Photon band structures: The plane-wave method

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Using both the plane-wave and the Korringa-Kohn-Rostoker method, the photon band structure is calculated within the scalar wave approximation for a fcc lattice of dielectric microspheres embedded within a uniform host medium. The plane-wave method is found to converge fairly rapidly. The optimal volume-filling fraction of spheres for the creation of a gap in the photon density of states is found to vary substantially with the relative dielectric constant r, and this gap persists for r as small as 3.

There has been growing interest in studying photon band structures in three-dimensional periodic dielectric media that exhibit a gap in the photon density of states.[1-3] There are important motivations for such studies. (1) Since electromagnetic modes are totally absent within the band gap, spontaneous emission is therefore strongly suppressed. This ability to inhibit spontaneous emission has some extremely important consequences since spontaneous emission plays a fundamental role in limiting the performance of many optical and electronic devices such as semiconductor lasers, heterojunction bipolar transistors, and solar cells.[1,4] In atomic physics, this phenomenon has in fact been demonstrates.[5-7] (2) It has also been pointed out that the basic properties of many atomic, molecular, and excitonic systems can be profoundly modified in a volume of space, where the most important electromagnetic processes are totally absent.[8] (3) There is also a proposal to study mobility edges and Anderson localization of photons within a related pseudogap in the presence of some randomness.[2]

The first calculation of photonic bands exhibiting the presence of a common gap in the photon density of states was carried out recently[2] based on the scalar wave equation and using the Korringa-Kohn-Rostoker[9,10] (KKR) method. The structure consists of a fcc lattice of microspheres embedded in a host medium. The main results of that study were (1) the gap in the photon density of states persists down to a relative dielectric constant r of about 7.8, and (2) the optimal volume filling fraction f, for the creation of this gap, is about 11%. In this work, we report results that are based on the plane-wave method. Results based on the KKR method are also presented. We find that our plane-wave calculation converges fairly rapidly. This is an important finding since the plane-wave method is comparatively much simpler than the KKR method, the computer program is much easier to write, and runs substantially much faster. Moreover, unlike the KKR method, which is limited to "muffin-tin"-like modulation of the "potential," the plane-wave method can readily handle all sorts of modulations. This capability is especially important since we believe that, besides requiring a high dielectric contrast, the shape of the dielectric structure is also a very crucial factor in determining the photon band structure and the existence of a gap in the density of states.

Although some of our results are somewhat similar to those reported earlier, there are two significant discrepancies. First, our results show that the gap persists done to an r value of about 3. Second, we find that the optimal value of f depends significantly on the value of r, and in general decreases with increasing r.

Following the previous work,[2] we start with the scalar wave equation

$$-\nabla^2\psi+V\psi=k_b^2\psi\ , \tag{1}$$

where the "potential" V is given by

$$V=k_b^2\left[1-\frac{\epsilon}{\epsilon_b}\right]\ , \tag{2}$$

with $\epsilon=\epsilon_a$ inside the spheres, $\epsilon=\epsilon_b$ inside the host, and $k_b=\sqrt{\mu\epsilon_b}\omega/c$. Although the equation is of scalar form, and therefore neglects the vector nature of the photon, it retains an important characteristic in that the "potential" is proportional to ω^2, and thus vanishes in the long-wavelength limit. This has some very important physical consequences in the present problem as well as in the photon localization problem.[11]

The plane-wave method is very straightforward. We work in Fourier space, where the Fourier coefficients

$$c_{\mathbf{k}}=\int d\mathbf{r}\, e^{-i\mathbf{k}\cdot\mathbf{r}}\psi(\mathbf{r})\ , \tag{3}$$

and

$$V_{\mathbf{k}}=\frac{1}{\Omega}\int_{\text{cell}} d\mathbf{r}\, e^{-i\mathbf{K}\cdot\mathbf{r}}V(\mathbf{r})\ , \tag{4}$$

with $\mathbf{K}$ as a reciprocal-lattice vector of the fcc lattice, and Ω the volume of the unit cell. The scalar wave equation can then be expressed in the form

$$[k_b^2-|\mathbf{k}-\mathbf{K}|^2]c_{\mathbf{k}-\mathbf{K}}-k_b^2\sum_{K} U_{\mathbf{K}-\mathbf{K}'}c_{\mathbf{k}-\mathbf{K}'}=0\ , \tag{5}$$

where we have defined $U=V/k_b^2$. This eigenvalue equation can be recast into the standard form if we divide it by $k_b^2|\mathbf{k}-\mathbf{K}|$, let $d_{\mathbf{k}-\mathbf{K}}=|\mathbf{k}-\mathbf{K}|c_{\mathbf{k}-\mathbf{K}}$, and treat k_b^{-2} as the eigenvalue. The result is

$$\left[\frac{1-U_0}{|\mathbf{k}-\mathbf{K}|^2}-\frac{1}{k_b^2}\right]d_{\mathbf{k}-\mathbf{K}}-\frac{1}{\Gamma}\sum_{\mathbf{K}'}{}'\frac{U_{\mathbf{K}-\mathbf{K}'}}{|\mathbf{k}-\mathbf{K}'|}d_{\mathbf{k}-\mathbf{K}'}=0\ , \quad (6)$$

where the prime over the summation sign signifies that the $\mathbf{K}'=\mathbf{K}$ term is to be omitted. The photon band structure is then obtained by solving this equation for the eigenvalues k_b^{-2} 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 on the band structure based on the above plane-wave band equation. First, it is clear that the equation has exactly the same form as the corresponding equation for electrons, if we identify $(1-U_0)/|\mathbf{k}-\mathbf{K}|^2$ with the free-particle energy, k_b^{-2} as the exact energy eigenvalue, and $U_{\mathbf{K}-\mathbf{K}'}/(|\mathbf{k}-\mathbf{K}||\mathbf{k}-\mathbf{K}'|)$ as the corresponding Fourier element of the electron potential. Thus, in the empty-lattice limit, i.e., $V\to 0$, the band structure can be obtained from most solid-state textbooks. It is clear 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 $k_b=k$.

There are two important effects when the "potential" is turned on. First, depending on the symmetry of V, some of these degeneracies are lifted. Second, the levels shift up away from zero if U_0 is positive, and shift down toward zero otherwise. As a result, 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 $\mathbf{K}$ of the lattice, and the slope of the straight portion is no longer unity, but should be given by $(\epsilon_b/\epsilon_{\text{eff}})$, where ϵ_{eff} is the effective dielectric constant of the entire medium in the long-wavelength limit. The exact expression for ϵ_{eff} can be easily derived from the plane-wave band equation because at low frequencies and long wavelengths, where k_b^2 and k are both small compared with the smallest nonzero reciprocal-lattice vector, only the coefficient $d_{\mathbf{k}-\mathbf{K}}$ with $\mathbf{K}=0$ is non-negligible. Thus one can easily show that

$$\epsilon_{\text{eff}}=(1-U_0)\epsilon_b\ . \quad (7)$$

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

$$U_{\mathbf{K}}=3f(1-r)g(Ka)\ , \quad (8)$$

where the function $g(x)=(\sin x-x\cos x)/x^3$, a is the radius of the sphere, and $U_0=f(1-r)$. Using these results and the plane-wave equation, we have calculated the photon band structures for various values of f and r. We find that the results for the lowest-lying bands converge fairly rapidly. To within an accuracy of 0.1%, we find that 70 $\mathbf{K}$ points are sufficient for convergence even for r as large as 12. For r around 3, only 30 points are needed. This rapid convergence is reasonable because the "potential" here is very smooth near the lattice points, and does not have a highly attractive part as that found in the corresponding solid state's problem. The band structure is shown in Fig. 1 for $f=0.375$ and $r=12.25$. We have used reduced units, where k_b is measured in units of $2\pi/c_0$, and c_0 is the length of the conventional unit cube of the fcc lattice. We have also repeated the band-structure calculation using the KKR method. We find that it is necessary to include terms up to $l_{\max}=3$, especially for large r values. The KKR results are shown by the circles in Fig. 1, and are in excellent agreement with those obtained by the plane-wave method. In addition, we have checked that our results in the low-frequency and long-wavelength region are, within our numerical accuracy, in perfect agreement with our analytical prediction in Eq. (7).

From the figure, we see that there is a common indirect gap in the band structure. This gap is determined by the top of the "valence band" at the W point and the bottom

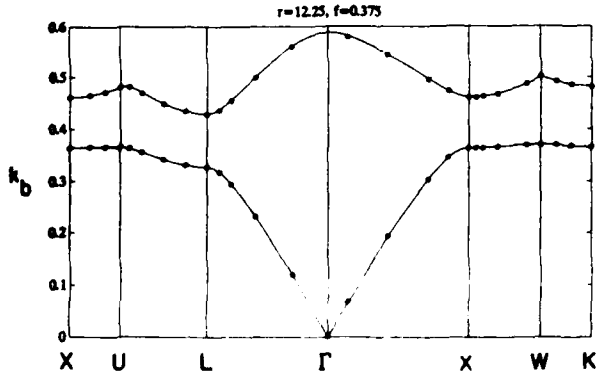

FIG. 1. The solid curves give the band structure calculated with the plane-wave method. The volume-filling fraction of spheres is 0.375 and the relative dielectric constant is 12.25. The solid circles are our results calculated with the KKR method.

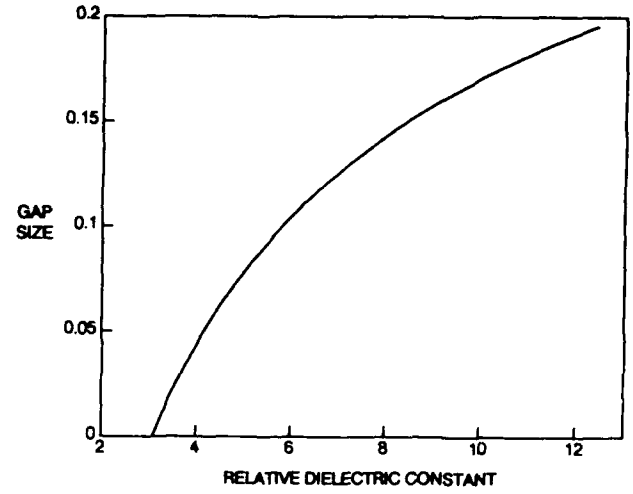

FIG. 2. The optimal volume-filling fraction of spheres for the creation of a gap in the photon density of states is plotted as a function of the relative dielectric constant.

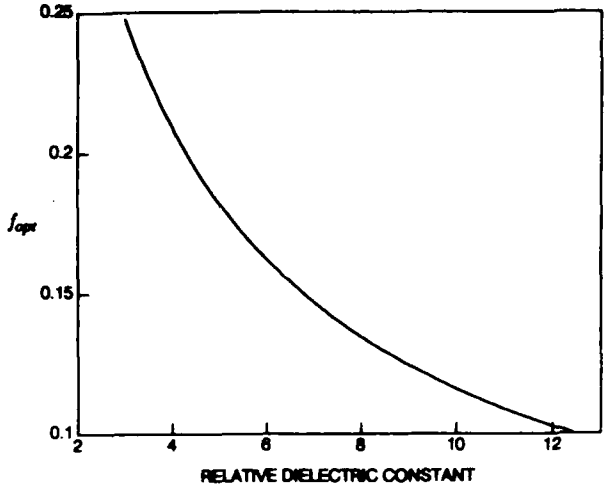

FIG. 3. The size of the gap at the optimal volume-filling fraction is shown as a function of the relative dielectric constant.

of the "conduction band" at the L point. According to our numerical results, this is true also for other values of f and r, as long as such a gap is finite. Note that in the empty-lattice limit, the lowest levels at the W point form a quadruplet, and are higher than those at the L point, which forms a doublet. Thus in order to have a gap, these levels must be splitted and shifted in such a way that the second level at L must be higher than the lowest level at W. We find that the gap persists down to an r value as small as 3, in contrast with the value of 7.8 reported by the earlier study.[2] Clearly at a fixed value of r, this gap do not exist if either f is too small or too large, because in either limit, the photon simply sees a uniform dielectric medium. But we find that for $r>3$, as f is increased from zero, the size of the gap first increases from negative to positive, and then it reaches a maximum. Further increases in f then decreases the gap size and eventually becomes negative again. Using the plane-wave method, the optimal value of f, f_{opt} is found, and the result is shown as a function of r in Fig. 2. At $r=3$, f_{opt} is 25% and it decreases with increasing r. For large r, we find that f_{opt} decreases as r^{-1}. For each r, the size of the gap at the optimal volume-filling fraction is calculated, and is found to increase monotonically with r, as shown in Fig. 3. This is clearly expected since the larger r is, the stronger is the scattering, and therefore the larger is the gap.

For the full vector wave, the degeneracy factor for all the levels is double that of the scalar case. Thus a much larger value of r is required to obtain a gap, and the lifting of the degeneracies due to the polarizations can become very important. Nevertheless, we can expect the plane-wave method to be also effective in the vector case.

Note added in proof. After submission of this work, we became aware of a recent publication with results very similar to those reported here. In that work, results were computed only with the plane-wave method. In addition, the transformation of the band equation into an eigenvalue problem was not used and thus a root searching method had to be used for the eigenvalues.

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