Full Vector Wave Calculation of Photonic Band Structures in Face-Centered-Cubic Dielectric Media

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(Received 17 April 1990)

The photonic band structure of a face-centered-cubic lattice of spheres is calculated using the plane-wave method for Maxwell's equations. Comparisons with the available experimental results show rather good agreement, except that we do not find a true gap for this configuration. This we believe is due to symmetry reasons at the W point.

PACS numbers: 41.10.Hv, 03.40.Kf, 78.20.Bh

The idea of employing three dimensionally periodic dielectric structures to create gaps in the photon density of states has recently been introduced.[1,2] The potential applications of such a forbidden frequency gap are fascinating. Examples include the inhibition of spontaneous emission,[1] the modification of basic properties of atomic, molecular, and excitonic systems,[3,4] and the possibility for studying mobility edges and Anderson localization of photons within the gap.[2,5]

A recent experiment with microwaves[6] has demonstrated the soundness of the basic idea of photonic bands in three-dimensional periodic structures. Moreover, in one of the samples, a gap that extends throughout the Brillouin zone was observed. Unfortunately, there was little theoretical guidance to help find optimal dielectric structures which will produce such gaps for these new artificial optical media, besides the fact that the dielectric contrast should be large and the Brillouin zone should be as close to spherical as possible. Consequently, the experimentalists had to adopt a tedious cut-and-try approach in which dozens of fcc structures with atomic volume filling fraction between 11% and 86% and various refractive-index ratios were painstakingly machined out of low-loss dielectric materials. This very time-consuming approach was necessary to help insure that no possibilities were overlooked. It was found that out of the 21 samples that were made, only one exhibits a true photonic band gap.

Here we show that the plane-wave method can be used to calculate the photonic bands in three-dimensionally periodic dielectric media. The structure we studied is the same as that investigated experimentally,[6] and consists of a face-centered-cubic lattice of spheres of refractive index n_a embedded in a homogeneous transparent host medium of refractive index n_b. The photon bands were calculated for various values of the relative refractive index, $r=n_a/n_b$, and volume filling fraction of spheres, f. We have also studied the case in which the spheres are air atoms which are so closely packed that they actually overlap. This case is especially interesting in that it was found experimentally to have a common photon band gap throughout the entire Brillouin zone. Overall our theoretical results are in reasonable agreement with those of the experiment.[6] This includes the effective long-wavelength refractive index as a function of the volume filling fraction, and the size of the gap at the L and X points for an 86% fraction of air atoms. However, there is a discrepancy for this case at the W point, where our result suggests that a gap does not exist because of symmetry, whereas a gap is observed experimentally. In addition, in the W to K direction away from the W point, the gap is much more feeble than measured experimentally.

We present here the *first* computation of photon band structures based on Maxwell's equations. Our results, therefore, fully take into account the vector nature of the photon. The importance of a full vector calculation has in fact been pointed out.[6] Here we see that calculations for scalar waves are inadequate and much too optimistic in predicting a gap to open up at a refractive-index contrast of about 1.7.[7-11] We should mention that the plane-wave method has recently been used successfully to calculate photonic band structures based on the scalar wave approximation.[7,8] Our present work shows that the method can be extended with similar success to the full vector case as well.[12] The method is extremely simple, and is capable of treating any form of dielectric modulation. We find that convergence is slower than in the scalar case, but is reasonably rapid enough for obtaining accurate band structures. This is unlike conventional electronic band calculations where a convergence problem arises for the plane-wave method because wave functions are rapidly oscillating near the highly attractive atomic core potentials and are plane-wave-like outside the atomic regions.

We start with Maxwell's equations and eliminate the magnetic field in favor of the electric field $\mathbf{E}$ to obtain, for monochromatic waves of frequency ω, the equation

$$\nabla\times(\nabla\times\mathbf{E})+k_b^2V\mathbf{E}=k_b^2\mathbf{E}\,, \tag{1}$$

where $V=1-(n/n_b)^2$, $k_b\triangleq\mu\omega n_b/c_0$, and $n=n_a$ inside the spheres and $n=n_b$ inside the host. We can identify k_b^2 as the energy and k_b^2V as the potential. Owing to the spin-1 nature of the photon, the above equation has a vector character and the potential is proportional to ω^2, and thus vanishes in the long-wavelength limit. This has

some very important consequences for the photonic band structures here, as well as in the photon localization problem.[13]

In the plane-wave method one works with the Fourier coefficients

$$\mathbf{E}_{\mathbf{k}}=\int d\mathbf{r}\, e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{E}(\mathbf{r}), \tag{2}$$

and

$$V_{\mathbf{K}}=\frac{1}{\Omega}\int d\mathbf{r}\, e^{-i\mathbf{K}\cdot\mathbf{r}}V(\mathbf{r}), \tag{3}$$

where $\mathbf{K}$ are the reciprocal-lattice vectors and Ω is the volume of the fcc primitive cell. Equation (1) can then be expressed in the form

$$[(|\mathbf{k}-\mathbf{K}|^2-k_b^2)\mathbf{1}-(\mathbf{k}-\mathbf{K})(\mathbf{k}-\mathbf{K})]\cdot\mathbf{E}_{\mathbf{k}-\mathbf{K}}+k_b^2\sum_{\mathbf{K}'}V_{\mathbf{K}'-\mathbf{K}}\mathbf{E}_{\mathbf{k}-\mathbf{K}'}=0. \tag{4}$$

This equation gives an infinite-order determinantal equation that can only be solved by truncation. If N reciprocal-lattice points are included, then a $3N\times 3N$ matrix equation has to be solved. However, it is important to note that this equation has zero eigenvalues that correspond to longitudinal-photon modes. This can be seen by setting k_b in Eq. (4) to zero and working in a coordinate system in which the z axis points along the vector $\mathbf{k}-\mathbf{K}$. Then it is clear that the resulting determinant is zero and the eigenvectors corresponding to the zero eigenvalues have $(\mathbf{k}-\mathbf{K})^x=(\mathbf{k}-\mathbf{K})^y=0$ and $(\mathbf{k}-\mathbf{K})^z\neq 0$. These zero eigenvalue modes can be eliminated by the condition $\nabla\cdot\mathbf{D}=0$, where $\mathbf{D}$ is the displacement field. This condition implies that

$$(\mathbf{k}-\mathbf{K})\cdot\sum_{\mathbf{K}'}(\delta_{\mathbf{K}-\mathbf{K}'}-V_{\mathbf{K}'-\mathbf{K}})\mathbf{E}_{\mathbf{k}-\mathbf{K}'}=0. \tag{5}$$

With this equation one of the Cartesian components of $\mathbf{E}_{\mathbf{k}-\mathbf{K}'}$ can be eliminated. The resulting determinantal matrix is therefore of order $2N\times 2N$. This procedure of eliminating the zero-eigenvalue modes is found to speed up our numerical calculation by at least a factor of 2, and enables us to include more $\mathbf{K}$ points to improve the accuracy of our results. The photon band structure is then obtained by finding the eigenvalues k_b^2 of the resulting matrix for each value of $\mathbf{k}$.

Before we give the results of our calculations that are specific to the present problem, we want to make a few general remarks. First, it is easy to see that in the empty-lattice limit, i.e., $V\rightarrow 0$, the eigenvalues are given by $k_b^2=|\mathbf{k}-\mathbf{K}|^2$ and are at least doubly degenerate, because the photon can have different states of polarization. The band structure can be found in most solid-state textbooks. It is also true that in this limit, most of the levels are highly degenerate, especially at high-symmetry points, and for $\mathbf{k}$ varying from the Γ point to the edge of the Brillouin zone, the dispersion curves are straight lines given by $k_b=k$. A detailed plot of the free-photon bands for the fcc lattice can be found in a recent paper,[8] except that the degeneracy factor for each level should be multiplied by a factor of 2.

For $V\neq 0$, depending on the symmetry of V, some of these degeneracies are lifted, and the dispersion curves originating from the Γ point are linear only near the Γ point, where k is small compared with the magnitude of the smallest nonzero reciprocal-lattice vector of the lattice. If we plot k_b vs k for the photon bands, then the slope of the straight portion is no longer unity, but should be given by n_b/n_{eff}, where n_{eff} is the effective long-wavelength refractive index of the entire medium.

For fixed values of the relative refractive index and volume filling fraction, the lowest-lying frequency gap is expected to have the largest width. We find that this is true in all the cases that we have studied, and therefore we shall only report results for the lowest few bands. Moreover, it is important to note that because of the two different states of polarization, the lowest gap can lie only between the second and the third bands. This situation is very different from the scalar wave case where the lowest gap lies between the first and the second bands.

Now we are ready to discuss the results for the present model. For the case of dielectric spheres considered here, we have

$$V_{\mathbf{K}}=3f(1-r)g(|\mathbf{K}|a), \tag{6}$$

where the function $g(x)=(\sin x-x\cos x)/x^3$, and a is the radius of the sphere. This result applies as long as the spheres do not touch. In the experimental work of Yablonovitch and Gmitter,[6] two types of models were studied. The first type consists of dielectric spheres of polycrystalline Al_2O_3 with a microwave refractive index of 3.06 embedded in a dielectric foam of refractive index 1.01. Samples were made with a variety of volume filling fractions, from 11% to the closed-packed value of 74%. The second type of samples were made by drilling spherical holes in a low-loss dielectric material which has a refractive index of 3.5. Various samples with volume filling fraction from 11% to 86% were fabricated. The voids are actually overlapping when the volume filling fraction is larger than the close-packed value of $f_c=0.74$. It turns out that when $f>f_c$, there are three separate cases that have to be considered. These three cases correspond to $c/\sqrt{8}<a<c/\sqrt{6}$, $c/\sqrt{6}<a<c\sqrt{3/16}$, and $c\sqrt{3/16}<a<c/2$, where c is the length of the side of the conventional unit cube for the fcc lattice. In the first case, both the spheres and the host material form an infinite multiply connected domain. In the last two cases, the host material breaks up into disconnected star-shape islands while the spheres form an infinite multiply connected domain. We find that for $a=c/\sqrt{6}$, the volume filling fraction is 0.964. Therefore, the sample which was found experimentally to have a gap in the photon density of states and has a volume filling fraction $f=0.86$ actually belongs to the first case.

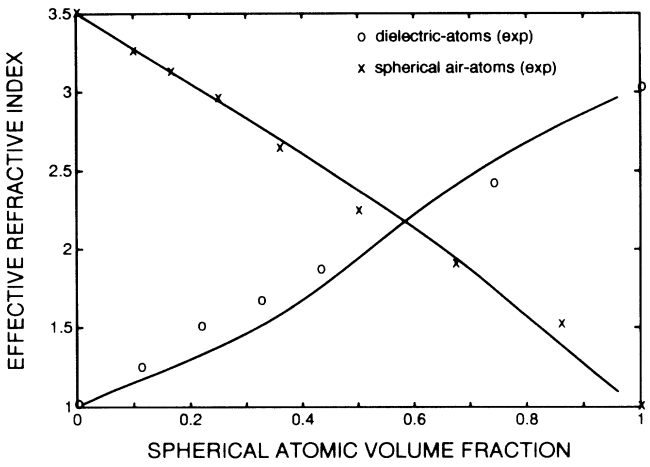

FIG. 1. The effective long-wavelength refractive index for two basic crystal structures as a function of the volume filling fraction. The solid lines are our computed results. The experimental values are shown by the o and × points, respectively, for spherical dielectric atoms and spherical air atoms.

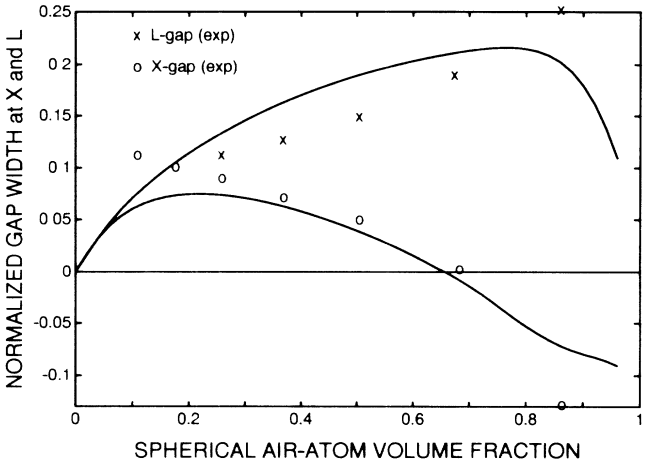

FIG. 2. The computed forbidden frequency gap width at the L and X points as a function of the volume filling fraction for air atoms embedded in a dielectric material with a refractive index of 3.5. The experimental values at the L and X points are labeled, respectively, by × and o. These results are all normalized to the center frequency of the lowest gap at the X point.

It can be shown that for this case

$$V_{\mathbf{K}}=(1-r)\left[3fg(|\mathbf{K}|a)-\frac{2}{\Omega}\sum_{\mathbf{Q}}I(\mathbf{Q})\right], \tag{7}$$

where

$$I(\mathbf{Q})=\frac{2\pi}{Q_\rho}\int_{a_c}^{a}dz\cos(Q_z z)(a^2-z^2)^{1/2} \times J_1(Q_\rho(a^2-z^2)^{1/2}). \tag{8}$$

In the above equations, J_1 is the first-order Bessel function, and two of the six $\mathbf{Q}$ vectors are given by $Q_\rho=[K_x^2+(K_y\pm K_z)^2/2]^{1/2}$ and $Q_z=(K_y\mp K_z)/\sqrt{2}$ in cylindrical coordinates. The remaining four vectors are given by cyclic permutations of x, y, and z. Although the integrals can be expressed in terms of Lommel's functions of two variables and various schemes for computing them are available,[14] we find it more convenient in our work to simply compute them numerically.

Using these results together with our plane-wave equations, we have calculated the photon band structure for various values of f and r. We find that the results for the lowest few bands converge reasonably fast. To within an accuracy of about a few tenths of 1%, we find that 400 $\mathbf{K}$ points are sufficient for r ranging from 1/12.25 to 9.179 and for f ranging from 0 to 0.96. First we show the results for the effective long-wavelength refractive index in Fig. 1 for both the dielectric and air atoms as a function of the volume filling fraction. The results are seen to be in excellent agreement with the experimental results of Yablonovitch and Gmitter.[6]

Next we present, in Fig. 2, the computed results for the eigenvalues for the second and third bands at the L and X points in the Brillouin zone as a function of the volume filling fraction for the case of air atoms. These results are normalized to the center frequency of the lowest gap at the X point. The agreement with the experimental results[6] is fairly good. In particular we find that the X gap goes to zero for $f\approx 0.66$. This is very close to the experimental value of 0.68. The physical origin of this behavior has been fully discussed by Yablonovitch and Gmitter, and accordingly we plot the gap width at the X point as a negative quantity for $f>0.66$. For $f=0.86$ our results for the gap sizes at L and X are both smaller than those observed in the experiment.

We have also calculated the entire photonic band structure for $\mathbf{k}$ along the symmetry directions in the Brillouin zone. Results are obtained for the refractive-index ratio r varying from $\frac{1}{4}$ to 1 for air atoms and from 1 to 4 for dielectric atoms. For each value of r, the volume filling fraction is varied from 0 to 0.96 for air atoms and from 0 to 0.74 for dielectric atoms. Figure 3 shows the results for an 86% volume filling fraction of air atoms embedded in a dielectric material with a refractive index of 3.5. These parameters correspond to the case in which a common gap was found experimentally. We see that although the overall band structure agrees reasonably well with the experiment, our computed band structure does not have a common gap. This is due to the fact that the second and third bands appear to be degenerate at the W point. Figure 3 also suggests that the second and third bands are degenerate along the W to K direction. (Note that the K and U points are connected by a reciprocal-lattice vector, and are therefore equivalent points in the Brillouin zone.) However, further investigation shows that this degeneracy away from the W point in the K direction is purely accidental and it is absent in general for other values of r and f. The same is

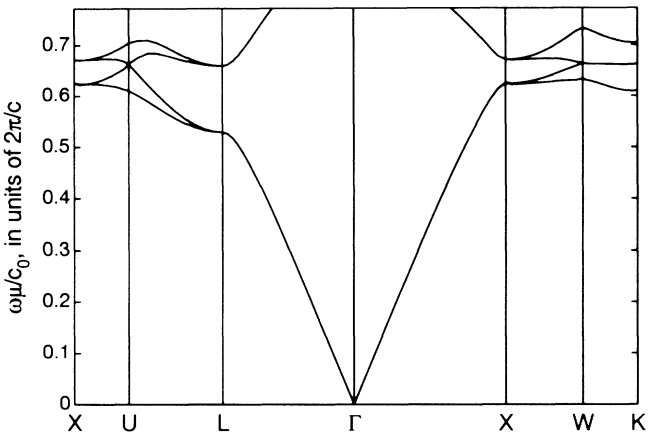

FIG. 3. The computed photonic band structure for an 86% volume filling fraction of air atoms embedded in a dielectric material with a refractive index of 3.5. The spherical voids are actually closer than close packed, and are overlapping.

also true for the near degeneracy of the second and third bands at the U point.

In trying to obtain a true photonic band gap, we find that the most troublesome result is at the W point where the degeneracy is found to persist for this value of refractive-index ratio of $r=1/3.5$ for f ranging from 0 to 0.96. Further calculation indicates that this remains true down to a value of $r=1/4$ for all values of f, and that this degeneracy appears to be symmetry related.

In the case of dielectric atoms, we find that the gap at the W point opens up for $r>2.8$; unfortunately there is no overlap in the gaps at the L and X points for a true gap to develop for these values of r. We have also checked that for r around 4 the second and third bands at X appear to be degenerate and therefore a common gap does not exist either. We have not gone to values of r too much larger than 4 because of the lack of suitable optical materials that are currently available in the laboratory, and because in our calculation the size of the matrix required for convergence becomes prohibitively large.

In summary, we found that for r ranging from $\frac{1}{4}$ to 4, thus including both the air- and dielectric-atom cases, there is no common gap in the photonic band structure for the fcc geometry at any volume filling fraction. Our work suggests that it is important to find a mechanism which will either redistribute the strength of the Fourier coefficients of the potential in such a way that degenerate levels at the W point do not occur for the second and third levels, or lift the degeneracy of these levels.

We are grateful to Dr. Eli Yablonovitch for many illuminating discussions, and for sending us preprints of unpublished results. This work is supported by the U.S. ONR under Contract No. N00014-88-0050, by the Naval Research Laboratory under Contract No. N00014-89-J-2078, and by the Joint Services Electronics Program.

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