Electromagnetic Wave Propagation in Periodic Structures: Bloch Wave Solution of Maxwell's Equations

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We examine the propagation of electromagnetic waves in periodic dielectric structures by solving the vector Maxwell equations with the plane-wave method. Contrary to experimental reports as well as results of scalar-wave calculations, we do not find a true gap extending throughout the Brillouin zone in the fcc structure. However, there is a depletion in the photon density of states, seemingly a remnant of the Mie resonance, giving rise to a pseudogap in the spectrum which is quite strong for dielectric-sphere packing fraction $\beta \sim 0.3$–0.4. An effect analogous to the Borrmann effect in x-ray diffraction is predicted where certain photon modes will propagate an anomalously long distance before getting absorbed.

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The propagation of electromagnetic (EM) waves in a medium with a collection of scatterers is an old problem[1,2] having to do with such diverse subjects such as x-ray diffraction in crystals, the blue color of the sky, the theory of rainbows, light scattering from interstellar dusts, rainfall measurement using radar, etc. In the last four examples the scatterers are randomly distributed in the medium. Recently, there has been growing interest in EM wave propagation in man-made structures with a periodic array of scatterers of macroscopic dimensions. New stimulus for this has been provided by the experiments of Yablonovitch and Gmitter,[3] where the existence of photon bands in the fcc crystal of dielectric spheres has been demonstrated and the possibility of the existence of a band gap in the "photonic band structure" has been raised.

In the frequency range of the photonic gap the EM wave would not propagate through the medium but rather would decay exponentially. Such a structure could exhibit potentially new physical phenomena such as inhibition of electron-hole radiative recombination if the corresponding photon frequency falls in the gap region.[4] For an atom or molecule left in such a medium, John and Wang have recently suggested that the single-photon spontaneous emission is inhibited and a qualitatively new quantum electrodynamic bound state of the photon in the vicinity of the atom is formed.[5] Kurizki and Genack[6] have earlier shown that the dipole-dipole interaction between two atoms is also suppressed in such a situation. Another interesting phenomenon is the possibility of Anderson localization for the EM waves.[7-10]

So far, the photon bands in periodic structures have been examined theoretically only in the scalar-wave approximation where the vector nature of the EM field is neglected. This has been studied by several authors using the plane-wave (PW),[11,12] the Korringa-Kohn-Rostoker (KKR),[13] or the augmented-plane-wave[14] (APW) method with the general result that for the face-centered-cubic structure a gap appears in the entire Brillouin zone (BZ) if the dielectric-constant ratio between the spheres and the background exceeds a critical value of ~ 3 or so. However, the vector nature of the EM waves as shown here has important consequences.

Scattering of vector EM waves from a single sphere has been studied in great detail since the pioneering work of Mie.[15] We consider here the wave equation for the electric displacement vector $\mathbf{D}$ in a periodic structure with a space-dependent real dielectric constant $\varepsilon(\mathbf{r})$ and with the magnetic permeability μ being uniform throughout. The dielectric constant $\varepsilon(\mathbf{r})$ is periodic with the value ε_a inside the spheres and ε_b in the background. The corresponding refractive indices are denoted by n_a and n_b, respectively. From Maxwell's equations, we have the wave equation for $\mathbf{D}$:

$$-\nabla^2\mathbf{D} = (\omega^2/c^2)\mathbf{D} + \nabla\times\nabla\times[V(\mathbf{r})\mathbf{D}]\,, \quad (1)$$

where the "potential" $V(\mathbf{r})$ is given by

$$V(\mathbf{r}) = 1 - 1/\varepsilon(\mathbf{r}) \quad (2)$$

and c is the vacuum speed of light. It is sufficient to solve Eq. (1) for the displacement field $\mathbf{D}$, since once it is known, the other EM field vectors, viz., $\mathbf{E}$, $\mathbf{H}$, and $\mathbf{B}$, are uniquely determined. For a periodic dielectric structure $V(\mathbf{r})$ can be expanded in terms of its Fourier components $V(\mathbf{G})$, $\mathbf{G}$ being a reciprocal-lattice vector. The electric displacement $\mathbf{D}$ which satisfies Bloch's theorem can be expanded in terms of the plane waves:

$$\mathbf{D} = \sum_{\mathbf{G}} \mathbf{d}_{\mathbf{G}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}\,, \quad (3)$$

where $\mathbf{k}$ is the Bloch momentum. The zero divergence condition for $\mathbf{D}$, $\nabla\cdot\mathbf{D}=0$, applied to Eq. (3), implies that each component in the plane-wave expansion is orthogonal to the wave vector of the corresponding plane wave:

$$\mathbf{d}_{\mathbf{G}}\cdot(\mathbf{k}+\mathbf{G}) = 0\,. \quad (4)$$

Substituting Eq. (3) into Eq. (1) one obtains the equation for the expansion coefficients $\mathbf{d}_{\mathbf{G}}$:

$$H_{\mathbf{G}}\mathbf{d}_{\mathbf{G}} + \sum_{\mathbf{G}'} V(\mathbf{G}-\mathbf{G}')\{(\mathbf{k}+\mathbf{G})\cdot\mathbf{d}_{\mathbf{G}'}(\mathbf{k}+\mathbf{G}) - |\mathbf{k}+\mathbf{G}|^2\mathbf{d}_{\mathbf{G}'}\} = 0\,, \quad (5)$$

where

$$H_{\mathbf{G}} = |\mathbf{k}+\mathbf{G}|^2 - \omega^2/c^2\,. \quad (6)$$

In fact, this equation is familiar from the dynamical theory of x-ray diffraction[1,16] in crystals, where it is used to describe the Bragg scattering of x rays using two plane waves. Here we solve for the electric displacement field **D** using many plane waves in the expansion (3) to study the eigenmodes of the EM waves in the periodic dielectric structure. Expressing $\mathbf{d}_\mathbf{G}$ in terms of its Cartesian components, it follows from Eq. (5) that the following determinant must vanish:

$$\det[H_\mathbf{G}\delta_{\mathbf{G},\mathbf{G}'}\delta_{i,j}+V(\mathbf{G}'-\mathbf{G})\{(\mathbf{k}+\mathbf{G}')_i(\mathbf{k}+\mathbf{G}')_j - |\mathbf{k}+\mathbf{G}'|^2\delta_{i,j}\}]=0\,, \quad (7)$$

where $i=x$, y, or z. If we retain N plane waves in the expansion (3), then Eq. (7) is a $3N\times 3N$ determinant the solution of which provides us with $3N$ eigenmodes. However, since EM waves are transverse waves with two distinct helicity modes for each plane wave, we should have in total only $2N$ modes. This apparent discrepancy in the number of eigenmodes is explained by taking the dot product of Eq. (5) with the vector $\mathbf{k}+\mathbf{G}$ and observing that the orthogonality condition, Eq. (4), is satisfied only for those solutions ω for which $H_\mathbf{G}\equiv|\mathbf{k}+\mathbf{G}|^2-\omega^2/c^2\neq 0$. Thus the orthogonality condition must be explicitly checked in the solution of Eq. (7) to discard the N unphysical solutions, one per plane wave in the expansion. The remaining $2N$ solutions are the true eigensolutions.

Our numerical calculations were performed for the fcc lattice with the dielectric constants varied between ~ 1 and 36 and for a number of sphere packing fractions $\beta=\Omega_{\text{sphere}}/\Omega_{\text{cell}}$. The value of $\beta=0.74$ corresponds to close packing of spheres beyond which they overlap. Ω_{cell} is the unit-cell volume and $\Omega_{\text{sphere}}=(4\pi/3)R_s^3$ when the spheres of radius R_s are not overlapping. We examined the cases of both "air atoms" ($\varepsilon_a=1$ with ε_b varied) and dielectric spheres ($\varepsilon_b=1$ with ε_a varied). We retained typically ~ 300 plane waves in the expansion which results in an accuracy better than $<3\%$ or so in the lower-lying eigenmodes.

A typical photon band structure for the vector waves is shown in Fig. 1. The parameters correspond to the case where a true gap was reported experimentally.[3] In striking contrast with the experiment, we do not find a true gap existing throughout the BZ. However, the calculated effective refractive index n_{eff} shown in Fig. 2 agrees reasonably well with the measured value. This was calculated from the average value of the frequencies of the first four modes at the X point to directly compare with the experimentally reported values. As in the experiment[3] we found n_{eff} calculated this way to be extremely close to that calculated using the long-wavelength limit, viz.,

$$n_{\text{eff}}^{-1}=\lim_{k\to 0}\frac{1}{c}\frac{d\omega_k}{dk}\,.$$

The calculated width of the forbidden gap at the X and L points (Fig. 3) does not agree very well with the experimental data, indicating a necessity for repeating the experiments with improved accuracy. The calculated widths tend to zero in the limit $\beta\to 0$ or 1 as they should since these limits correspond to a uniform medium without scatterers.

For the entire range of ε_a and ε_b we did not find a true gap of significant magnitude in the fcc structure. This is in marked contrast to the scalar-wave result where for ratios of the two dielectric constants exceeding a critical value of ~ 3 a true gap was found.[11-14]

Even though a gap is absent throughout the BZ, in

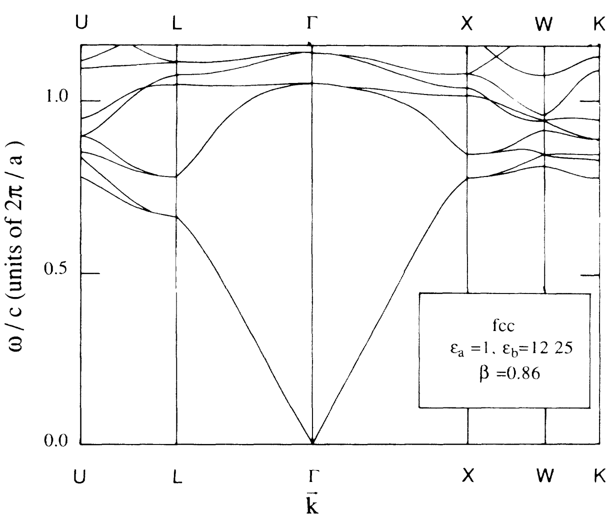

FIG. 1. Typical photon bands in the fcc structure. In the long-wavelength limit the dispersion is linear and the frequencies of the two helicity modes are nearly degenerate. There is no true photonic gap extending throughout the BZ. The basic features of the bands may be understood as perturbation of the free photon bands folded into the fcc BZ (Ref. 11).

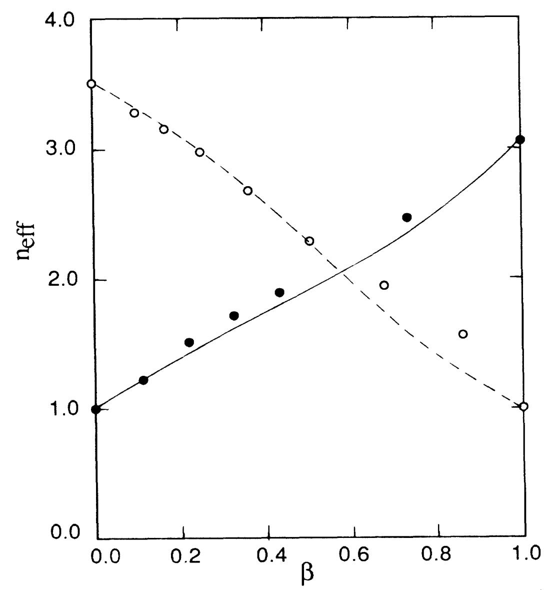

FIG. 2. The effective refractive index n_{eff} for the two dielectric structures: "air atoms" with $n_a=1.0$, $n_b=3.5$ (solid line), and dielectric spheres with $n_a=3.06$, $n_b=1.01$ (dashed line). Data points are experimental values from Ref. 3.

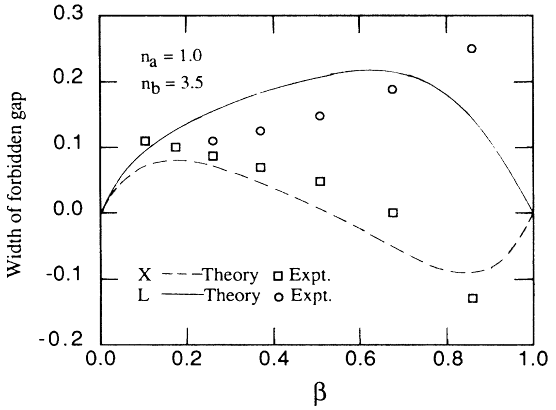

FIG. 3. Calculated width of the forbidden gap at the X and L points normalized to the center frequency at X as a function of sphere packing fraction β. Data points are from Ref. 3.

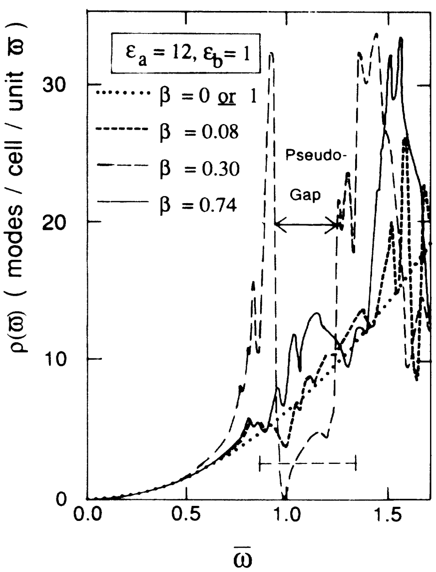

FIG. 4. The calculated DOS of the photon modes, $\rho(\bar{\omega})$, for $\varepsilon_a=12$, $\varepsilon_b=1$, and several values of packing fraction β. The dotted line corresponds to a uniform medium with the DOS varying as $\bar{\omega}^2$. A well-developed pseudogap, seemingly a remnant of the single-sphere Mie resonance, is seen for the sphere packing fraction $\beta=0.3$. The dashed horizontal line indicates the region of strong Mie scattering for this case.

certain situations there is a strong pseudogap present in the density of states for the photon modes. The density of states $\rho(\omega)$ is defined such that $\rho(\omega)d\omega$ is the number of photon modes including both helicities between the frequency ω and $\omega+d\omega$. It may be calculated by integrating over the irreducible BZ in a standard manner.[17] The density of states was calculated using the tetrahedron intgegration scheme[18] with 120 **k** points in the irreducible BZ and ~ 100 plane waves.

First, we note that for a homogeneous medium, the linear dispersion relation is linear, $\omega=\bar{c}k$, gives rise to an ω^2 dependence of the density of states (DOS):

$$\rho(\bar{\omega})=2\pi\bar{\omega}^2\,, \tag{8}$$

where the dimensionless quantity $\bar{\omega}$ is defined as $\bar{\omega}\equiv(2\pi/a)^{-1}\omega/\bar{c}$, where $\bar{c}$ is the speed of light, $\bar{c}\equiv c/n_{\text{eff}}$. Since the linear dispersion relation is followed in the long-wavelength limit, for sufficiently small values of ω the density of states has a similar ω^2 dependence.

Figure 4 shows the gradual evolution of a pseudogap in the DOS as the strength of the scatterers is varied by changing the sphere packing fraction β. Even though there is no true gap extending throughout the BZ we find that the depletion of the DOS can be very large. Unlike the corresponding scalar case where the magnitude of the gap is optimized for a packing fraction β of $\sim 10\%$–15%, we find in the vector case that the magnitude of the pseudogap is optimized generally for $\beta\sim 30\%$–40%. A true gap in the entire BZ, although absent for the fcc structure, could conceivably exist in other periodic structures.

The photon bands are the result of interplay between the coherent scattering due to the periodic structure and the scattering due to the individual spheres, the latter exhibiting characteristic Mie resonances for certain incident wavelengths.[2,15] A relevant question, therefore, is how much of the Mie resonance effect is retained in the photon bands. Clearly, if the spheres are too large, single-sphere scattering is expected to be a poor approximation for the periodic structures; on the other hand, for small spheres the scattering strength, which scales as πR_s^2, is small enough that any Mie resonance effect is likely to be blurred by the lattice effects. In fact, by definition, in the limit $\beta=0$ or 1, the Mie resonance effects would obviously be absent since in those limits we do not have any scatterers. For the case $\beta\sim 0.3$ shown in Fig. 4, the first three Mie resonances occur at $\bar{\omega}\approx 0.91$, 1.19, and 1.33 and the scattering coefficient is significantly large in the entire range of $\bar{\omega}$ between ~ 0.87 and 1.35. The position and width of the pseudogap compares well with the single-sphere Mie resonances as indicated in Fig. 4. This suggests that the pseudogap is a remnant of the single-sphere Mie resonances.

An interesting phenomenon associated with x-ray diffraction is the Borrmann absorption.[19] It occurs when the Bragg condition is nearly satisfied, with one of the doubly refracted rays avoiding the region of the atoms where photoelectric absorption takes place. Absorption is thereby minimized for this ray while the other ray behaves in just the opposite way.[20] Thus, the first ray propagates an anomalously longer distance than expected while the second one is absorbed anomalously faster.

A similar phenomenon is expected to occur for the periodic dielectric structures as well. This is illustrated in Fig. 5 where we plot the electric displacement vector **D** on the x-y plane for the modes belonging to the lowest two branches at the X point. Each branch consists of two helicity modes with nearly identical frequencies. For the lower two modes the magnitude of **D** inside the

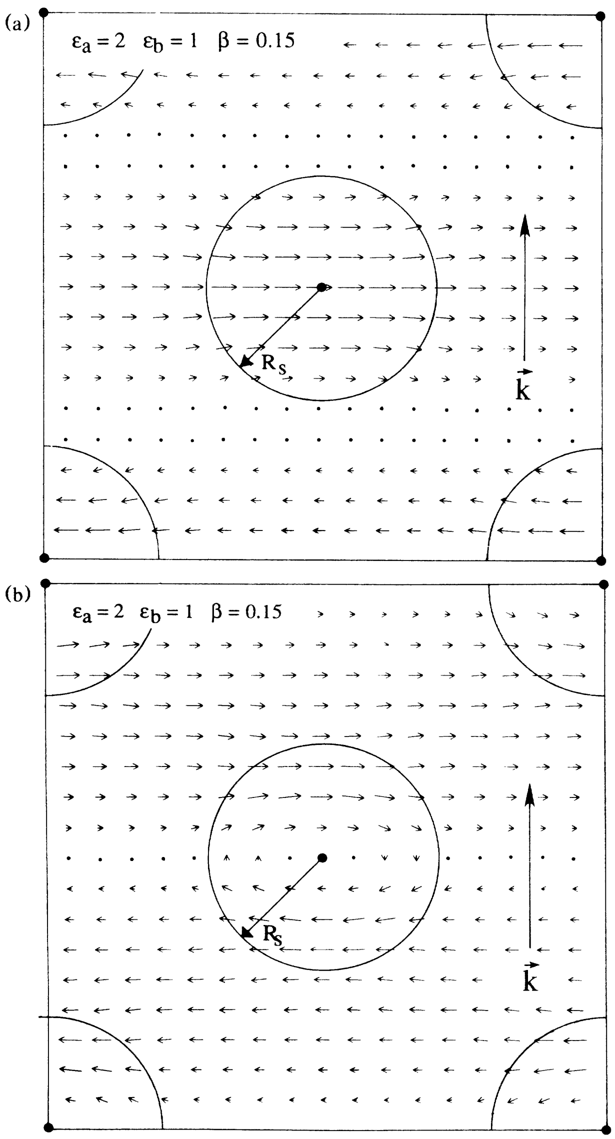

FIG. 5. Electric displacement vector **D** for the photon modes belonging to the lowest two branches at the *X* point. Each branch contains two modes which are close in frequency and in the nature of the **D** field and only one of these is shown for each branch: (a) lower branch and (b) higher branch. The plane of the plot is the (100) plane. Note that different modes have different magnitudes of **D** inside the spheres, leading to the possibility of Borrmann absorption.

dielectric spheres is larger compared to the magnitude in the background region while for the higher two modes it is the reverse. This implies that if the dielectric spheres were more absorbing compared to the background dielectric material, then the lower two modes would be absorbed much faster while the higher two modes would be absorbed much less. This is the analog of the Borrmann effect and should be observable in the periodic dielectric structures as well.

In conclusion, contrary to the reported experimental results, we do not find a true gap extending throughout the BZ for the fcc structure when the vector nature of the EM waves is taken into account. However, even though a true gap is absent, we find that for moderate values of the dielectric constants a pseudogap develops in the photon spectrum, the optimal value for which is in the range of $\beta \sim 30\%$–40%. We have also illustrated the existence of the Borrmann effect in the periodic dielectric structure.

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