Photonic band gaps in body-centered-cubic structures

R. M. Hornreich and S. Shtrikman*
Department of Electronics, Weizmann Institute of Science, 76100 Rehovot, Israel

C. Sommers
Laboratoire de Physique des Solides, Université de Paris-Sud, Bâtiment 510, F-91405 Orsay CEDEX, France
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Photonic energy bands in body-centered-cubic bcc materials are analyzed by considering structures having O^8 ($I4_132$) space-group symmetry. Such structures can be realized physically by interlacing cylindrical elements oriented along $\langle 111\rangle$ crystallographic axes. In addition to heterogeneous systems composed entirely of dielectric materials, the possibility of using conducting materials (particularly at microwave frequencies) is studied. We find that (a) band gaps occur in heterogeneous dielectric systems when materials having a dielectric constant of 10 or more are properly placed in the O^8 unit cell, and (b) utilizing conducting materials can significantly widen the excluded frequency band, the result being that band gaps of more than 20% should be attainable with O^8 structures at microwave frequencies. Experimental verification of these results should be possible in this spectral region.

In a series of theoretical studies, the feasibility of designing solids capable of exhibiting "photonic band gaps" has been analyzed for different structure groups and cellular geometries.[1–7] Based upon these studies, it has proved possible to design materials possessing such band gaps and they have been successfully fabricated and tested.[7–10] All of these studies, both theoretical and experimental, have been based upon two basic conceptions: One, the best (and perhaps only possible) structure for the solids is face-centered cubic (fcc) and two, only electrical insulators or semiconductors (but not metallic conductors) should be used in fabricating the heterogeneous structure.

In this work, we demonstrate that these two restrictions are not always applicable and that it may be possible to produce useful "photonic crystals" in other ways. In particular, we (a) present the results of photonic band calculations showing the existence of photonic band gaps in body-centered-cubic (bcc) structures, and (b) show, by considering bcc composites containing both conducting and insulating materials, that they can possess band gaps as wide as those found using fcc insulating or semiconducting structures.[6,7] In addition, the particular bcc structure we analyze may have advantages over fcc solids in ease of fabrication.

The starting point of our study was noting that the nonsymmorphic and noncentrosymmetric space group O^8 ($I4_132$) can be realized as an interlaced assembly of identical $\langle 111\rangle$ oriented cylinders, each having an internal chiral character.[11] This internal structure is important when the cylinders are completely uniform along their length as otherwise the relevant space group would be centrosymmetric O_h^{10} ($Ia\bar{3}d$). This higher symmetry is *not* desirable as it results, for example, in $\langle hk0\rangle$ Bragg reflections being forbidden unless[12] $k,l=2n$. There can then be no $\langle 110\rangle$ Fourier components in the position-dependent dielectric constant and, consequently, it is difficult to significantly break certain degeneracies in the "free photon bands" (e.g., the degeneracy existing in the absence of spatial dielectric variations in the photon bands at the point N in the bcc Brillouin zone).

Since ordinary materials are generally nonchiral, the desired O^8 space-group symmetry was obtained by "decorating" the cylindrical elements[11] forming the solid. Consider, for example, a [111] direction cylinder whose axis is on a main diagonal of the unit cell. In[12] O^8, the point pairs $(\frac{1}{8},\frac{1}{8},\frac{1}{8})$ and $(\frac{5}{8},\frac{5}{8},\frac{5}{8})$ are distinct from $(\frac{3}{8},\frac{3}{8},\frac{3}{8})$ and $(\frac{7}{8},\frac{7}{8},\frac{7}{8})$. In centrosymmetric O_h^{10}, on the other hand, all four of those points are related by elements of the space group.[12] We therefore "decorate" this cylinder by making the segments $(0,0,0)$ to $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ and $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ to $(\frac{3}{4},\frac{3}{4},\frac{3}{4})$ one "color" and those between $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ to $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ and $(\frac{3}{4},\frac{3}{4},\frac{3}{4})$ to $(1,1,1)$ a different one. In practice, this reduces to forming a given cylinder by alternating two different materials and/or using different radii for the cylindrical segments in each of the two distinct regions. The O^8 space-group symmetry elements then uniquely fix the corresponding positional patterns of all the other cylinders.

To calculate the photon band structure, we used the standard method of linear combination of plane waves as adopted to the photon problem by Ho *et al.*[6] The relevant equations for the magnetic field vector $\mathbf{H}$ are

$$\sum_{\mathbf{G}'}\sum_{\lambda'=1,2} F^{\lambda,\lambda'}_{\mathbf{G},\mathbf{G}'} h_{\mathbf{G}',\lambda'} = \frac{\omega^2}{c^2} h_{\mathbf{G},\lambda}, \tag{1}$$

$$[F_{\mathbf{G},\mathbf{G}'}] = |\mathbf{K}+\mathbf{G}||\mathbf{K}+\mathbf{G}'|\epsilon^{-1}_{\mathbf{G},\mathbf{G}'} \begin{vmatrix} \hat{e}_1\cdot\hat{e}_{1'} & \hat{e}_1\cdot\hat{e}_{2'} \\ \hat{e}_2\cdot\hat{e}_{1'} & \hat{e}_2\cdot\hat{e}_{2'} \end{vmatrix}. \tag{2}$$

Here the $H_{\mathbf{G},\lambda}$ and $\hat{e}_\lambda$ are the Fourier components and basis vectors of the magnetic field

$$\mathbf{H}(\mathbf{r}) = \sum_{\mathbf{G}} \sum_{\lambda=1,2} h_{\mathbf{G},\lambda} \hat{\xi}_{\lambda} e^{i(\mathbf{K}+\mathbf{G})\cdot\mathbf{r}}, \quad (3)$$

where $\mathbf{G}$ are reciprocal lattice vectors, $\mathbf{K}$ is a vector in the first Brillouin zone, $\epsilon^{-1}_{\mathbf{G},\mathbf{G}'} = \epsilon^{-1}(\mathbf{G}-\mathbf{G}')$ are the Fourier components of the inverse dielectric constant $\epsilon^{-1}(\mathbf{r})$, and $\omega = \omega(\mathbf{K})$ is the frequency (i.e., energy) of the monochromatic electromagnetic plane wave. The solution now reduces to numerically diagonalizing the matrix $[F_{\mathbf{G},\mathbf{G}'}]$ for selected $\mathbf{K}$ values and determining, in particular, the low lying photon bands of the structure. The only input required is the position-dependent dielectric constant $\epsilon(\mathbf{r})$. Given the latter, the $\epsilon^{-1}_{\mathbf{G},\mathbf{G}'}$ are obtained by discretizing $\epsilon^{-1}(\mathbf{r})$ on an appropriate grid and Fourier transforming numerically.

In addition to considering a bcc structure, the other innovation in our work was to explore the possibility of forming the structure from metallic conductors as well as (or instead of) conventional dielectrics or semiconductors. This is particularly applicable to microwave frequencies where, as is well known, good conductors are essentially reflectors of electromagnetic radiation. In other words, since the skin depth is small compared with the thickness of the conductor (which is of the order of the radiation's wavelength), the high frequency spatial field configuration outside the conductor is analogous to that outside a superconductor in the presence of a magnetic field.[13] As far as electromagnetic propagation outside the metallic regions is concerned, this is formally equivalent to characterizing these regions of the structure by an effective dielectric constant much smaller than unity. This equivalence is easily understood when it is recognized that at an interface between regions with different dielectric properties, the electromagnetic field intensities are *strongest* in the region having the *higher* dielectric constant (see, e.g., Ref. 10). Therefore, fields incident upon a region having a dielectric constant much smaller than unity will be essentially *totally reflected* into neighboring regions having ϵ's of $O(1)$ or more, just as occurs when microwave radiation is incident upon a conducting region since such radiation's wavelength is much larger than the skin or penetration depth. This is the basis for the equivalence noted above. (At optical frequencies, the calculation of the field distribution when conductors are present is much more complex. The reason for this is that here the skin depth to wavelength ratio is not necessarily small. We shall not consider this spectral region here in the context of metallic materials.)

In the numerical calculations, the two alternating regions making up each of the cylinders and the interstitial region outside the cylinders were each characterized, in principle, by distinct dielectric constants. The results were not sensitive to the ϵ value chosen to model the metallic regions as long as it was less than 0.04. The results presented here were all obtained using 0.01 as the effective value. The cylinders were taken to be tightly packed—their radius was therefore $r_m = \sqrt{2}a/8 = 0.177a$ where a is the cubic unit cell edge dimension. Then $\epsilon^{-1}(\mathbf{r})$ was calculated on a net of 32^3 points and a fast Fourier transform package was used to obtain $\epsilon^{-1}(\mathbf{G})$. The matrix $[F_{\mathbf{G},\mathbf{G}'}]$ was calculated using up to 381 plane waves (i.e., matrix sizes of 762 × 762) and 221 points in the Brillouin zone and partially diagonalized to yield the ten lowest lying photon bands. Average CPU time for the largest matrices was 1.3 min per $\mathbf{K}$ value on an RS6000/320H workstation. By comparing results obtained with 141, 177, 249, and 381 plane waves and extrapolating, we concluded that the results obtained with the latter were converged to better than 1% for each of the different configurations studied. (Note that the convergence we are referring to relates to the ten lowest-lying bands only; the higher lying bands are certainly not converged nor are the field values very close to the interfaces between regions having very different dielectric properties. For both of the latter, many more plane waves would be required in order to obtain reliable results. However, it is the low-lying bands which are of interest to us here.)

Results obtained using only conventional (i.e., nonmetallic) materials are shown in Fig. 1(a). Here the alternating cylindrical segments were taken to be composed of materials[14] with $\epsilon = 25$ and $\epsilon = 1.1$, respectively, with the interstitial regions filled with a dielectric having $\epsilon = 3$. A photon band gap having a relative width of 12.5% was obtained. The minimum ϵ required for the high dielectric constant regions of the cylindrical elements in order to obtain a band gap was 10; for $\epsilon = 15$, the band gap was 8.2% when the interstitial region had $\epsilon = 4$. If, for the case of alternating cylindrical segments with $\epsilon = 25$ and $\epsilon = 1.1$, respectively, the interstitial regions are filled with material having $\epsilon = 5$ rather than $\epsilon = 3$, a band gap of 16.2% is reached.

In Fig. 1(b), we show results obtained using only metallic (i.e., conducting) cylinders. Here we took alternating segments with radii of r_m and $0.2r_m$, respectfully; a low-lying photon band gap with a relative width of 13.8% was obtained. Interestingly, a second band gap lying (counting from the bottom) between bands 6 and 7 was also found for this configuration. It had a relative gap width of 8.3%. This second band gap was particularly sensitive to the magnitude of the smaller cylinder radius. A similar calculation in which the latter was reduced to zero (i.e., the system was composed of appropriately located and oriented cylindrical "plugs") did not yield a secondary gap. This result is shown in Fig. 1(c), where the single band gap has a relative width of 23.4%.

The latter, in fact, was the largest photonic band gap we obtained. Alternating strong dielectric ($\epsilon = 25$) and conducting segments in compound cylinders of uniform radius r_m with $\epsilon = 1$ in the interstitial region give similar but not better results for the relative band gap [20.1%—see Fig. 1(d)].

The band gaps obtained by us for the O^8 bcc structure are of the same magnitude (about 20%) as those obtained using an fcc structure produced by drilling holes in a microfabricated semiconductor superlattice.[7,9,10] Indeed, these two structures are similar in one respect—they are both based upon using nonspherical "atoms." The bcc one differs in that it uses nonintersecting cylindrical units as building blocks. In addition, our results suggest that, at least at microwave frequencies, good conductors can be efficaciously used to obtain structures with large photonic

band gaps.

In Fig. 1, the frequencies are given in units of (c/a), where a is the dimension of the bcc unit cell. Since $d_m = 2r_m = \sqrt{2}a/4$, the center frequency of the photonic band gap is set by fixing the maximum diameter of the cylindrical units used to construct the structure. For example, using the metallic "plug" structure whose bands are shown in Fig. 1(c) and setting the center of the gap at a typical microwave frequency of 10 GHz, we find that cylindrical elements of diameter $d_m = 3.64$ mm and length 4.46 mm are required.

This diameter may be compared with the skin depth, which is given by[13]

$$\delta = \sqrt{(1/\pi f \sigma \mu_0)}. \quad (4)$$

Taking (for Cu) $\sigma = 5 \times 10^7$ mho/m and $\mu_0 = 4\pi \times 10^{-7}$ h/m, the skin depth at 10 GHz is $\delta = 0.7$ μm. Thus our basic requirement that $\delta \ll d_m$ is easily satisfied.

In summary, we have shown that photonic band gaps can be obtained by interlacing cylindrical elements into a bcc structure. To obtain these gaps, it is crucial that these elements be formed by alternating units of different dielectric properties and/or diameter in order to obtain a noncentrosymmetric O^8 structure. We also found, for the case of microwave frequencies, that particularly large band gaps can be obtained by utilizing high conductivity materials. We suggest that experimental tests of the predicted band gaps at these frequencies could confirm the feasibility of using bcc structures in practical applica-

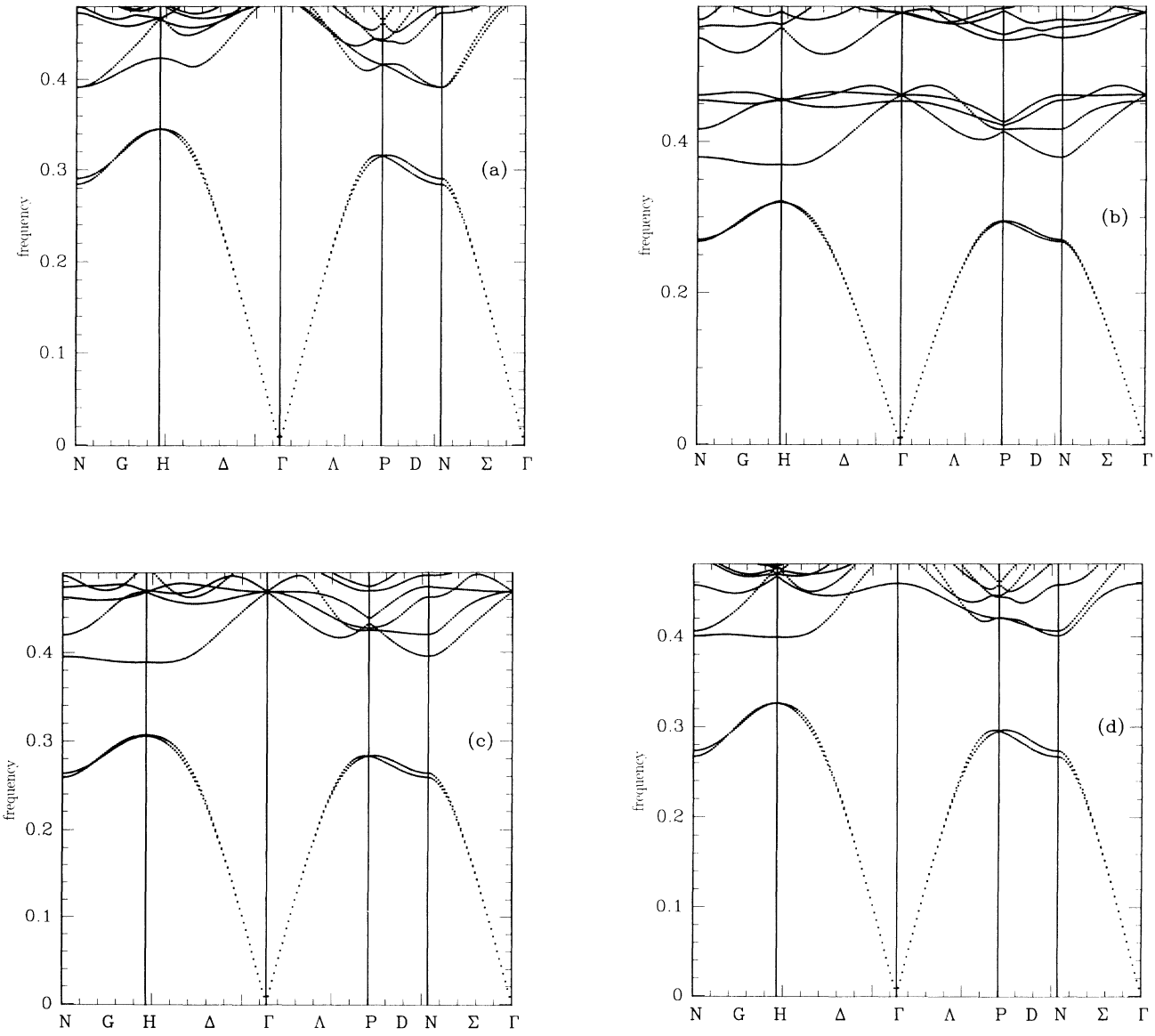

FIG. 1. Photon frequency bands in the O^8 body-centered-cubic structure. The frequency is given in units of (c/a), where c is the velocity of light and a is the cubic lattice dimension. The solid is constructed by interlacing cylindrical elements composed of (a) dielectric materials, (b) conducting materials, (c) short conducting segments, (d) alternating dielectric and conducting materials. See text for details.

tions. Among these are the integration of antennas and electronic components[10] and the fabrication of antennas operating at different microwave frequencies as a single multilayer unit.

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* Also with the Department of Physics, University of California at San Diego, La Jolla, CA 92093.

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