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Brief Reports

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Photonic band structure: The case of oval holes

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The photonic bands of a face-centered-cubic structure with a basis consisting of three intersecting cylinders with oval cross section are computed using the plane-wave method. The optimal band-gap size to midgap frequency ratio is found to be 12% larger than the case of circular holes for a refractive-index contrast of 3.6. A contour plot is computed that gives this ratio as a function of both the refractive-index contrast and the major diameter of the oval holes.

Since its inception a few years ago,[1] the idea of photonic band structure in a three-dimensional periodic dielectric medium is rapidly gaining acceptance, especially after the experimental work of Yablonovitch and Gmitter[2] on face-centered-cubic (fcc) arrays of spheres. During this time, theoretical photonic-band-structure calculations have also appeared. Although scalar-wave-band calculations are often used in electronics, it is clear from the initial scalar-wave calculations[3–7] that they are inadequate here for the description of photonic bands. These works were very soon followed by full vector band calculations based on Maxwell's equations.[8–10] The results of these calculations not only agreed with experiment,[2] but also highlighted some discrepancies in experiment, and suggested structures that permit the opening up of a full photonic band gap.

One of such structures[10] places two spheres into the Wigner-Seitz unit cell of fcc lattice, forming the diamond structure. The structure permits a very wide photonic band gap, however, its fabrication on the scale of optical wavelengths would be somewhat difficult. The other structure[11] can also be considered as fcc, but the Wigner-Seitz cell contains three cylinders running along the $\langle 110\rangle$, $\langle 101\rangle$, and $\langle 011\rangle$ directions and passing through the center of the cell.[12] For experiment in the microwave regime, the structure was made by direct drilling three sets of holes at polar angles $\theta_0=\cos^{-1}\sqrt{2/3}$ off normal and with azimuthal angles $\phi=120°$ apart into the top surface of a dielectric slab. Excellent agreement between theory and the available experimental data[11] was obtained. The three-dimensional forbidden photonic band-gap width is about 19% of its center frequency at a refractive index contrast of 3.6. Calculations indicate that the gap remains open for the refractive index $n>2.1$. Besides having a sizable band gap, this basic structure is also interesting in that it lends itself readily to microfabrication on the scale of optical wave lengths by techniques such as reactive ion etching.[13] However, as a result of the fabrication process, the cylinders will have an oval rather than circular cross section. The purpose of this paper is to compute the photonic bands of this structure using the plane-wave method

There are thus far three slight variations of the plane-wave method that have been used for vector wave calculations. In one of these works,[9] the transversality condition $\nabla\cdot\mathbf{D}=0$ was not imposed. As a result, if one keeps N plane waves in the calculation, then matrices of order $3N$ by $3N$ have to be diagonalized. Moreover, one obtains N zero-frequency longitudinal photon modes that must be discarded. On the other hand, in the works of Ho, Chan, and Soukoulis[10] (HCS) and Leung and Liu[8] (LL) the transversality condition was strictly imposed. The dimension of the matrices is reduced to $2N$ by $2N$, and there are no zero-frequency longitudinal photon modes. The main difference between these two studies was that the magnetic field was used by HCS, while LL chose to work with the electric field. We have checked that both variations of the plane-wave method yield the same results to within six to seven significant figures and are therefore basically equivalent. The method of HCS is however better than that of LL in that the matrices involved are naturally in a symmetric form. This allows the eigenvalues and eigenfunctions to be computed more efficiently. We therefore adopt their method in all of our calculations here.

Thus we expand the magnetic field in a plane-wave basis,[10]

$$\mathbf{H}(\mathbf{r})=\sum_{\mathbf{G}}\sum_{\lambda=1}^{2} h_{\mathbf{G},\lambda}\hat{\mathbf{e}}_{\lambda}e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}, \tag{1}$$

where $\mathbf{k}$ is a wave vector in the Brillouin zone, $\mathbf{G}$'s are the reciprocal lattice vectors, and the vectors $\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2$ and $\mathbf{k}+\mathbf{G}$ form a triad. Maxwell's equations then yield the eigenvalue equation

$$\sum_{\mathbf{G}',\lambda'} H^{\lambda,\lambda'}_{\mathbf{G},\mathbf{G}'} h_{\mathbf{G}',\lambda'} = (\omega^2/c^2) h_{\mathbf{G},\lambda} , \tag{2}$$

where

$$H_{\mathbf{G},\mathbf{G}'} = |\mathbf{k}+\mathbf{G}||\mathbf{k}+\mathbf{G}'| \epsilon^{-1}_{\mathbf{G},\mathbf{G}'} \begin{bmatrix} \hat{\mathbf{e}}_2 \cdot \hat{\mathbf{e}}_{2'} & \hat{\mathbf{e}}_2 \cdot \hat{\mathbf{e}}_{1'} \\ -\hat{\mathbf{e}}_1 \cdot \hat{\mathbf{e}}_{2'} & \hat{\mathbf{e}}_1 \cdot \hat{\mathbf{e}}_{1'} \end{bmatrix} , \tag{3}$$

and $\epsilon^{-1}_{\mathbf{G},\mathbf{G}'}$ is the inverse of the dielectric function in reciprocal space. The normal mode frequencies and their coefficients are obtained by solving this eigenvalue equation.

We want to consider here a three-dimensional periodic dielectric medium which is fabricated, for example, using reactive ion etching, in the following way.[14] A mask with a hexagonal array of circles with diameter d is first placed on top of a dielectric medium. The distance between the holes is $a/\sqrt{2}$, where a is the length of the conventional unit cube of the resulting fcc structure. Etching is performed at an angle θ_0 with respect to the normal. This process is repeated twice with the sample rotated at an angle of 120° around the normal each time before etching. As a result, a fcc lattice is formed. The basic repeating unit can be considered as a fcc Wigner-Seitz cell with three hollow cylinders lying in the $\langle 101 \rangle$, $\langle 110 \rangle$, and $\langle 011 \rangle$ directions. The three cylinders have an oval cross section and intersect at the center of the cell. For a very thin mask, the eccentricity of the oval holes is given by $1/\sqrt{3}$.

In our calculation, a fine mesh is set up with the Wigner-Seitz cell to represent the structure in real space. Its Fourier transform is then computed to obtain the dielectric function in reciprocal space. The number of plane waves used in our calculation is varied from 113 to 169, 259, and then to 531 to test for convergence. The results reported below are obtained using 169 plane waves, which we find to be a suitable compromise between numerical accuracy and the required amount of computational time. The largest change in the lowest several eigenvalues is less than 0.1%, as compared with the corresponding results obtained using 531 plane waves. That only happens for the largest value of refractive-index ratio of 5 which we have studied, and for a few $\mathbf{k}$ points within the Brillouin zone.

We have computed the photonic bands for n between 1.9 and 5, and for the ratio of the diameter of the holes in the mask to the length of the conventional unit cube d/a between 0.30 and 0.58. We find that there is no true band gap for $n < 2.05$. Due to the lack of suitable nonabsorbing optical material whose refractive index is larger than 5, we have not explored the region $n > 5$. As d/a is increased above 0.58, the structure becomes more and more fragile as it is getting closer to becoming not self-supporting.

In Fig. 1, we show the photonic bands for $n = 3.6$ and for $d/a = 0.53$, which is the optimal ratio for this refractive-index contrast. We have adopted the same labeling of the symmetry points in the Brillouin zone as in Ref. 11. In Fig. 1(b) $\mathbf{k}$ varies within a mirror plane and the electric field can be classified as either s-polarized ($\mathbf{E}$ is perpendicular to the mirror plane) or p-polarized ($\mathbf{E}$ lies within the mirror plane). The s-polarized bands and the p-polarized bands are shown by the solid and dashed lines, respectively. In Fig. 1(a) there is no separation into s and p-polarized bands. These bands of mixed polarizations are shown by solid lines. In both plots, the darker shaded regions denote the absolute band gap for any polarization. The lighter shaded regions either above or below the absolute gap in Fig. 1(a) represent forbidden

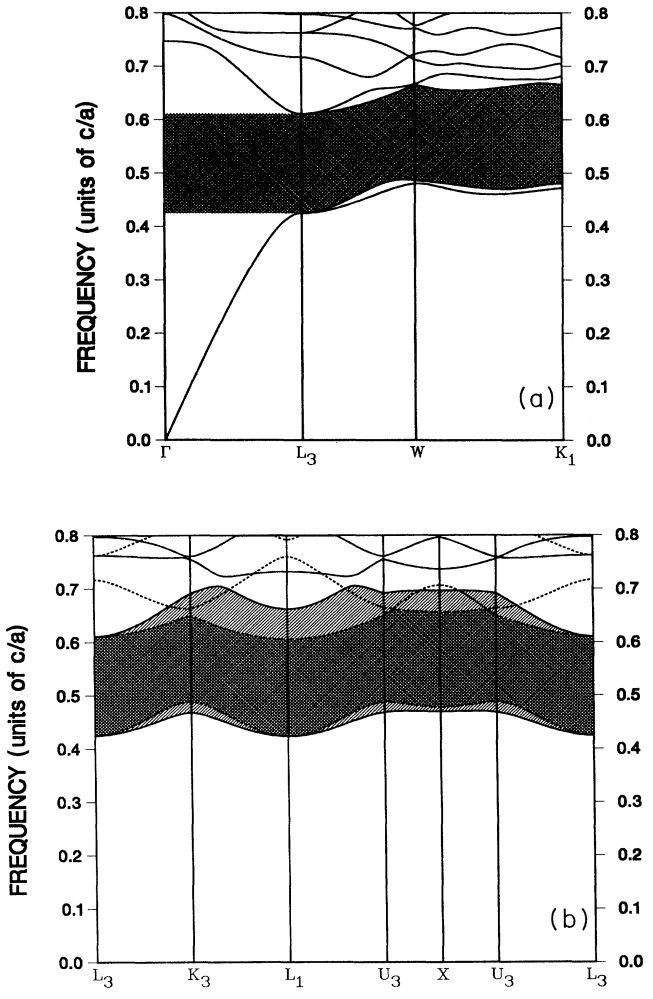

FIG. 1. The photonic bands for the present structure with oval holes. The refractive-index contrast is 3.6 and the major diameter of the holes is 0.53 in units of the length of the conventional unit cube. The darker shaded regions denote the absolute band gap for any polarization. (a) There is no separation into s- and p-polarized bands. These bands of mixed polarizations are shown by solid lines. (b) The s-polarized and p-polarized bands are shown by the solid and dashed lines, respectively. The lighter shaded regions either above or below the absolute gap represent forbidden gaps for the s-polarized wave only.

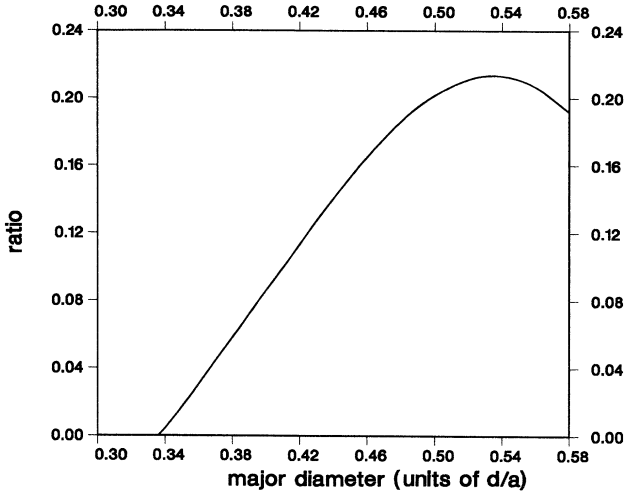

FIG. 2. The band-gap size to midgap frequency ratio as a function of the major diameter of the oval holes at a refractive index contrast of 3.6.

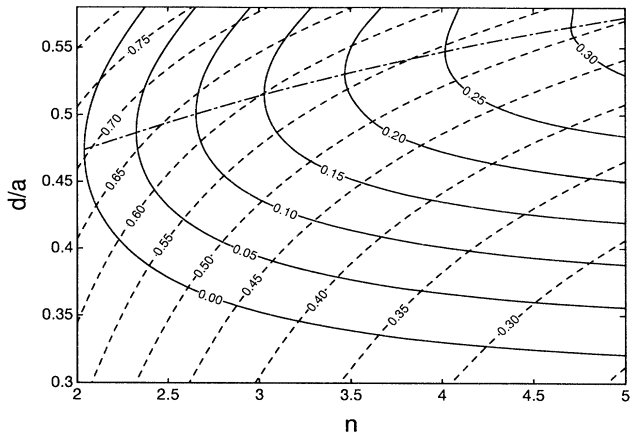

FIG. 3. Contour plot showing the gap size to midgap frequency ratio (solid lines) and the midgap frequency in reduced units (dashed lines) as a function of both the refractive index contrast and the major diameter of the oval holes. The dash-dotted line gives the optimum diameter as a function of the refractive index.

gaps for the s-polarized wave only. The gap size to midgap frequency ratio Δ is found to be 21.3%, which is about 12% larger than the optimal value in the case of circular holes for this value of n. The volume filling fraction of air here is 80.5%, which is very close to the corresponding optimal fraction for the case of circular holes. The top of the valence band occurs close to W, and the bottom of the conduction band occurs at L_1. This is exactly the same as that found for circular holes. The overall band structure is also quite similar as compared to that of circular holes. The most noticeable difference is in the ordering of the two valence bands. The s-polarized band is actually lower than the p-polarized band here. However, the frequency at the top of the valence remains almost identical in both cases. It is the bottom of the conduction band situated at L_1 which is pushed slightly upward; this accounts for the 12% improvement in the reduced gap size.

The variation of the gap size to midgap frequency ratio as a function of d/a for $n=3.6$ is shown in Fig. 2. In general, for all the values of n and d/a that we have computed, the top of the valence band occurs either at K_3 or near U_3 or W. In any case we find that these eigenvalues are very close to each other. The bottom of the conduction band is located either at L_3 or L_1. Again the eigenvalues differ only very slightly in either case.

In Fig. 3, we show a contour plot of Δ and the midgap frequency as a function of n and d/a. The minimum threshold value of n for the present structure to exhibit a true band gap is found to be 2.05, and this occurs at an optimal value of d/a of about 0.47. The optimal value of d/a is seen to shift monotonically upward with increasing n while the optimal value of Δ also increases monotonically. For $n=5$, the optimal value of Δ is about 32%, and that occurs when d/a is about 0.58.

In the fabrication of the material, by using a thicker mask during the etching process, it is possible to increase the eccentricity of the oval holes to values larger than $1\sqrt{3}$. It turns out that it is not profitable to do so because the optimal values for Δ actually decrease with increasing eccentricity.

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