A_2(\mathbf{k}_\parallel|\mathbf{G}'_\parallel)\right\}=\frac{\omega^2}{c^2}A_1(\mathbf{k}_\parallel|\mathbf{G}_\parallel) , \tag{3.6a}$$

$$\sum_{\mathbf{G}'_\parallel}\left\{-(k_1+G_1)(k_2+G_2)\delta_{\mathbf{G}_\parallel,\mathbf{G}'_\parallel}A_1(\mathbf{k}_\parallel|\mathbf{G}'_\parallel)+\left[(k_1+G_1)^2\delta_{\mathbf{G}_\parallel,\mathbf{G}'_\parallel}+f\frac{\omega_p^2}{c^2}\frac{2J_1(|\mathbf{G}_\parallel-\mathbf{G}'_\parallel|R)}{(|\mathbf{G}_\parallel-\mathbf{G}'_\parallel|R)}\right]A_2(\mathbf{k}_\parallel|\mathbf{G}'_\parallel)\right\}=\frac{\omega^2}{c^2}A_2(\mathbf{k}_\parallel|\mathbf{G}_\parallel) . \tag{3.6b}$$

Equations (3.6) constitute a standard eigenvalue problem for a real symmetric matrix. However, the size of the matrix to be diagonalized in the case of H polarization, is twice that of the matrix to be diagonalized in the case of E polarization, when the same number of plane waves is used in the expansions (2.4) and (3.4).

IV. RESULTS

A. E Polarization

We first consider the case of E polarization for both a simple square lattice of lattice parameter a for which the primitive translation vectors are

$$\mathbf{a}_1=a(1,0), \quad \mathbf{a}_2=a(0,1) , \tag{4.1a}$$

while the primitive translation vectors of the reciprocal lattice are

$$\mathbf{b}_1=\frac{2\pi}{a}(1,0) , \quad \mathbf{b}_2=\frac{2\pi}{a}(0,1) , \tag{4.1b}$$

and for a triangular lattice for which the primitive translation vectors are

$$\mathbf{a}_1=a(1,0), \quad \mathbf{a}_2=a(\tfrac{1}{2},\tfrac{1}{2}\sqrt{3}) , \tag{4.2a}$$

and the corresponding primitive translation vectors of the reciprocal lattice are

$$\mathbf{b}_1=\frac{2\pi}{a}(1,-\tfrac{1}{3}\sqrt{3}) , \quad \mathbf{b}_2=\frac{2\pi}{a}(0,\tfrac{2}{3}\sqrt{3}) . \tag{4.2b}$$

The filling fractions of the metallic rods are $f=\pi R^2/a^2$ and $f=(2\pi/\sqrt{3})R^2/a^2$ for these two lattices, respectively.

In Fig. 1(a) we present the photonic band structure of a square lattice when the filling fraction of the rods is $f=0.001$. A total of 197 plane waves was used in obtaining this result. We have taken $\omega_p a/2\pi c=1$, which is the value of $\omega a/2\pi c$ at which the change in sign of $\epsilon(\omega)$ occurs. For small filling fractions, namely up to $f=0.1$, we have obtained a band structure that is not significantly different from the dispersion curves for electromagnetic waves in vacuum. However, for higher values of the filling fraction, the band structure differs substantially from the dispersion relation for electromagnetic waves in vacuum and reveals the existence of an absolute band gap between the first and second bands, which appears for values of the filling fraction $f \gtrsim 0.25$. The presence of the band gap is illustrated in Fig. 1(b), where the photonic band structure for E polarization when $f=0.7$ is shown. The variation of the width of the band gap with the filling fraction is nonmonotonic. We have found that the optimal filling fraction, which is defined as the value of f that gives the largest width of the band gap, is $f=0.7$. In Fig. 2(a) we plot the width of the band gap as a function of the filling fraction. In Fig. 2(b) we plot the ratio of the width of the band gap to the frequency at the center of the band gap as a function of the filling fraction. From the latter figure, we see that this ratio can be as large as 17% for a filling fraction $f \cong 0.65$. A total of 197 plane waves was used in obtaining the results for all values of the filling fraction.

In Fig. 3(a) we present the photonic band structure of a triangular lattice when the filling fraction of the rods is $f=0.001$. A total of 271 plane waves was used in obtaining this result. The band structure for small values of the filling fraction resembles the dispersion curves for electromagnetic waves in vacuum. It changes as the filling

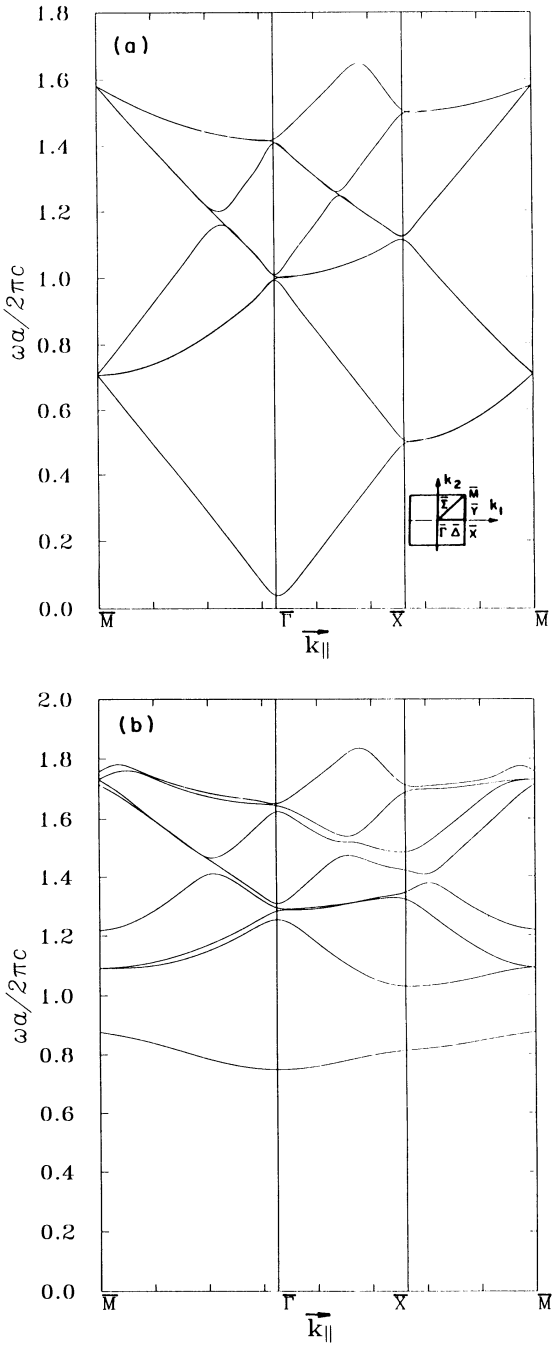

FIG. 1. The photonic band structure of a square lattice of metal cylinders in vacuum. E polarization: (a) $f=0.001$. (b) $f=0.7$. A band gap is present in the latter structure. The number of plane waves used in these calculations is (NG) = 197.

fraction increases. However, in contrast to the band structure for the square lattice, we have not found an absolute band gap in the frequency range studied, as is seen from Fig. 3(b), where we present the photonic band structure for a filling fraction of $f=0.5$. A total of 271 plane waves was used to obtain this result.

It should be noted that the convergence of these calculations is rapid, and relatively small matrices are required for an accurate determination of the photonic band structure for the case of E polarization.

A notable feature of the results for the photonic band structures for electromagnetic waves of E polarization in square and triangular lattices of metallic cylinders in vacuum presented in Figs. 1 and 3, respectively, is the presence of a band gap below the lowest frequency band. The existence of this gap is a consequence of the metallic nature of the cylinders, and has its origin in the second term inside the braces on the left-hand side of Eq. (2.6). Its width is seen to increase with increasing filling fraction f.

B. H Polarization

In Figs. 4 and 5 we present the photonic band structure for the case of H polarization for the square and triangular lattices, respectively, when the filling fraction of the rods is $f=0.001$. A total of 197 plane waves for the square lattice and a total of 271 plane waves for the triangular lattice was used to obtain these results.

In contrast to the case of E polarization, we have also found flats bands in the region $0<\omega<\omega_p$, which are superimposed on a band structure that resembles the

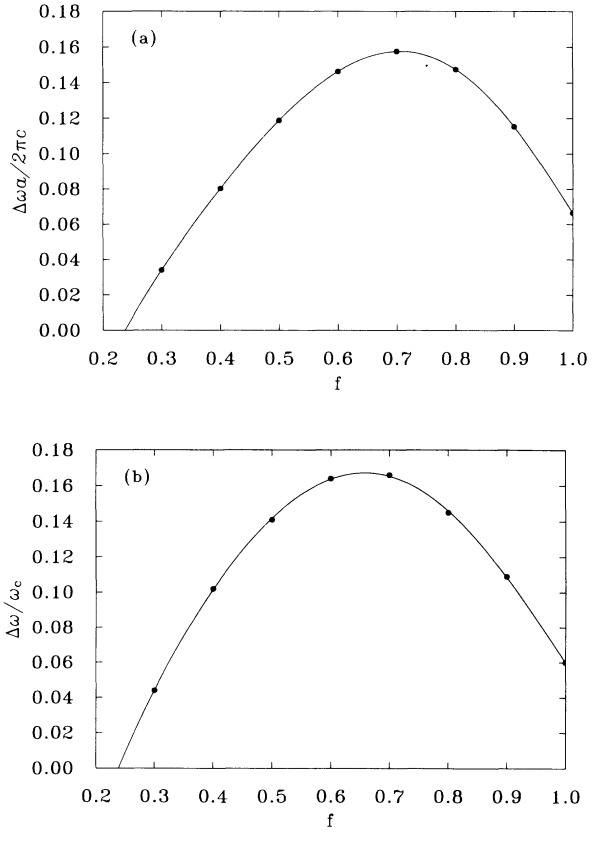

FIG. 2. (a) The width of the band gap present in the results displayed in Fig. 1(b) is plotted as a function of the filling fraction f. (b) The ratio of the width of this band gap ($\Delta\omega$) to the frequency at the center of the gap ω_c is plotted as a function of the filling fraction f.

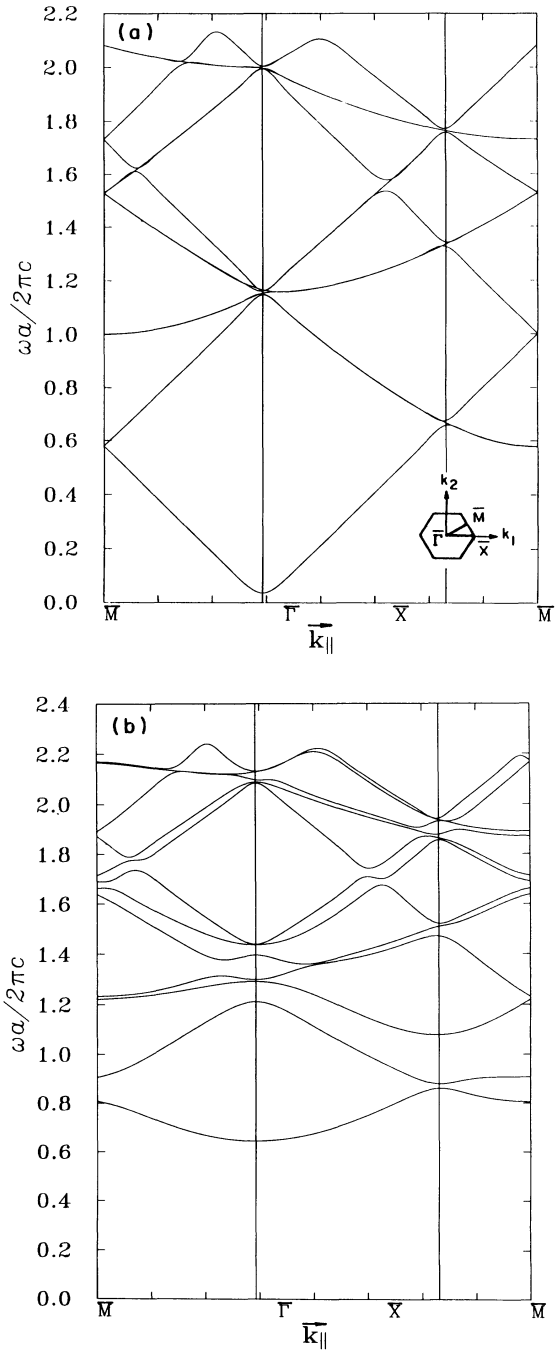

FIG. 3. The photonic band structure of a triangular lattice of metal cylinders in vacuum. E polarization (a) $f=0.001$. (b) $f=0.5$. NG = 271.

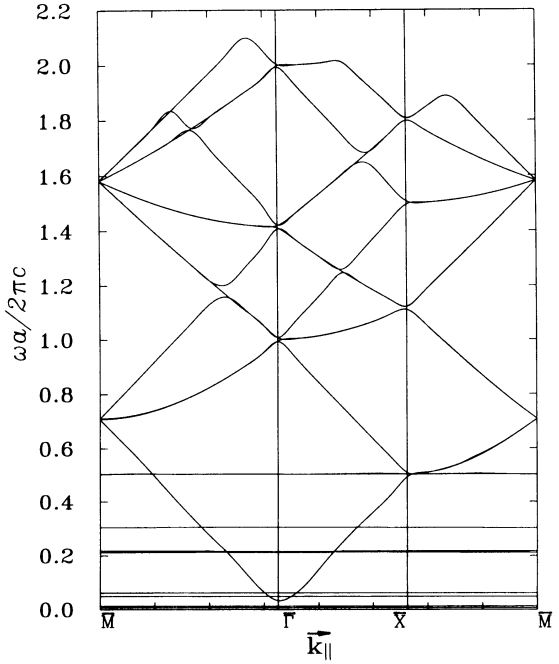

FIG. 4. The photonic band structure of a square lattice of metal cylinders in vacuum. H polarization: $f=0.001$. NG = 697.

dispersion curves for electromagnetic waves in vacuum. The existence of the flat bands confirms the results of the calculation of the photonic band structure for the case of H polarization for the identical system reported recently,[31] although a different method was used to obtain those results. We have found that the vacuumlike part of the band structure converges rapidly, but that the flat bands, in contrast, converge very slowly with an increasing number of plane waves. In fact, even the use of up to $\simeq 4500$ plane waves, together with a extrapolation procedure, failed to yield results for flat bands that we felt had converged. Thus, the flat bands depicted in Figs. 4 and 5 are not reliably calculated, and should be regarded only as indicative of the true flat-band structure that exists in the frequency range $0<\omega<\omega_p$.

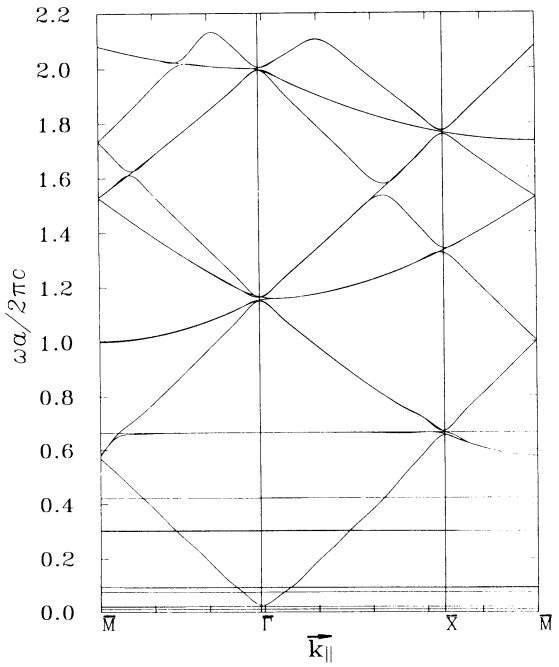

FIG. 5. The photonic band structure of a triangular lattice of metal cylinders in vacuum. H polarization: $f=0.001$. NG = 709.

This disappointing result for the flat-band portion of the photonic band structure in H polarization obtained by the use of Eqs. (3.6) prompted us to seek another approach for the determination of the band structure in this case. The method that was eventually used is based on eliminating E_1 and E_2 from Eqs. (3.2) to obtain the equation satisfied by H_3, which we write in the form

$$\frac{\partial}{\partial x_1}\left[\frac{1}{\epsilon(\mathbf{x}_\parallel)}\frac{\partial H_3}{\partial x_1}\right]+\frac{\partial}{\partial x_2}\left[\frac{1}{\epsilon(\mathbf{x}_\parallel)}\frac{\partial H_3}{\partial x_2}\right]+\frac{\omega^2}{c^2}H_3=0\ . \tag{4.3}$$

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

$$\frac{1}{\epsilon(\mathbf{x}_\parallel)}=\sum_{\mathbf{G}_\parallel}\hat{\kappa}(\mathbf{G}_\parallel)e^{i\mathbf{G}_\parallel\cdot\mathbf{x}_\parallel}\ , \tag{4.4}$$

$$H_3(\mathbf{x}_\parallel|\omega)=\sum_{\mathbf{G}_\parallel}A(\mathbf{k}_\parallel|\mathbf{G}_\parallel)e^{i(\mathbf{k}_\parallel+\mathbf{G}_\parallel)\cdot\mathbf{x}_\parallel}\ . \tag{4.5}$$

In the general case of metal cylinders of arbitrary cross section, the Fourier coefficients $\{\hat{\kappa}(\mathbf{G}_\parallel)\}$ are given by

$$\hat{\kappa}(\mathbf{G}_\parallel)=1+f\frac{\omega_p^2}{\omega^2-\omega_p^2}\ ,\quad \mathbf{G}_\parallel=0\ , \tag{4.6a}$$

$$\hat{\kappa}(\mathbf{G}_\parallel)=\frac{\omega_p^2}{\omega^2-\omega_p^2}\frac{1}{a_c}\int d^2x_\parallel S(\mathbf{x}_\parallel)e^{-i\mathbf{G}_\parallel\cdot\mathbf{x}_\parallel}\ ,\quad \mathbf{G}_\parallel\neq 0\ . \tag{4.6b}$$

In the case of metallic cylinders whose cross section is a circle of radius R, we obtain for $\hat{\kappa}(\mathbf{G}_\parallel)$

$$\hat{\kappa}(\mathbf{G}_\parallel)=1+f\frac{\omega_p^2}{\omega^2-\omega_p^2}\ ,\quad \mathbf{G}_\parallel=0\ , \tag{4.7a}$$

$$\hat{\kappa}(\mathbf{G}_\parallel)=\frac{\omega_p^2}{\omega^2-\omega_p^2}f\frac{2J_1(G_\parallel R)}{G_\parallel R}\ ,\quad \mathbf{G}_\parallel\neq 0\ . \tag{4.7b}$$

When we substitute the expansions (4.4) and (4.5) into Eq. (4.3), we obtain as the equation satisfied by the coefficients $\{A(\mathbf{k}_\parallel|\mathbf{G}_\parallel)\}$

$$\sum_{\mathbf{G}'_\parallel}(\mathbf{k}_\parallel+\mathbf{G}_\parallel)\cdot(\mathbf{k}_\parallel+\mathbf{G}'_\parallel)\hat{\kappa}(\mathbf{G}_\parallel-\mathbf{G}'_\parallel)A(\mathbf{k}_\parallel|\mathbf{G}'_\parallel)=\frac{\omega^2}{c^2}A(\mathbf{k}_\parallel|\mathbf{G}_\parallel)\ . \tag{4.8}$$

The use of the results given by Eqs. (4.7) in Eq. (4.8) transforms the latter into

$$\frac{(\omega^2-\omega_p^2)}{\omega_p^2}\left[\frac{\omega^2}{c^2}-|\mathbf{k}_\parallel+\mathbf{G}_\parallel|^2\right]A(\mathbf{k}_\parallel|\mathbf{G}_\parallel)=f\sum_{\mathbf{G}'_\parallel}(\mathbf{k}_\parallel+\mathbf{G}_\parallel)\cdot(\mathbf{k}_\parallel+\mathbf{G}'_\parallel)\frac{2J_1(|\mathbf{G}_\parallel-\mathbf{G}'_\parallel|R)}{(|\mathbf{G}_\parallel-\mathbf{G}'_\parallel|R)}A(\mathbf{k}_\parallel|\mathbf{G}'_\parallel)\ . \tag{4.9}$$

At this point we define

$$\frac{\omega^2}{\omega_p^2}=\mu\ , \tag{4.10}$$

and rewrite Eq. (4.9) in the form

$$(\mu^2\vec{\vec{I}}-\mu\vec{\vec{M}}+\vec{\vec{N}})\,\mathbf{A}=0\ , \tag{4.11}$$

where the elements of the matrices $\vec{\vec{M}}$ and $\vec{\vec{N}}$ are given by

$$M(\mathbf{G}_\parallel|\mathbf{G}'_\parallel)=\delta_{\mathbf{G}_\parallel,\mathbf{G}'_\parallel}\left[1+\frac{c^2|\mathbf{k}_\parallel+\mathbf{G}_\parallel|^2}{\omega_p^2}\right]\ , \tag{4.12a}$$

$$N(\mathbf{G}_\parallel|\mathbf{G}'_\parallel)=\delta_{\mathbf{G}_\parallel,\mathbf{G}'_\parallel}\frac{c^2|k_\parallel+\mathbf{G}_\parallel|^2}{\omega_p^2}-f\frac{c^2}{\omega_p^2}(\mathbf{k}_\parallel+\mathbf{G}_\parallel)\cdot(\mathbf{k}_\parallel+\mathbf{G}'_\parallel)\frac{2J_1(|\mathbf{G}_\parallel-\mathbf{G}'_\parallel|R)}{(|\mathbf{G}_\parallel-\mathbf{G}'_\parallel|R)}\ . \tag{4.12b}$$

Equation (4.11) can be written in the factored form

$$(\mu\vec{\vec{I}}-\vec{\vec{B}})(\mu\vec{\vec{I}}-\vec{\vec{C}})=0\ , \tag{4.13}$$

where the matrices $\vec{\vec{B}}$ and $\vec{\vec{C}}$ satisfy the pair of equations

$$\vec{\vec{B}}+\vec{\vec{C}}=\vec{\vec{M}}\ ,\quad \vec{\vec{B}}\vec{\vec{C}}=\vec{\vec{N}}\ . \tag{4.14}$$

If we write

$$\vec{\vec{C}}=\vec{\vec{M}}-\vec{\vec{B}}\ , \tag{4.15}$$

the equation satisfied by $\vec{\vec{B}}$ becomes

$$\vec{\vec{B}}=\vec{\vec{N}}\vec{\vec{M}}^{-1}+\vec{\vec{B}}^2\vec{\vec{M}}^{-1}\ . \tag{4.16}$$

We solve Eq. (4.16) by iteration by writing it as

$$\vec{\vec{B}}=\epsilon\vec{\vec{N}}\vec{\vec{M}}^{-1}+\vec{\vec{B}}^2\vec{\vec{M}}^{-1}\ , \tag{4.17}$$

expressing $\vec{\vec{B}}$ as an expansion in powers of ϵ,

$$\vec{\vec{B}}=\sum_{r=1}^{\infty}\epsilon^r\vec{\vec{B}}_r\ , \tag{4.18}$$

and setting $\epsilon=1$ at the end of the calculation. The matrices $\{\vec{\vec{B}}_r\}$ can be calculated recursively;

$$\vec{\vec{B}}_1=\vec{\vec{N}}\vec{\vec{M}}^{-1} \tag{4.19a}$$

$$\vec{\vec{B}}_r=\sum_{s=1}^{r-1}\vec{\vec{B}}_{r-s}\vec{\vec{B}}_s\vec{\vec{M}}^{-1}\ ,\quad r\geq 2\ . \tag{4.19b}$$

Once $\vec{\vec{B}}$ has been calculated, $\vec{\vec{C}}$ is obtained from Eq. (4.15). In this way the problem of calculating the photonic band structure in H polarization is reduced to the diagonalization of the two matrices $\vec{\vec{B}}$ and $\vec{\vec{C}}$.

It is found that the eigenvalues of the matrix $\vec{\vec{B}}$ yield the flat bands, while the eigenvalues of $\vec{\vec{C}}$ produce the dispersive bands which, for small filling fractions, are not significantly different from the dispersion curves for electromagnetic waves in vacuum. The complete band structure is then the superposition of the band structures associated with each of the eigenvalue problems.

The convergence of the calculation of the band structure was monitored by increasing the number of the plane waves used in the expansion (4.5), and by increasing the number of terms retained in the expansion (4.18) for $\vec{\vec{B}}$ (with $\epsilon=1$).

In Figs. 6 and 7 we present the photonic band structure for the case of H polarization for the square and triangular lattices, respectively, when the filling fraction of the rods is $f=0.001$. A total of 529 plane waves for the square lattice and 535 plane waves for the triangular lattice was used to obtain these results, and the first 12 terms in the expansion (4.18) for $\vec{\vec{B}}$ were kept. The dispersive part of the band structure is essentially identical with the dispersive part of the band structure depicted in Figs. 4 and 5. We have found that the nearly dispersionless part of the photonic band structure converges slowly, and we have used up to 1373 and 1417 plane waves for the square and triangular lattices, respectively, together with an extrapolation procedure to obtain converged results. In Figs. 8 and 9, we present results displaying the convergence of the average of the frequencies of the flat bands calculated at the $\bar{M}$, $\bar{\Gamma}$, and $\bar{X}$ points as the number of plane waves used in the calculation is

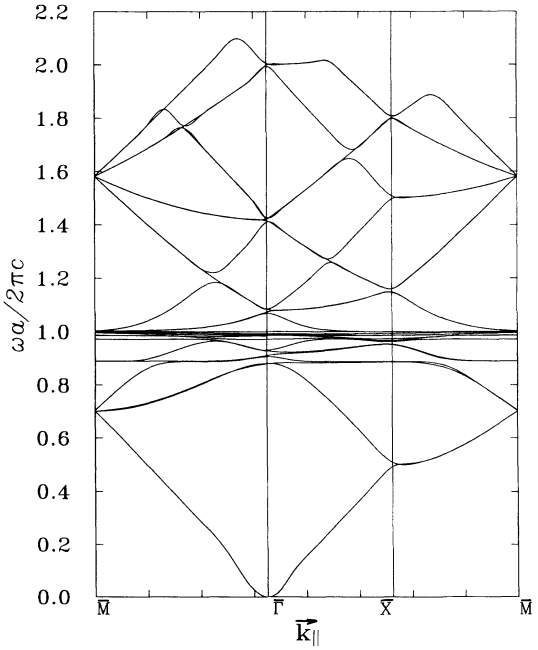

FIG. 6. The photonic band structure of a square lattice of metal cylinders in vacuum calculated by diagonalizing the $\vec{\vec{B}}$ and $\vec{\vec{C}}$ matrices. H polarization: $f=0.001$. NG = 529.

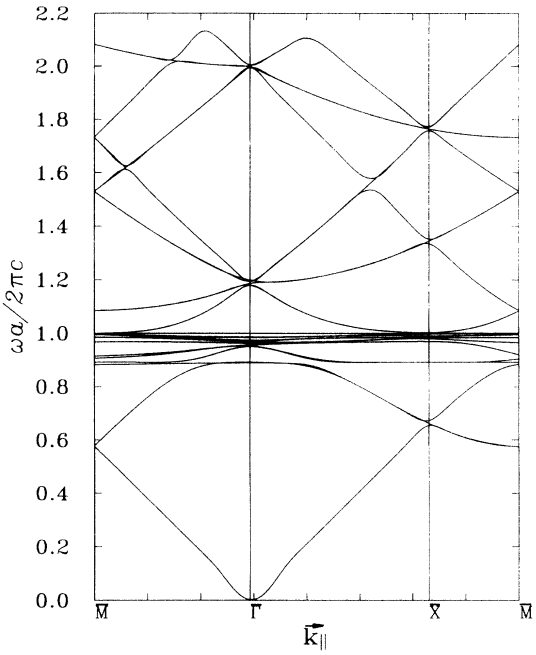

FIG. 7. The photonic band structure of a triangular lattice of metal cylinders in vacuum calculated by diagonalizing the $\vec{B}$ and $\vec{C}$ matrices. H polarization: $f=0.001$. NG = 535.

increased for the square and triangular lattices, respectively. One sees that at this filling fraction there is no absolute band gap in the frequency range investigated. In fact, the flat bands fill the frequency range from $(\omega a/2\pi c)\cong 0.7$ to $(\omega a/2\pi c)=1$. By the use of the approach just described, it is possible to calculate the photonic band structures for electromagnetic waves of H polarization for larger filling fractions than can be treated by the use of Eqs. (3.6).

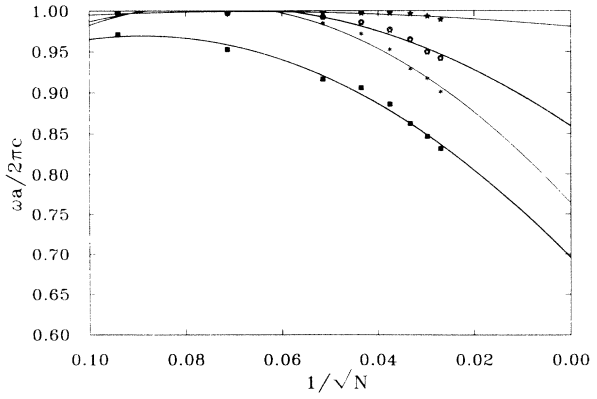

FIG. 8. Convergence of the frequencies of the flat bands present in the results displayed in Fig. 6 as the number of plane waves used in the calculation is increased.

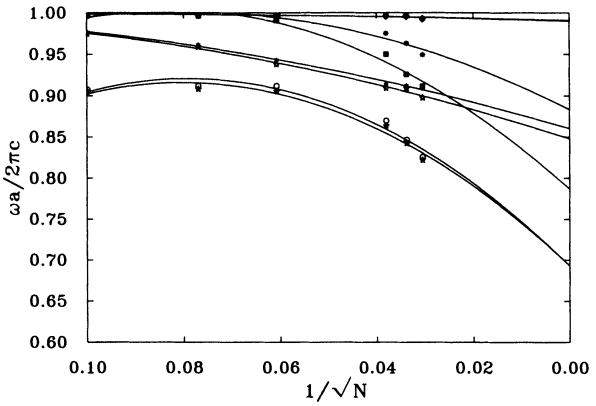

FIG. 9. Convergence of the frequencies of the flat bands present in the results displayed in Fig. 7 as the number of plane waves used in the calculation is increased.

V. CONCLUSIONS

The results presented in this paper show that the plane-wave method can be used successfully for obtaining the photonic band structure for electromagnetic waves of E polarization in two-dimensional, periodic structures consisting of an infinite array of identical, infinitely long, parallel, metal cylinders embedded in vacuum, whose intersections with a perpendicular plane form a two-dimensional crystal structure, even for large values of the volume filling fraction. The use of a modest number of plane waves (~ 200) appears to be sufficient to yield converged bands. The calculated photonic band structures resemble qualitatively those that are obtained when the metal cylinders are replaced by dielectric cylinders. For large values of the filling fraction, a band gap for waves of E polarization is obtained for the square lattice, but none is observed in the results for the triangular lattice, in the frequency range investigated. However, the photonic band structures for both lattices display an absolute band gap below the lowest frequency band, whose dispersion curve does not tend to zero frequency at the $\bar{\Gamma}$ point. The width of this gap grows with increasing filling fraction, and is a consequence of the metallic nature of the cylinders from which the periodic structures are constructed.

The situation is quite different in calculations of the photonic band structure for electromagnetic waves of H polarization in the two-dimensional periodic structures considered here. In this case, the use of a comparatively small number of planes waves (~ 200) is sufficient to yield converged results for the majority of the bands calculated, which are dispersive. However, unlike the case for E-polarized electromagnetic waves, the photonic band structures for waves of H polarization also possess a number of rather flat, nearly dispersionless, bands in the frequency range $\omega<\omega_p$, effectively superimposed on the dispersive band structure. These flat bands were also obtained in our earlier calculations of the photonic band structure of H-polarized electromagnetic waves in a two-

dimensional, square lattice array of metallic cylinders.[31] The convergence of the frequencies of these bands with increasing number of plane waves is very slow when the eigenvalue problem defined by Eqs. (3.6) is solved. A somewhat more rapid rate of convergence of these bands is obtained by the diagonalization of the matrix $\overleftrightarrow{B}$, although even in this approach a large number of plane waves and an extrapolation procedure is required to obtain accurate results.

In view of the fact that these flat bands occur in the case of H polarization but not in the case of E polarization it is tempting to identify their origin as the (weak) overlap of H-polarized excitations associated with each metal cylinder in isolation and characterized by discrete frequencies, when an infinite number of cylinders is brought together to form the kind of periodic structure considered in this paper. The overlap of these excitations broadens the discrete frequencies into narrow bands.

The frequencies of the electromagnetic modes of H polarization of a metal cylinder of radius R, characterized by the dielectric function (1.1), embedded in vacuum, are the roots of[33]

$$D_n^{(H)}(\omega)=I_n\left[|\epsilon(\omega)|^{1/2}\frac{\omega}{c}R\right]'H_n^{(1)}\left[\frac{\omega}{c}R\right]+|\epsilon(\omega)|^{1/2}I_n\left[|\epsilon(\omega)|^{1/2}\frac{\omega}{c}R\right]\times H_n^{(1)}\left[\frac{\omega}{c}R\right]'=0\ ,\quad n=0,12,\ldots, \tag{5.1a}$$

where $H_n^{(1)}(z)$ is a Hankel function, $I_n(z)$ is a modified Bessel function, and the prime denotes differentiation with respect to argument. Our notation emphasizes the fact that we are seeking frequencies in the range $0\le\omega\le\omega_p$, i.e., in the range in which $\epsilon(\omega)<0$. We have also assumed that the magnetic field in the region outside the cylinder has the nature of an outgoing wave at infinity, as would be the case in the scattering of a plane wave propagating perpendicularly to the axis of the cylinder. The frequencies of the electromagnetic modes of E polarization of the same system are the roots of[33]

$$D_n^{(E)}(\omega)=I_n\left[|\epsilon(\omega)|^{1/2}\frac{\omega}{c}R\right]H_n^{(1)}\left[\frac{\omega}{c}R\right]'-|\epsilon(\omega)|^{1/2}I_n\left[|\epsilon(\omega)|^{1/2}\frac{\omega}{c}R\right]'\times H_n^{(1)}\left[\frac{\omega}{c}R\right]=0\ ,\quad n=0,1,2,\ldots\ . \tag{5.1b}$$

The solutions of both of these dispersion relations for each n are, in general, complex $\omega_{n,s}=\omega_{n,s}^{(R)}-i\omega_{ns}^{(I)}$ ($n=0,1,2\ldots,s=1,2,3,\ldots$), and we have searched for them by plotting $|D_n^{(H,E)}(\omega)|^{-2}$ as functions of real ω in the range $0\le\omega\le\omega_p$. Such plots will have Lorentzian peaks centered at $\omega_{n,s}^{(R)}$ whose full width at half maximum is $2\omega_{n,s}^{(I)}$. In the case of E polarization, no such peaks were found in the range $0\le\omega\le\omega_p$, for a value of R corresponding to a filling fraction of 0.001. This is consistent with the absence of any flat bands in the photonic band structure for electromagnetic waves of this polarization. In the case of H polarization, a multitude of such peaks were found in the frequency range $\omega_p/\sqrt{2}<\omega_{n,s}<\omega_p$, for values of $n=1,2,3,\ldots$. This is consistent with the existence of flat bands in the photonic band structure for electromagnetic waves of H polarization in this frequency range.

The preceding discussion has an admittedly heuristic nature, but may help in understanding the origin of the curious feature of the nearly dispersionless bands present in the photonic band structure for electromagnetic waves of H polarization but not in the band structure of waves of E polarization.

Finally, we note that the reduction of the problem of obtaining photonic band structures of periodic, two-dimensional structures containing metallic components to the solution of a standard eigenvalue problem used here in the case of E polarization can also be used in calculations of the photonic band structures of periodic, three-dimensional structures containing metallic components, if one works with the equations satisfied by the components of the electric field. Whether this approach will be competitive with the transfer-matrix method used by Pendry[32] in such a calculation remains to be determined. However, it should be emphasized that this method works because of the particular form of the dielectric function given by Eq. (1.1). Thus, in the present work if the cylinders were fabricated from a cubic, polar crystal containing two ions in a primitive unit cell, for which the dielectric function has the form

$$\epsilon(\omega)=\epsilon_\infty\frac{\omega_L^2-\omega^2}{\omega_T^2-\omega^2}\ , \tag{5.2}$$

where ϵ_∞ is the optical frequency dielectric constant, while ω_L and ω_T are the frequencies of the longitudinal-optical and transverse-optical vibration modes of infinite wavelength, respectively, the method employed here would not lead to a standard eigenvalue problem even in E polarization. However, for electromagnetic waves of both E- and H polarization a generalization of the kind of eigenvalue problem obtained in Sec. IV B can be obtained in this case.

It should be noted that Sigalas *et al.*[34,35] by using a transfer-matrix method[8,36] have calculated the transmission coefficient as a function of frequency for the propagation of E-polarized electromagnetic waves through a finite two-dimensional square lattice of cylinders fabricated from a polar semiconductor characterized by the dielectric function (5.2). By this approach, the frequency ranges in which band gaps occur can be determined fairly simply. However, the photonic band structure for this system has not yet been obtained. Sigalas *et al.*[35] have also used the same method to calculate the transmission coefficient as a function of frequency for the propagation of E-polarized electromagnetic waves through a finite two-dimensional square lattice of cylinders fabricated

from a lossy polar semiconductor whose dielectric function has the form

$$\epsilon(\omega)=\epsilon_i+(\epsilon_0-\epsilon_i)\frac{\omega_T^2}{\omega_T^2-\omega^2-i\Gamma\omega}\ , \tag{5.3}$$

where ϵ_0 is the static dielectric constant and Γ the damping constant, and have obtained the frequency regions in which band gaps occur.

If dissipation is introduced into the metallic components of periodic two- or three-dimensional structures through the use of a dielectric function of the form

$$\epsilon(\omega)=1-\frac{\omega_p^2}{\omega(\omega+i\gamma)}\ , \tag{5.4}$$

where $\gamma=1/\tau$ is an inverse electron relaxation time, the reduction of the band-structure calculation to the solution of a standard eigenvalue problem is not possible. However, a generalization of the type of eigenvalue problem obtained in Sec. IV B can again be obtained to yield complex values of ω for each value of $\mathbf{k}_\parallel$. It is hoped that such problems will be studied in the near future.

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