Photonic band gaps in periodic dielectric structures: The scalar-wave approximation

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Using a plane-wave expansion method we have computed the band structure for a scalar wave propagating in periodic lattices of dielectric spheres (dielectric constant ϵ_a) in a uniform dielectric background (ϵ_b). All of the lattices studied (simple cubic, bcc, fcc, and diamond) do possess a full band gap. The optimal values of the filling ratio f of spheres and of the relative dielectric contrast for the existence of a gap are obtained. The minimum value of the relative dielectric contrast for creating a gap is also obtained. These results are applicable to the problem of classical-wave propagation in composite media and relevant to the problem of classical-wave localization.

I. INTRODUCTION

Recently, there has been growing interest[1,2] in the studies of the propagation of electromagnetic (EM) waves in three-dimensional (3D) periodic and/or disordered dielectric structures (photonic band structures). The reasons for this interest are both fundamental and practical. The possibility of the observation of Anderson localization of EM waves in disordered dielectric structures, where the strong *el-el* interaction effects entering the electron-localization problem are absent, is of fundamental interest.[1] Also in analogy to the case of electron waves propagating in a crystal, classical EM waves traveling in periodic dielectric structures will be described in terms of photonic bands with the possibility of the existence of frequency gaps where the propagation of EM waves is forbidden. The potential applications of such photonic band gaps are very interesting. It has been suggested[3] that the inhibition of spontaneous emission in such gaps can be utilized to substantially enhance the performance of semiconductor lasers and other quantum electronic devices. Photonic band-gap materials can also find applications in frequency-selective mirrors, bandpass filters and resonators. Moreover, electromagnetic interaction governs many properties of atoms, molecules and solids. The absence of EM modes inside the photonic gap can lead to unusual physical phenomena.[4–6] For example, atoms or molecules embedded in such a material can be locked in excited states if the photons to be emitted to release the excess energy have frequency within the forbidden gap. In addition, John[2] has proposed that Anderson localization of light near a photonic band gap might be achieved by weak disordering of a periodic arrangement of spheres.

It is therefore, very important to obtain structures with a frequency gap where the propagation of EM waves is forbidden for all wave vectors. Yablonovitch and Gmitter[7] have demonstrated the soundness of the basic idea of photonic bands in 3D periodic structures in an experiment using microwave frequencies, where the periodic structures can be fabricated by conventional machine tools. In addition, a photonic gap in a face-centered-cubic (fcc) dielectric structure was reported.[7] During the same period, theoretical studies of the propagation of EM waves in 3D periodic structures began.[8–16] At first, the photonic band structures have been examined theoretically in the scalar-wave approximation[8–12] in which the vector nature of the EM field is ignored. It soon became apparent[10–11] that not so many aspects of the experimental photon bands in periodic dielectric structures can be understood in terms of scattering of scalar waves. However, the scalar-wave approach is directly applicable to the scattering of acoustic waves, an area of equally active interest and to the localization of acoustic waves.[1,2,17] Recently, by expanding the EM fields with a plane-wave basis set, Maxwell's equations were solved exactly,[13–16] taking the vector nature of the EM field fully into account. Comparison of the calculated[13–15] results of the fcc structure with experiment[7] indicated that, while the experimental data and theory agree very well over most of the Brillouin zone, there are two symmetry points (W and U) where the experiment indicates a gap, while calculations show that propagating modes exist. It is now believed that the fcc structure does not possess a full photonic band gap in the lowest bands, instead there is a region of low density of states rather than a forbidden frequency gap.

We discovered a group of periodic dielectric structures[15] that possessed full photonic band gaps. This proposed structure is an arrangement of dielectric spheres in a diamond lattice structure. A systematic examination[15] of the photonic band structures for dielectric spheres and air spheres on a diamond lattice as a function of refractive index contrasts and filling ratios was made. It was found that photonic band gaps exist over a wide region of filling ratios for both dielectric and air spheres for refractive-index contrasts as low as 2. However, this diamond dielectric structure is not too easy to fabricate, especially in the micron or submicron length scales relevant for infrared and optical devices. We have also determined[18] new periodic dielectric structures, which can be regarded as a practical implementation of the diamond structure, that possess full photonic gaps, but at the same time are easier to fabricate. One of these structures, the "3-cylinder structure," which consists of three sets of cylinders drilled into a dielectric material at 35.26

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degrees off normal, has been fabricated[19] in the millimeter length scale and shown to possess full photonic gaps in the microwave region, in agreement with the predictions[18] of our theoretical calculations.

In spite of the extensive attention that the question of classical-wave localization had received recently,[1] there is no conclusive evidence yet that classical-wave localization is indeed possible in disordered systems characterized by a positive definite random dielectric function. In a recent paper, Soukoulis *et al.*[17] demonstrated numerically that classical-wave localization does take place in a lattice model. This numerical work, together with approximate calculations based on the coherent-potential approximation[17] (CPA) and the potential-well analogy[20] (PWA), provided for the first time strong evidence that classical-wave localization is possible in a composite system consisting of spheres of radius r_s and of dielectric constant ϵ_a embedded randomly into a medium of dielectric constant ϵ_b ($\epsilon_a > \epsilon_b$). Drake and Genack[21] reported measurements of the optical diffusion coefficient in a system of close-packed titania spheres strongly suggesting that the critical regime very close to localization has been reached for the first time. However, Albada *et al.*[22] have recently argued that the reported[21] exceptionally small diffusion constants can be attributed to small transport velocities rather than to small mean free paths.

Thus, the outstanding problem in classical-wave localization is to find the optimal conditions for its realization. The relevant parameters are the filling fraction f, the ratio of the two dielectric constant ϵ_a/ϵ_b and the frequency ω (in units $2\pi c/a\sqrt{\epsilon_b}$). The numerical results and the CPA-PWA treatment[17] show that the single sphere Mie resonances persist in strongly influencing the transport properties even for rather high values of f, which for the CPA-PWA approximate results can reach up to the close-packed limit. However, for the high-f regime, there is no way of systematically estimating the accuracy of the CPA-PWA results, since this high-f regime cannot be easily studied by the numerical technique of Ref. 17 or by any other numerical method. Therefore, there is a great need for an independent reliable way to check existing results[1] and also different theoretical methods,[1,23] in the area of classical-wave localization, within the scalar-wave approximation. We can very reliably calculate the bands and gaps if the dielectric spheres form a periodic lattice. It is very plausible that a connection between the gaps in a periodic system and the ranges of localized states in a random system exist. At least for weak disorder, and/or for high-f (approaching the close-packed limit), the regions of localized states practically coincide with the positions of the gaps. This is exactly the reason that John[2] has proposed that classical-wave localization might be achieved near a gap by weak disordering of a periodic arrangement of spheres. Finally, the photonic band structure within the scalar-wave approximation of periodic lattices of dielectric spheres in a uniform dielectric background is also directly applicable to the scattering of acoustic waves, an area of equal importance.

The purpose of this paper is to make a systematic study of the band structure for a scalar wave propagating in periodic lattices, such as the simple cubic, bcc, fcc, and diamond of dielectric spheres in uniform dielectric background. Both the cases of dielectric spheres and air spheres are examined. In all the cases we examined, the lattice constant a was kept constant and the radius r_s of the spheres was varied to change the filling fraction f. All of the lattices studied do possess photonic band gaps for both dielectric spheres and air spheres for reasonable values of the relative dielectric contrast. The optimal values of the filling ratio f and of the dielectric contrast for the creation of a gap are obtained. We find that when we fixed the dielectric contrast at 15, photonic band gaps exist over a wide range of filling ratios for both dielectric spheres and air spheres. For dielectric spheres for the lattices studied the largest gap occurs at $f \simeq 0.08$, while for the case of air spheres the largest gap occurs at $f \simeq 0.95$. The minimum value of the relative dielectric contrast for creating a gap is also obtained for all the lattices studied for both dielectric and air spheres. We find that photonic band gaps exist when the dielectric contrast exceeds four. The fcc lattice gives a gap when dielectric ratio exceeds three, for $f \simeq 0.08$.

In Sec. II, we describe the scalar-wave approximation and the plane-wave method. In Sec. III, we present and discuss the results and in Sec. IV, we summarize the conclusions of this work.

II. PHOTONIC BAND STRUCTURE IN THE SCALAR-WAVE APPROXIMATION

We consider the scattering of a scalar classical wave propagating in periodic lattices of dielectric spheres with dielectric constant ϵ_a and radius r_s in a uniform dielectric background of ϵ_b. The wave equation for a classical scalar wave of amplitude $E(\mathbf{r})$ and frequency ω propagating in such a dielectric medium can be described by the following equation,

$$\nabla^2 E(\mathbf{r}) + \frac{\omega^2}{c^2}\epsilon(\mathbf{r})E(\mathbf{r}) = 0 \tag{1a}$$

or

$$-\nabla^2 E(\mathbf{r}) + \frac{\omega^2}{c^2}\epsilon_b V(\mathbf{r})E(\mathbf{r}) = \frac{\omega^2}{c^2}\epsilon_b E(\mathbf{r}) , \tag{1b}$$

where the "effective potential" $V(r)$ in Eq. (1b) given

$$V(\mathbf{r}) = \left[1 - \frac{\epsilon(\mathbf{r})}{\epsilon_b}\right] , \tag{2}$$

with $\epsilon(\mathbf{r}) = \epsilon_a$ inside the spheres and $\epsilon(\mathbf{r}) = \epsilon_b$ inside the host and c is the vacuum speed of light. Although the equation is of scalar form, and therefore neglects the vector nature of the photon, it retains an important characteristic, which is that the effective potential is proportional to ω^2 and thus vanishes in the long-wavelength limit. This has some important physical consequences in the present problem as well as in the photon localization problem.[2] In addition, this scalar-wave approximation is usually applicable to the scattering of acoustic waves and also forms the basis of the diffraction theory of Kirchoff in optics.

The scalar-wave equation [Eq. (1)] was studied in connection with the photonic band-gap problem and the

classical-wave localization problem by a number of authors using a variety of band-structure methods such as the Korringa-Kohn-Rostoker method,[8] the augmented-plane-wave method,[9] and the plane-wave method.[10–12] It is by now well understood[13–16] that the scalar-wave equations, which neglect the coupling between the two polarization modes of the EM field, do not describe key features such as the existence of band gaps in the propagation of EM waves in periodic dielectric structures. For example, in the fcc structure the scalar-wave approximation predicts the existence of a photonic gap where no gap exists in the full vector wave equation. For the diamond lattice,[15] where the full vector wave equation gives a gap, the double degeneracy of the states along the W and X prohibits the opening of a gap in the scalar approximation. Thus, important symmetry information is lost when the vector nature of the EM field is neglected.

For a periodic arrangement of the spheres $V(\mathbf{r})$, and therefore, $\epsilon(\mathbf{r})$ can be expanded in terms of its Fourier coefficients $\epsilon_{\mathbf{G}}$, where $\mathbf{G}$ is the reciprocal-lattice vector.

$$\epsilon(\mathbf{r})=\sum_{\mathbf{G}} \epsilon_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} . \tag{3}$$

The wave function $E(\mathbf{r})$ follows the standard Bloch theorem and can be also expanded in terms of the plane waves

$$E(\mathbf{r})=\frac{1}{\sqrt{\Omega}} \sum_{\mathbf{G}} \psi_{\mathbf{G}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} , \tag{4}$$

where $\mathbf{k}$ is a wave vector in the Brillouin zone of the lattice. Ω denotes the normalization volume. The wave equation [Eq. (1a)] can be expressed as a matrix equation

$$[-T+(\omega^2/c^2)\epsilon]\psi=0 , \tag{5}$$

where

$$T_{GG'}=|\mathbf{k}+\mathbf{G}|^2\delta_{GG'}, \quad \epsilon_{GG'}=\frac{1}{\Omega}\int e^{-i(\mathbf{G}-\mathbf{G}')\cdot\mathbf{r}}\epsilon(\mathbf{r})d^3r .$$

Now for nonzero k, T is positive definite and we can rewrite the Eq. (5) as

$$(T^{-1/2}\epsilon T^{-1/2})\psi'=\frac{c^2}{\omega^2}\psi' , \tag{6}$$

with $\psi'=T^{1/2}\psi$. The problem then is transformed to an eigenvalue problem. The $k=0$ case can be easily treated by a simple subspace projection. Hence, the eigenvalues of the matrix $T^{-1/2}\epsilon T^{-1/2}$ will give the allowed photon modes at the wave vector. We note that in our method the structure of the dielectric crystal enters the calculation only through the position-dependent dielectric function $\epsilon(\mathbf{r})$, which is evaluated on a fine grid in the real-space unit cell and Fourier transformed into reciprocal space. Thus, our method is able to treat any periodic arrangements of objects with arbitrary shapes and filling ratios. We find that the results for the lowest ten bands converge fairly rapidly. 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 attractive atomic core potentials and are plane-wave-like outside the atomic re-

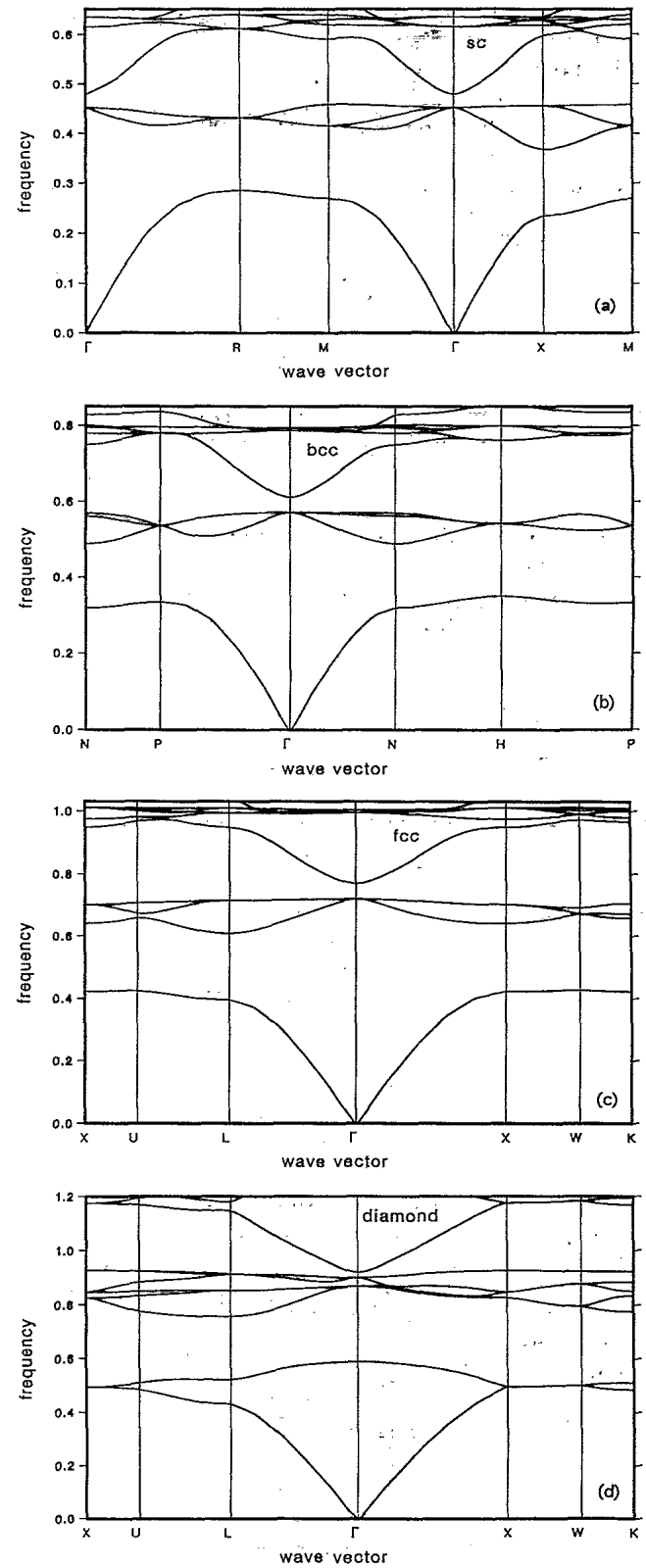

FIG. 1. Calculated photonic band structure along important symmetry lines in the Brillouin zone for (a) simple cubic, (b) bcc, (c) fcc, and (d) diamond dielectric structure composed of dielectric spheres of dielectric constant 15 in air background. The filling ratio of the dielectric material is 10%. The frequency ω is given in units of $2\pi c/a$, where a is the cubic lattice constant.

gions. Results reported in this paper were obtained with matrix sizes of the order of 750. Frequencies are converged to better than 1%.

Finally, we want to mention that the form of Eq. (6) is very useful in deriving analytically the dispersion relation ω vs k in the long-wavelength limit $k \to 0$. Using Eq. (6) within the second-order perturbation theory we obtain that

$$\frac{c^2}{\omega^2} = \frac{1}{k^2}\epsilon_{\rm av} + \sum_G \frac{|\epsilon(G)|^2}{G^2 \epsilon_{\rm av}} \tag{7a}$$

and

$$\frac{\omega}{c} = \frac{k}{\sqrt{\epsilon_{\rm av}}}\left[1 - \frac{k^2}{2\epsilon_{\rm av}^2}\sum_G \frac{|\epsilon(G)|^2}{G^2}\right], \tag{7b}$$

where $\epsilon_{\rm av}$ is the average value of the dielectric constant, i.e., $\epsilon_{\rm av} = f\epsilon_a + (1-f)\epsilon_b$. Our numerical results, discussed below, have verified Eq. (7b).

III. NUMERICAL RESULTS

We have made a systematic examination of the photonic band structures for dielectric spheres and air spheres on the simple cubic (sc), bcc, fcc, and diamond lattices as a function of the dielectric constant ratios and filling ratios. In all the cases we examined, the lattice constant a was kept constant and the radius r_s of the spheres was varied to change the filling fraction f. f is equal to $4\pi r_s^3/3\Omega_{\rm cell}$, where $\Omega_{\rm cell}$ is the unit-cell volume of the lattice under examination.

In Fig. 1, we show typical photon bands for the simple cubic, bcc, fcc, and diamond structure. The bands are shown along important symmetry lines in the Brillouin zone for the case of dielectric spheres with dielectric constant $\epsilon_a = 15$ in air background and sphere filling ratio $f = 0.10$. The frequency ω is given in units of $2\pi c\sqrt{\epsilon_b}/a$, where a is the cubic lattice constant for all the structures. Notice that within the scalar-wave approximation all these structures give a full band gap in which scalar waves are forbidden to propagate in any direction. For the diamond lattice there is a degeneracy at X and W and one has to open a gap to higher frequencies. Of course, in the long-wavelength limit $k \to 0$, we see the linear dispersion relation, $\omega = ck/\sqrt{\epsilon_{\rm av}}$, with the average dielectric constant given by $\epsilon_{\rm av} = f\epsilon_a + (1-f)\epsilon_b$. This linear dispersion relation[24] follows from Eq. (6) within the perturbation theory in the $k \to 0$ limit, as was shown briefly in Eq. (7).

We have made a systematic effort to obtain the optimal

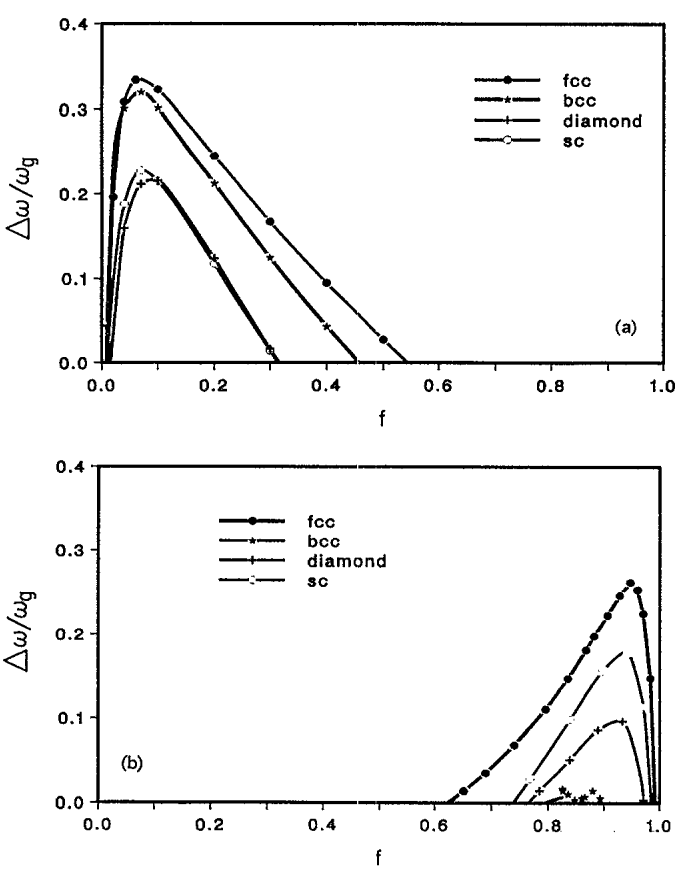

FIG. 2. Gap to midgap frequency ratio ($\Delta\omega/\omega_g$) as a function of the filling ratio for the case of (a) dielectric spheres in air and (b) air spheres in dielectric. The dielectric constant of the material is chosen to be 12.

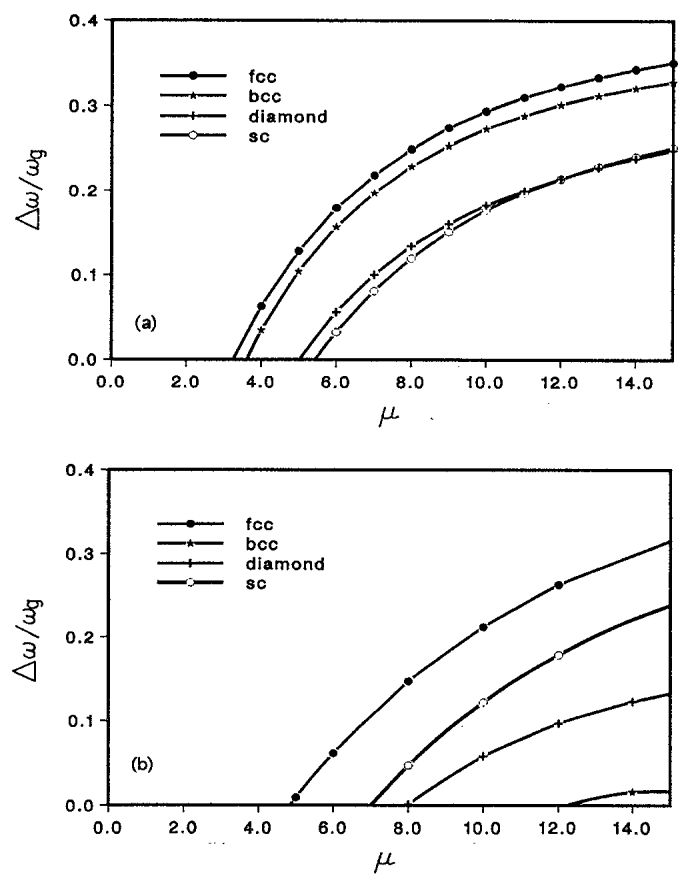

FIG. 3. Gap to midgap frequency ratio ($\Delta\omega/\omega_g$) as a function of the dielectric constant ratio for the case of (a) dielectric spheres in air and (b) air spheres in dielectric. The filling ratio f is 10% for the case of the dielectric spheres and 95% for the case of air spheres.

values of f and $\mu=\epsilon_a/\epsilon_b$ for the creation of a gap for all the four lattices. There is a wide range of filling ratios f and dielectric constant ratios that give a full band gap. For example, we find that when we fix the dielectric constant ratio at 12, band gaps exist over a wide region of filling ratios f for both dielectric spheres and air spheres. In Fig. 2, the calculated size of the forbidden gap normalized to the midgap frequency for both cases is given. For dielectric spheres [Fig. 2(a)] a maximum gap to midgap ratio ($\Delta\omega/\omega_g$) of 35% for the fcc and bcc lattice and of 25% for the simple cubic and diamond is found. In all the four lattices the optimum volume-filling fraction f is at around 0.08. At the optimum f of 0.08, the nearest-neighbor distance of the dielectric spheres with radius r_s

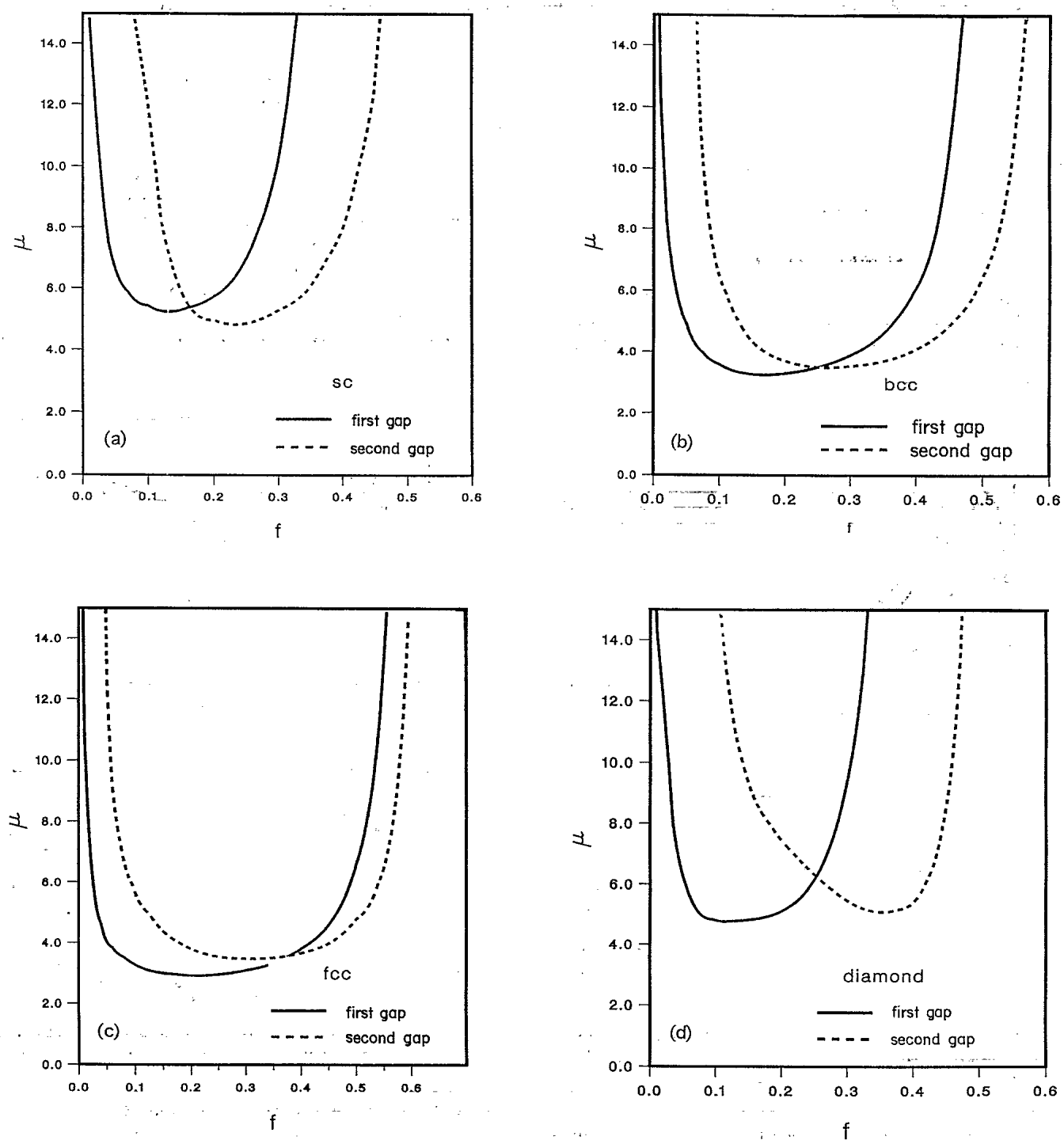

FIG. 4. The threshold value of the dielectric constant ratio $\mu=\epsilon_a/\epsilon_b$. A band gap just opened up is plotted as a function of the filling ratio f, for the (a) sc, (b) bcc, and (c) fcc, and (d) diamond lattice composed of dielectric spheres in air background.

is roughly four times the radius of the sphere. The wavelength λ corresponding to the midgap frequency ω_g at the optimum f is roughly equal to $12r_s$. Clearly at a fixed value of $\mu=\epsilon_a/\epsilon_b$, a gap does not exist if either f is too small or too large, because in either limit, the wave simply sees a uniform dielectric medium. For the case of air spheres [Fig. 2(b)], $\Delta\omega/\omega g$ can reach 18%, 1%, 29%, and 10% for the simple cubic, bcc, fcc, and diamond lattice, respectively. The optimum filling ratio f for all the four lattices of air spheres is rough equal to 95%. We do not understand the low value of $\Delta\omega/\omega_g$ for the bcc lattice.

Another interesting information that our detailed numerical results give is how easily a band gap can be formed. In particular, for a fixed value of f, what is the lowest dielectric constant that forms a gap? We plot in Fig. 3, $\Delta\omega/\omega_g$ as a function of the dielectric constant ratio μ for the sc, bcc, fcc, and diamond lattices. We keep $f=10\%$ for the case of dielectric spheres [Fig. 3(a)] and $f=95\%$ for air spheres in a dielectric background [Fig. 3(b)]. For the dielectric spheres, we find that the band gap persists down to a ratio ϵ_a/ϵ_b of 5, 4, 3, and 5 for the sc, bcc, fcc, and diamond lattice, respectively. For the case of air spheres in a uniform dielectric background the band gap persists down to a dielectric constant ratio of 7, 12, 5, and 8 for the sc, bcc, fcc, and diamond lattice, respectively. Such contrasts are easily accessible for acoustic waves with existing dielectric materials.

We observe [Fig. 3(a)] for the case of solid spheres, that for increasing contrasts $\Delta\omega/\omega_g$ saturates to different values of 25% or higher depending on the lattice under examination. For the fcc lattice the saturation value is close to 36%. For the case of air spheres, $\Delta\omega/\omega_g$ saturates to lower values than the solid spheres, but also the air spheres in a fcc arrangement give the highest saturation value of roughly 30%.

In a number of previous investigations,[1,9,17] it was suggested that the photon band gap obtained for the periodic structure is in fact the remnant of a Mie resonance obtained for a single sphere. In addition, there is an interconnection of the gaps in periodic systems and the range of localized states in random systems. At least for weak disorder, and/or for high f the region of localized states practically coincide with the position of the gaps. This is the reason of the proposal[1,2] that classical-wave localization near a gap can be achieved by weak disordering of a periodic arrangement of spheres.

We have calculated the dependence of the first two band gaps on ϵ_a/ϵ_b and f, for all the four lattices under examination. Comparing our present band-structure results for the band gaps with our previous CPA-PWA results for localized states, we find that indeed there is a connection between them. The CPA-PWA values of the optimum f are $f_{\rm opt}\simeq 0.20$, 0.30, and 0.35 with corresponding minimum values of $\mu\simeq 6.7$, 6.2, and 9 for the first three resonances. The band structure results (see Fig. 4) give $f_{\rm opt}\simeq 0.15$ and 0.30 with corresponding minimum values of $\mu=3$ and 4 for the first two gaps. Can the behavior of the band gaps be interpreted by the Mie resonant scattering from a single sphere? For a single sphere of dielectric constant ϵ_a in a dielectric background ϵ_b there are an infinite number of resonance frequencies ω, which are given as solutions of the equation

$$J_{l-1}\left[\frac{\omega}{c}\sqrt{\epsilon_a}r_s\right]=0 \quad (l\geq 1)$$

where J_l is spherical Bessel function corresponding to angular momentum l. For $l=0$, the Mie resonance frequencies are given by

$$\omega\sqrt{\epsilon_a}r_s/c=(2n+1)\pi/2 ,$$

where r_s is the radius of the sphere. Thus for each value of l, there are infinitely many values of Mie resonance frequencies. The explicit values of ω (in units of $c/r_s\sqrt{\epsilon_a}$) are the following: for s waves ($l=0$), $\omega=1.57$, 4.71, 7.85 for the first three resonances; for p waves ($l=1$), $\omega=3.14$, 6.28, 9.42; for d waves ($l=2$), $\omega=4.49$, 7.72, 10.90; and for f waves ($l=3$), $\omega=5.76$, 9.09, 12.32. These ω values are in close correspondence with the values of the frequencies that gaps appear in the periodic arrangement of dielectric spheres. This is clearly seen in Fig. 5 where we plot the midgap frequency for the first two gaps versus f, for all the lattices we have examined. As can be clearly seen from Fig. 4, there are no true gaps for very small and high values of f, for all the lattices studied, for $\mu=13$. Therefore, the values of midgap frequencies given in Fig. 5 for these f's, represent "pseudogaps", i.e., there is a drop in the density of states at this f. We have presented the midgap frequency as d/λ_a, where $d=2r_s$ is the diameter of the sphere and $\lambda_a=2\pi c/\omega\sqrt{\epsilon_a}$ is the wavelength inside the sphere. Notice that the resonances appear when the diameter of the spheres is about equal to half an integer the wavelength for the sphere material. Of course, this correspondence is exactly when $f\to 0$ and $\epsilon_a/\epsilon_b\to\infty$. As f increases, the values of the resonances not only shift, but they become broader and may even mix together. However, one can associate the band gaps in the periodic dielectric structures with the Mie resonance frequencies. Economou and Zdetsis[9] have checked this by omitting

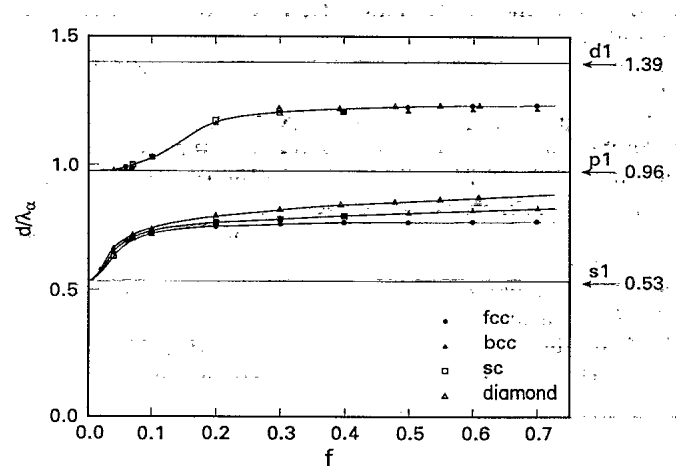

FIG. 5. The midgap frequency of the first two gaps vs f for the sc, bcc, fcc and diamond lattices composed of dielectric spheres of $\epsilon_a=13$ in air background. d is the diameter of the sphere and λ_a is the wavelength of the wave inside the sphere.

the corresponding partial wave in their augmented-plane-wave calculation. Indeed the corresponding gap disappears, providing enough support that the appearance of gaps is due to strong resonant scattering by each sphere. It must be also pointed out that numerical and the CPA-PWA treatment show[17] that the single-sphere Mie resonances persist even for rather high values of f, which for the CPA-PWA results[17] can reach up to the close-packed limit. It is rather surprising that the single-sphere scattering is the dominant factor in determining the band gaps and the range of localized states even for high values of f. A possible explanation[9,17] for this dominant role of the single-sphere scattering may be associated with its spherical symmetry. It is true, that the spherical scatterers, as opposed, e.g., to the cubic scatterers, cannot form new well connected shapes by clustering together. Thus, new cluster resonances cannot appear easily. It must be pointed out that it is the persistence of the dominant role of the single scatterer even for very high f that makes the CPA approach more reliable.

IV. CONCLUSIONS

In conclusion, we made a systematic study of the band structure for a classical wave propagating in a periodic arrangement of spheres of radius r_s and dielectric constant ϵ_a in a uniform dielectric background ϵ_b. All of the lattices studied (sc, bcc, fcc, and diamond) do possess a full band gap for an appreciable range of f and ϵ_a/ϵ_b values. The minimum value of the relative dielectric contrast for creating a gap is obtained and can be as low as 3. We have also argued that the positions of the band gaps in the periodic dielectric structures are closely related with the range of localized states in a random dielectric system, obtained by a weak disordering of a periodic arrangement of spheres, and are reminiscent of the Mie resonance of a single dielectric sphere.

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