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Photonic band gaps of three-dimensional face-centred cubic lattices

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Abstract. We show that the photonic analogue of the Korringa–Kohn–Rostoker method is a viable alternative to the plane-wave method for analysing the spectrum of electromagnetic waves in a three-dimensional periodic dielectric lattice. Firstly, in the case of a fcc lattice of homogeneous dielectric spheres, we reproduce the main feature of the spectrum obtained by the plane-wave method, namely that for a sufficiently high dielectric contrast a full gap opens in the spectrum between the eighth and ninth bands if the dielectric constant ε_s of the spheres is lower than the dielectric constant ε_b of the background medium. If $\varepsilon_s > \varepsilon_b$, no gap is found in the spectrum. The maximal value of the relative band-gap width approaches 14% in the close-packed case and decreases monotonically as the filling fraction decreases. The lowest dielectric contrast $\varepsilon_b/\varepsilon_s$ for which a full gap opens in the spectrum is determined to be 8.13. Eventually, in the case of a fcc lattice of coated spheres, we demonstrate that a suitable coating can enhance gap widths by as much as 50%.

1. Introduction

Under certain conditions, a gap can open in the spectrum of electromagnetic waves in a dielectric medium, independently of the direction of their propagation [1, 2]. Dielectric structures possessing such a photonic band gap are promising candidates for various technological applications [1]. Moreover, such structures offer a new laboratory for studying various atomic processes. Indeed, if a gap opens in the spectrum of electromagnetic waves, all parameters and characteristics of an atom placed in such a medium, such as the atomic radius and its spontaneous emission rates, are expected to change.

In order to open such a gap, one considers Maxwell's equations in a dielectric with a spatially periodic dielectric function, in full analogy to the Schrödinger equation with a periodic potential [1, 2]. In the latter case, the spectrum can be classified according to the Bloch momentum $\boldsymbol{k}$. The energy (frequency) levels ν_n are continuous functions of the Bloch momentum $\boldsymbol{k}$ in the (first) Brillouin zone. We say that there is a full gap, or simply a *gap*, between the nth and $(n+1)$th levels when $\nu_{n+1}(\boldsymbol{k}) > \nu_n(\boldsymbol{k}')$ for all $\boldsymbol{k}$ and $\boldsymbol{k}'$. We say that there is a *direct gap* between the nth and $(n+1)$th levels when $\nu_{n+1}(\boldsymbol{k}) > \nu_n(\boldsymbol{k})$ for all $\boldsymbol{k}$. For the Schrödinger equation in one space dimension, the number of gaps is in general infinite, and the only periodic potential which does not open any gap in the spectrum is a constant potential [3]. However, the situation changes dramatically for two and higher dimensions. One can prove

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rigorously that the number of gaps in the spectrum can only be finite, and, if the potential is not strong enough, no gap opens in the spectrum [4]. If electromagnetic waves are considered, opening a gap in the spectrum is even more difficult, and it took several years of intensive searching to achieve this experimentally for microwaves [5]. Note that Maxwell's equations enjoy scale invariance so, in principle, by scaling all of the sizes of a given structure, one can shift a gap theoretically to whatever frequency range is required.

So far, the plane-wave method [6–10] has been the main tool used for calculating the spectrum of electromagnetic waves in three-dimensional dielectric lattices. However, the plane-wave method is numerically rather unstable for a set-up used in experiments—namely, that in which the dielectric function is piecewise constant and changes discontinuously [5, 11, 12]. The main culprit as regards this behaviour is the Gibbs instability—the dielectric constant is poorly estimated near its spatial discontinuities by a truncated Fourier series, which oscillates wildly even if more than a thousand plane waves are retained (see, for example, figure 2 of [8]). Also, the plane-wave expansion becomes impractical if the dielectric constant exhibits a large imaginary part. Another approach used to calculate the spectrum of electromagnetic waves in three-dimensional dielectric lattices uses a discretization of Maxwell's equation inside the primitive cell of the lattice [14]. However, both methods are difficult to apply in the presence of impurities and to the calculation of Green's functions.

In order to obtain a universal method which can deal with the problems of the behaviour of electromagnetic waves in a periodic dielectric medium in their full complexity, we have developed and employed a photonic analogue of the first-principles on-shell multiple-scattering theory (MST) and of the Korringa–Kohn–Rostoker (KKR) method [15]. The unique feature of the on-shell MST is that, for nonoverlapping (muffin-tin) scatterers [17] (the present situation), it disentangles single-scattering and multiple-scattering effects (see [18] for a recent discussion). The KKR method [16] uses explicitly scattering matrices and Green's functions which are expanded in the basis of spherical harmonics, and the spectrum is determined by finding the zeros of a determinant. For electrons on a Bravais lattice and a muffin-tin potential, inclusion of spherical waves with angular momentum just up to $l_{max} = 2$ already gives for the lowest two bands a result within a few per cent of that from the exact calculation [16]. Expansion in the basis of spherical harmonics does not mean that scatterers have to be spherically symmetric. Indeed, scatterers of arbitrary shape are allowed; in such cases the scattering matrices are simply nondiagonal in the angular momentum indices [20]. The main advantage of the KKR method is that it gives directly the total Green's function from which the density of states (DOS) and the so-called local density of states can be easily extracted. The local DOS, which is proportional to the imaginary part of the total Green's function at the coinciding points in the coordinate space, is an important quantity which determines the decay of the excited states of atoms and molecules embedded in the lattice [19]. Also, the frequency dependence of the dielectric constant can be easily incorporated in the formalism.

The outline of our paper is as follows. In the following section, we show that the photonic KKR method is a viable alternative for calculating the photonic band structure by reproducing the main features of the spectrum obtained by the plane-wave method. The lowest dielectric contrast $\varepsilon_b/\varepsilon_s$ for which a full gap opens in the spectrum is found to be 8.13, which is slightly lower than the value 8.4 obtained by the plane-wave method [10]. In section 3 we discuss the case of coated spheres, i.e. spheres made out of several spherical shells with different dielectric constants. We demonstrate that even just a suitable single coating can enhance some of the gap widths by as much as 50%. Our conclusions are summarized in section 4.

2. The face-centred cubic lattice of dielectric spheres

In this section, we shall present the results of our numerical calculation for a face-centred cubic (fcc) lattice of dielectric spheres with a single sphere per lattice primitive cell. This case is very interesting from the experimental point of view, since such dielectric lattices form when silicon matrices, synthetic opals, and colloidal crystals are used [11–13]. Some of the structures were shown to exhibit the so-called *stop gap* (the gap in the spectrum for a fixed direction of the incident light) at optical frequencies [11, 12], and are the natural candidates to consider if one wishes to achieve a full photonic band gap [12].

At the same time, the case of a fcc lattice of dielectric spheres has been controversial since the first experimental results were published [21]. Results for a sample consisting of polycrystalline Al_2O_3 spheres, 6 mm in diameter, with a microwave refractive index of 3.06, in thermal-compression-moulded dielectric foam of refractive index 1.01 indicated the presence of a 'photonic band gap' in the microwave regime [21]. However, subsequent numerical calculations using the plane-wave method [6, 7] supported the claim that no gap opens in the spectrum and only a pseudo-gap (a sharp drop in the DOS) exists [6]. Nevertheless, two years later, using the plane-wave method, Sözüer, Haus, and Inguva [8] found a full gap for the fcc lattice of dielectric spheres between the eighth and ninth bands. The discrepancy between the results of [6, 7] and those of [8] follows from the fact that, unlike in the case of electrons, a gap for electromagnetic waves opens in an intermediate region, and the authors of [6, 7] stopped their calculation just beneath that region (see figure 1 in [6, 7]). Later, the results of Sözüer, Haus, and Inguva [8] were confirmed by two other groups using the plane-wave method [9, 10].

The latter deserves some discussion. In the case of electrons, the formation of bands results from the broadening of individual atomic levels when the atoms start to 'feel' each other's presence. The largest gap between atomic levels is that between the lowest-lying energy levels. Therefore, for a lattice of atoms, one expects to find a gap essentially between the first and the second energy band with the gap between higher bands scaling down to zero [3]. However, for electromagnetic waves a gap opens not between the lowest-lying bands but in an intermediate region. This phenomenon can be rather easily understood, since for a dielectric scatterer and Maxwell's equations, bound states are absent. They are replaced by resonances, and the above argument for locating the position of a band gap no longer holds. Moreover, if the wavelength is small compared to the size of the spheres, one can use geometric optics, while in the opposite limit of long wavelengths, the Rayleigh approximation applies. In neither case does a gap open in the spectrum. Therefore, if a gap is present in the spectrum, it should be in the intermediate region between the two limiting cases (see, however, the case of a diamond lattice (reference [7], figure 2), which is a complex lattice). The same is also expected to apply for the localization of light [2, 22].

2.1. Results

Sözüer, Haus, and Inguva [8] were well aware of the convergence problems of the plane-wave method, and they called for the recalculation and confirmation of their results by a more precise method. The latter is provided by the first part of our results. Using the photonic KKR method, we were able to confirm the plane-wave method result [8] that, in the case of air spheres and for a sufficiently high dielectric contrast,

- a full gap opens between the eighth and ninth bands, and
- a direct gap opens between the fifth and sixth bands.

If the dielectric constant of spheres is larger than that of a background medium, no gap opens in the spectrum. This situation is realized, for example, if dielectric spheres in air are considered.

We did not find any compelling explanation for this behaviour. In general, the higher the frequency, the higher the l_{max} that has to be adopted. Taking $l_{max} = 1$ is sufficient to account for the linear part of the band structure around the Γ point. The intermediate region requires then $l_{max} = 3$–5, and $l_{max} = 6$ is needed to ensure good convergence for the range considered.

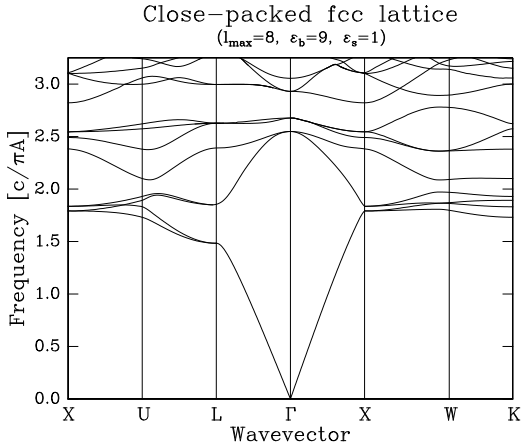

Figure 1. The photonic band structure for a close-packed fcc lattice of air spheres in a background dielectric medium with $\varepsilon_b = 9$ ($n_b = 3$). Frequency is plotted in dimensionless units; A is the lattice constant, c is the speed of light in the vacuum. Only a single gap with the central gap frequency $\nu = 2.796$ and the width $\Delta\nu = 0.044$ opens in the spectrum.

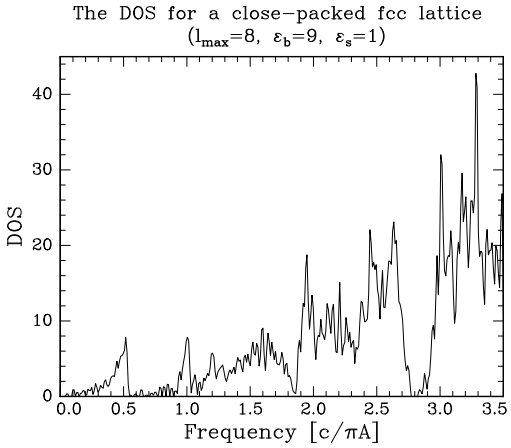

Figure 2. The DOS per primitive cell for a close-packed fcc lattice of air spheres in a background dielectric medium with $\varepsilon_b = 9$ ($n_b = 3$). Note the gap in the spectrum centred at $\nu = 2.796$.

In figures 1 and 2 we present our results for a three-dimensional close-packed fcc lattice of air spheres in a dielectric medium with the dielectric constant $\varepsilon_b = 9$. We choose this configuration for two reasons. First, it is sufficiently representative to show the presence of a full gap in the spectrum, and, secondly, the value of the background dielectric constant $\varepsilon_b = 9$ is close to that of rutile (TiO_2) at optical frequencies, which is used in experiments. Figure 1 shows the band structure. Frequency ν is plotted in scale-invariant units $c/\pi A$, where A is the

lattice constant† and c is the speed of light in the vacuum.

Only a single gap with a middle-of-gap frequency $\nu = 2.796$ and the width $\Delta\nu = 0.044$ opens in the spectrum in the range considered. The error is determined from the convergence properties of the KKR method. In the close-packed case, the lower gap boundary takes on its maximal value at the W point of the Brillouin zone, while the upper gap boundary takes on its minimal value at the X point, in agreement with the plane-wave calculations (see [24] for the classification of special points of three-dimensional lattices). In general, the photonic bands show much more branching than the electronic bands, and the actual classification of different bands can be quite involved. Group-theoretical classification of eigenmodes in three-dimensional photonic lattices is discussed in [25].

The presence of the gap in the $\varepsilon_b = 9, \varepsilon_s = 1$ case is also transparent from the calculation of the DOS per primitive unit cell. The latter was calculated using the Monkhorst–Pack integration scheme [26]. Integration over the Brillouin zone started from a mesh of $12 \times 12 \times 12$ uniformly spaced points, which was subsequently reduced to 182 points with weights calculated using the symmetries of the lattice. The resulting DOS per primitive cell is plotted in figure 2.

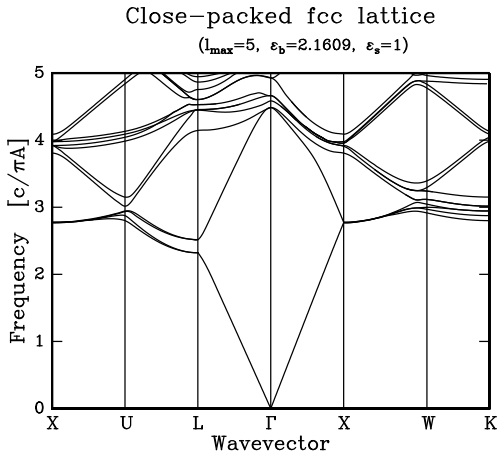

Figure 3. The photonic band structure for a close-packed fcc lattice of air spheres in a background dielectric medium with $\varepsilon_b = 2.1609$ ($n_b = 1.47$)—the experimental set-up reported in [11].

Figure 3 shows the band structure for a close-packed fcc lattice of air spheres in a dielectric medium with the dielectric constant $\varepsilon_b = 2.1609$ ($n_b = 1.47$). The latter case corresponds to the experimental set-up of [11] and is also close to that of [12]. Our calculation shows no gap in the spectrum. Only stop gaps are present. In agreement with the experimental observation, the most pronounced stop gap is seen between first bands at the L point of the Brillouin zone. For comparison with experiment, in table 1 we give the width $\Delta\nu_L$ of the stop gap at the L point and the effective refractive index n_{eff} for a close-packed fcc lattice of air spheres in background media with $n_b = 1.33, 1.37, 1.47$, and 1.6 used in recent experiments [11, 12], together with the results for the case with $n_b = 3$.

The effective refractive index n_{eff} is determined as the inverse of the slope of the band structure around the Γ point,

$$n_{eff}^{-1} = \lim_{k\to 0} \frac{1}{c}\frac{\mathrm{d}\omega}{\mathrm{d}k} \tag{1}$$

† Note that A is the side of the conventional unit cell of the cubic lattice, which has four times the volume of a primitive fcc unit cell, and not the lattice spacing [23].

Table 1. The width $\Delta\nu_L$ of the stop gap at the L point, effective refractive indices n_{eff} and n_{eff}^{MG}, and strength parameters ε_r and Ψ for a close-packed fcc lattice of air spheres in different background media.

	$n_b = 1.33$	$n_b = 1.37$	$n_b = 1.47$	$n_b = 1.6$	$n_b = 3$
$\Delta\nu_L$	0.145	0.159	0.195	0.236	0.368
n_{eff}	1.084	1.094	1.120	1.153	1.567
n_{eff}^{MG}	1.085	1.096	1.122	1.158	1.607
ε_r	0.281	0.313	0.391	0.487	1.140
Ψ	−0.376	−0.410	−0.485	−0.566	−0.935

where ω is the angular frequency. In the third row of table 1, we show the refractive index n_{eff}^{MG} calculated by using the Maxwell-Garnett formula [27],

$$n_{eff} = \left[\varepsilon_b\left(\frac{2\varepsilon_b + \varepsilon_s + 2f(\varepsilon_s - \varepsilon_b)}{2\varepsilon_b + \varepsilon_s - f(\varepsilon_s - \varepsilon_b)}\right)\right]^{1/2} \tag{2}$$

where f is the filling fraction ($f = 0.7405$ for a close-packed fcc lattice). In accordance with the plane-wave results [28] (see figure 2 there), n_{eff}^{MG} gives the upper bound on n_{eff}. For $\varepsilon_b < \varepsilon_s$ the situation is reversed, and n_{eff}^{MG} is expected to give the lower bound on n_{eff} [28]. For completeness, we also show the parameters

$$\varepsilon_r = \left[\frac{f\varepsilon_s^2 + (1-f)\varepsilon_b^2}{[f\varepsilon_s + (1-f)\varepsilon_b]^2} - 1\right]^{1/2} \tag{3}$$

introduced in [8], and

$$\Psi = 3f\frac{\varepsilon_s - \varepsilon_b}{\varepsilon_s + 2\varepsilon_b} \tag{4}$$

introduced in [12], which should characterize the scattering strength of a dielectric lattice.

From the experimental point of view, it is interesting to know what the threshold dielectric contrast $\varepsilon_{max}/\varepsilon_{min}$ is, where ε_{max} (ε_{min}) is the larger (smaller) of ε_s and ε_b, for which a full gap opens in the spectrum. Obviously, this threshold value changes with the radius of the spheres, and also depends on whether the dielectric constant of the spheres is larger or smaller than that of the background medium. Using the photonic KKR method, we scanned different configurations between the X and W points of the Brillouin zone. For close-packed air spheres, the lower and upper bounds of the full gap are set at the W and X points, respectively. For smaller filling fractions, at $f = 0.70$, and close to the threshold dielectric contrast, the gap width is already completely determined by the band structure at the W point. We determined the lowest threshold dielectric contrast $\varepsilon_b/\varepsilon_s$ for a fcc lattice of dielectric spheres to be 8.13 ($\varepsilon_r = 1.096$ and $\Psi = -0.918$ in this case). This can for example be realized for the case of close-packed air spheres in a background dielectric medium with the dielectric constant $\varepsilon_b = 8.13$. In all other cases—i.e., if the radius of the spheres is lowered—the threshold dielectric contrast is higher. The threshold dielectric contrast obtained by the photonic KKR method implies that the threshold refractive index contrast is 2.8506, which is significantly higher than the early theoretical estimates of 1.21 given by Yablonovitch [1] and 1.46 given by John [2]. On the other hand, the threshold dielectric contrast is slightly lower than the value 2.9 obtained by the plane-wave method [10].

A plot of the relative gap width, which is the gap width divided by the mid-gap frequency, as a function of the refractive index contrast is presented for different filling fractions in figure 4. The maximal value of the relative gap width approaches 14% in the close-packed case and

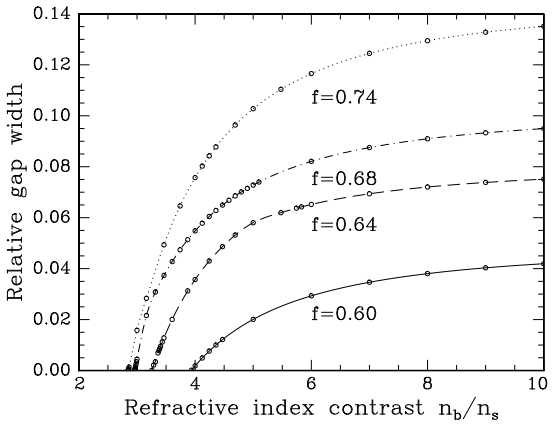

Figure 4. The relative band-gap width, which is the band-gap width divided by the mid-gap frequency, as a function of the refractive index contrast for different filling fractions f.

decreases monotonically as the filling fraction decreases. The relative gap width as a function of the refractive index contrast shows a rapid saturation. For example, in the close-packed case the relative gap width at 5.48 is already 80% of its maximal value.

3. The face-centred cubic lattice of coated spheres

After showing in the previous section that the photonic analogue of the KKR method is a viable alternative to the plane-wave method for calculating a photonic band structure, we shall proceed by investigating the case of coated spheres. A coated sphere is a sphere with the dielectric constant ε_1 and the radius r_1 embedded in a larger sphere with the dielectric constant ε_2 and the radius $r_2 > r_1$, which in turn can be embedded in a larger sphere, etc. Let ε_b be, as above, the background dielectric constant. Our interest in this system comes from the fact that there is an intensive experimental activity aimed at producing lattices of coated spheres by using them as basic particles in colloidal crystals. As in the previous section, due to its experimental relevance, we shall investigate only a simple fcc lattice (one scatterer per unit cell). It turns out that a coating alone does not help to create a full gap extending over the whole Brillouin zone as long as the fcc lattice remains a simple lattice. Nevertheless, following a suggestion made by A van Blaaderen, we shall show that a suitable coating of spheres forming a dielectric lattice can significantly enhance (by as much as 50%) some of the stop gaps. We looked mainly at the so-called lowest L-gap width (see [24] for the classification of special points of three-dimensional lattices), which corresponds to the (111) crystal direction (see [29] for a related theoretical discussion of the L gap). The reason for this is that experimental techniques make it possible for one to grow colloidal crystals such that the L direction corresponds to normal incidence on the crystal surface. Another reason is that recently [30], in the case of air spheres, a simple formula has been found for the L-gap width Δ_L of a fcc lattice. For the case of dense spheres such an explanation is lacking. There is hope that fcc lattices of coated spheres could provide some insight into the L-gap behaviour.

At first it seems that a coating will not have any significant effect on gap widths. One can arrive at this conclusion by looking at the effective dielectric constant ε^c_{eff} for a lattice of coated spheres. As we have seen in the previous section, the effective dielectric constant is a measure of the scattering strength of a dielectric lattice almost up to the first stop gap (the

Bragg reflection peak). Let us begin with the case of a coated sphere with a single coating, in which case we shall denote the dielectric constant and radius of the outer shell by ε and r_s, respectively. Defining $x = r_1^3/r_s^3$, and

$$\alpha_1 = \frac{\varepsilon_1 - \varepsilon}{\varepsilon_1 + 2\varepsilon} \qquad \alpha_0 = \frac{\varepsilon - \varepsilon_b}{\varepsilon + 2\varepsilon_b} \tag{5}$$

we have that the polarization factor α_c of a coated sphere with a single coating is

$$\alpha_c = \frac{\alpha_0 + x\alpha_1(\varepsilon_b + 2\varepsilon)/(\varepsilon + 2\varepsilon_b)}{1 + 2x\alpha_1\alpha_0}. \tag{6}$$

Here $0 \leqslant x \leqslant 1$ and $0 \leqslant \alpha_j < 1$. The Maxwell-Garnett formula [27] then gives

$$\varepsilon_{eff}^c \approx \varepsilon_b(1 + 2f\alpha_c)/(1 - f\alpha_c). \tag{7}$$

One can verify that for $x = 1$, i.e. if the radius of the interior sphere coincides with that of the entire sphere,

$$\alpha_c = \frac{\varepsilon_1 - \varepsilon_b}{\varepsilon_1 + 2\varepsilon_b}. \tag{8}$$

That is, one reproduces the polarization factor of a homogeneous sphere with the dielectric constant ε_1 in the host with the dielectric constant ε_b. The same result is also recovered in the special case where $\varepsilon_1 = \varepsilon$. In the limit $x \to 0$, i.e. if the radius of the interior sphere shrinks to zero, $\alpha_c \to \alpha_0$, which is the polarization factor of a homogeneous sphere with the dielectric constant ε in the host with the dielectric constant ε_b. It is important to realize that as a function of the parameter x, $\alpha_c(x)$ is a monotonic function continuously interpolating between α_0 and α_1. The latter follows from the fact that the first derivative $\mathrm{d}\alpha_c(x)/\mathrm{d}x$ has a constant sign determined by the sign of $\varepsilon - \varepsilon_b$. Since

$$\frac{\mathrm{d}\varepsilon_{eff}^c}{\mathrm{d}\alpha_c} = \frac{3f\varepsilon_b}{(1 - f\alpha_c)^2} > 0 \tag{9}$$

the effective dielectric constant ε_{eff}^c is also a monotonic function of x which smoothly interpolates between the two limiting cases of homogeneous spheres with the dielectric constants ε_1 and ε in the background with the dielectric constant ε_b. Therefore, for any x the effective dielectric constant ε_{eff}^c for a lattice of coated spheres is always smaller than the largest of the effective dielectric constants obtained for the two limiting cases for a lattice of homogeneous spheres. Using a transfer-matrix method to calculate the polarization factor α_c for a coated sphere with an arbitrary number of coatings, one can show that this restriction on the values of the effective dielectric constant ε_{eff}^c for a lattice of coated spheres holds also in the general case. Indeed, let us consider a coated sphere made out of N spherical shells with the dielectric constant ε_j, $j = 1, \ldots, N$. Then

$$\varepsilon_{eff}^c \leqslant \max_j\{\varepsilon_{eff}^j\} \tag{10}$$

where ε_{eff}^j is the effective dielectric constant of a lattice of homogeneous spheres with the dielectric constant ε_j in the background with the dielectric constant ε_b. Therefore, one would naively expect that a coating merely has the effect of interpolating between the limiting cases for homogeneous spheres.

Nevertheless, considerations based on the value of ε_{eff}^c can be deceptive. In figure 5 we show a plot of the relative L-gap width Δ_L for a close-packed fcc lattice of coated spheres as a function of r_1/r_s, the ratio of the interior and entire sphere radii. The solid curve corresponds to the case in which the refractive index of the core sphere is $n_1 = 2$ (ZnS) and that of the shell is $n = 1.45$ (silica). The dashed curve shows the opposite case, i.e., that for which

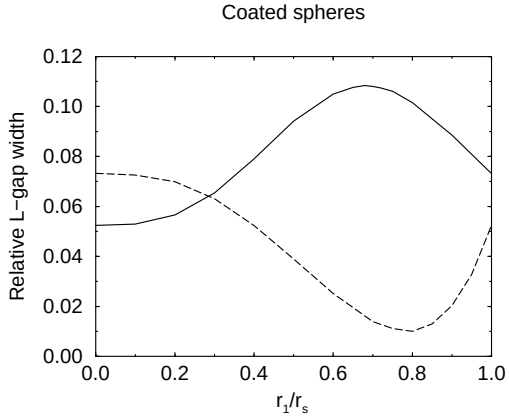

Figure 5. The relative L-gap width for a simple close-packed fcc lattice of coated spheres as a function of the ratio r_1/r_s of the interior and entire sphere radii. The solid curve corresponds to the case in which the refractive index of the core sphere is $n_1 = 2$ (ZnS) and that of the shell is $n = 1.45$ (silica). The dashed curve shows the opposite case, i.e., that for which $n_1 = 1.45$ and $n = 2$. Note that in the first case the relative L-gap width can be increased by as much as 50% if $r_1/r_s \approx 0.68$. The cases in which $r_1/r_s = 0$ and 1 correspond to the limiting cases for homogeneous spheres.

$n_1 = 1.45 < n = 2$. Obviously, the cases in which $r_1/r_s = 0$ and 1 correspond to the limits for homogeneous spheres. Let us denote by Δ_+ the larger relative L-gap width of the two limiting homogeneous spheres cases. Then in the first case ($n_1 > n$), at around $r_1/r_s \approx 0.68$ the relative L-gap width can be increased by as much as 50% with respect to Δ_+. In the second case ($n_1 < n$), the relative L-gap width remains smaller than Δ_+ for all values of r_1/r_s.

In the following, we test the Maxwell-Garnett formula (7) against the exact value of the effective dielectric constant ε^c_{eff} (refractive index $n_{eff} = \sqrt{(\varepsilon^c_{eff})}$) obtained directly from a band structure. In table 2 we collect together the effective refractive indices n_{eff} and n^{MG}_{eff} (the Maxwell-Garnett value) for those values of r_1/r_s which are near to the maximum and minimum of the relative L-gap width Δ_L (cf. figure 5). Here one expects the largest deviations of n^{MG}_{eff} from n_{eff}, because n^{MG}_{eff} is a monotonic function of r_1/r_s, and hence it does not have local minima and maxima.

Table 2. The effective refractive indices n_{eff} and n^{MG}_{eff} for a simple close-packed fcc lattice of coated spheres in air. The first three columns are for $n_1 = 2$ and $n = 1.45$; the last three columns are for the opposite case, in which $n_1 = 1.45$ and $n = 2$.

r_1/r_s	0.65	0.68	0.72	0.75	0.8	0.85
n_{eff}	1.419	1.434	1.444	1.540	1.507	1.469
n^{MG}_{eff}	1.414	1.428	1.438	1.525	1.494	1.460

It is interesting to note that n^{MG}_{eff} continues to approximate the exact value n_{eff} very well. Like in the case of homogeneous spheres in air [28], in the case of coated spheres in air the Maxwell-Garnett formula (7) slightly *underestimates* the exact value of the effective refractive index n_{eff} obtained from a band structure:

$$n^{MG}_{eff} < n_{eff}. \tag{11}$$

4. Conclusions

We have shown that the photonic KKR method is a viable alternative for calculating the photonic band structure, by reproducing the main features of the photonic band structure obtained by the plane-wave method for a simple three-dimensional fcc lattice of homogeneous spheres [8–10]. We confirmed that for a sufficiently high dielectric contrast a full gap opens between the eighth and ninth bands, a direct gap opens between the fifth and sixth bands, and no gap opens in the spectrum if $\varepsilon_b < \varepsilon_s$. To obtain a good convergence over the frequency range considered, it was sufficient to retain multipole fields with angular momenta up to $l_{max} = 6$. In general, the higher the frequency, the higher the value of l_{max} needed. In order to reproduce the first band and the linear part of the spectrum, $l_{max} = 1$ is enough. The size of the secular equation is reduced by almost a factor of 10 compared to that in the plane-wave method [6, 10], which customarily requires well above a thousand plane waves. The precision of the elements of the secular equation is determined by the standard Ewald summation [16] which yields structure constants [15] up to six digits.

For close-packed air spheres, the lower and upper bounds of the full gap are set at the W and X points, respectively. For filling fractions less than 0.7 and close to the threshold dielectric contrast for which a full gap opens in the spectrum, the gap width is completely determined at the W point. The lowest dielectric contrast $\delta = \varepsilon_b/\varepsilon_s$ for which a full gap opens in the spectrum is found to be 8.13, which occurs for a close-packed fcc lattice. This value is slightly lower than that of 8.4 obtained by the plane-wave method [10]. The maximal value of the relative gap width approaches 14% in the close-packed case and decreases monotonically as the filling fraction decreases. Readers interested in the role of Mie's resonances in the formation of a band structure could refer to [31].

The open question remains of what causes such a different behaviour of a lattice of dense spheres compared to that of a lattice of air spheres. It can be partially attributed to the fact that, for a lattice of spheres, it is the effective dielectric constant ε_{eff} rather than ε_b which describes the dielectric constant of the medium surrounding a given sphere. Therefore, the bare dielectric contrast δ is renormalized to $\delta_{eff} = \max(\varepsilon_s/\varepsilon_{eff}, \varepsilon_{eff}/\varepsilon_s)$, where $1 < \varepsilon_{eff} < \delta$ for $\varepsilon_s \neq \varepsilon_b$. Given the bare dielectric contrast δ, one finds that the renormalized dielectric contrast $\delta^d_{eff} = \varepsilon_s/\varepsilon_{eff}$ in the case of dense spheres is always smaller than the renormalized dielectric contrast $\delta^a_{eff} = \varepsilon_{eff}$ in the case of air spheres (see figure 6). The latter is easy to verify in the limit of very high bare dielectric contrast $\delta \to \infty$, where Maxwell-Garnett's formula (7) implies

$$\delta^d_{eff} \sim \delta(1-f)/(1+2f) < \delta^a_{eff} \sim \delta(1-f)/(1+f/2).$$

Nevertheless, a full understanding of the differences between the lattices of air and dense spheres still remains a theoretical challenge.

As in the case of homogeneous spheres in air, in the case of a simple fcc lattice of coated spheres in air no full gap opens in the spectrum. However, we have shown that even just a single coating can enhance the relative L-gap width Δ_L by as much as 50% with respect to Δ_+, the larger relative L-gap width of the two limiting cases for homogeneous spheres. This suggests the use of coated spheres to reduce the threshold dielectric contrast for which a full gap opens in the spectrum in the case of the so-called complex fcc lattice (having more than one scatterer in the primitive cell), which will be dealt with elsewhere. Note that in contrast to the case for a simple fcc lattice, in the latter case a full gap does open in the spectrum [10]. In general, Δ_L is not a monotonic function of the effective refractive index n_{eff}, and, for a single coating, shows one local maximum (minimum) as r_1/r_s is varied from zero to one (cf. figure 5).

It is interesting to note that the Maxwell-Garnett formula (7) provides a very good

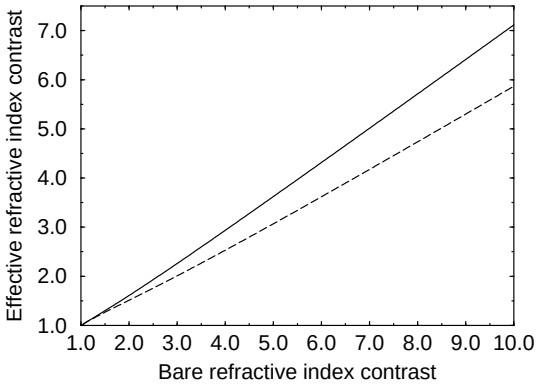

Figure 6. In a medium with a finite density of scattering spheres, such as that constituted by spheres on a lattice, the bare refractive index contrast gets renormalized. This may give a partial explanation for the fact that the band structures of fcc lattices of dense and air spheres show such different behaviours. This figure shows a typical behaviour of the effective refractive index contrast as a function of the bare refractive index contrast for air spheres in a dielectric (solid line) and dense dielectric spheres in air (dashed curve). Note that the latter is always smaller than the former. This plot was made for filling fraction $f = 0.4$. The Maxwell-Garnett formula overestimates ε_{eff} for the case of air spheres and underestimates ε_{eff} for the case of dielectric spheres in air. As a result, the exact curves are rotated slightly to the right with respect to the layout for the case in which the Maxwell-Garnett value is taken for ε_{eff}.

approximation to the exact value of the effective refractive index n_{eff} for coated spheres also. Like in the case of homogeneous spheres in air [28], in the case of coated spheres in air the Maxwell-Garnett formula [27] slightly *underestimates* the exact value of the effective refractive index n_{eff} obtained directly from a band structure. The Maxwell-Garnett formula holds well even beyond the limit $\omega r_s \ll 1$, r_s being the sphere radius for which it was originally derived. It describes n_{eff} well almost up to the lowest L gap, and can also be used to determine the mid-L-gap angular frequency ω_c [30]. In the case of coated spheres considered here (cf. figure 5), the ratio $n_{eff}\omega_c/k_L \in (0.973, 0.995)$, where k_L is the length of the Bloch vector corresponding to the L point.

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References

[1] Bykov V P 1975 *Sov. J. Quantum Electron.* **4** 861
Yablonovitch E 1987 *Phys. Rev. Lett.* **58** 2059
[2] John S 1987 *Phys. Rev. Lett.* **58** 2486

[3] Eastham M S P 1973 *The Spectral Theory of Periodic Differential Equations* (Edinburgh: Scottish Academy Press)
[4] Skriganov M M 1985 *Inventione Math.* **80** 107
[5] Yablonovitch E, Gmitter T J and Leung K M 1991 *Phys. Rev. Lett.* **67** 2295
[6] Leung K M and Liu Y F 1990 *Phys. Rev. Lett.* **65** 2646
Zhang Z and Satpathy S 1990 *Phys. Rev. Lett.* **65** 2650
[7] Ho K M, Chan C T and Soukoulis C M 1990 *Phys. Rev. Lett.* **65** 3152
[8] Sözüer H S, Haus J W and Inguva R 1992 *Phys. Rev.* B **45** 13 962
[9] Suzuki T and Yu P K 1995 *J. Opt. Soc. Am.* B **12** 804
[10] Biswas R, Sigalas M M, Subramania G and Ho K M 1998 *Phys. Rev.* B **57** 3701
[11] Astratov V N *et al* 1995 *Nuovo Cimento* D **17** 1349
Astratov V N *et al* 1996 *Phys. Lett.* A **222** 349
Vlasov Yu A, Astratov V N, Karimov O Z and Kaplyanski A A 1997 *Phys. Rev.* B **55** R13 357
[12] Vos W L, Sprik R, van Blaaderen A, Imhof A, Lagendijk A and Wegdam G H 1996 *Phys. Rev.* B **53** 16 231
Vos W L, Megens M, van Kats C M and Bösecke P 1996 *J. Phys. C: Solid State Phys.* **8** 9503
Wijnhoven J E J G and Vos W L 1998 *Science* **281** 802
[13] Tarhan I I and Watson G H 1997 *Phys. Rev. Lett.* **76** 315
[14] Pendry J B and MacKinnon A 1992 *Phys. Rev. Lett.* **69** 2772
[15] Moroz A 1995 *Phys. Rev.* B **51** 2068
Moroz A 1995 *Confined Electrons and Photons: New Physics and Applications* ed E Burstein and C Weisbuch (New York: Plenum) p 741
See also
Wang X, Zhang X-G, Yu Q and Harmon B N 1993 *Phys. Rev.* B **47** 4161
[16] Korringa J 1947 *Physica* **13** 392
Kohn W and Rostoker N 1954 *Phys. Rev.* **94** 1111
[17] Beeby J L 1964 *Proc. R. Soc.* A **279** 82
[18] Moroz A and Tip A 1997 *Phys. Lett.* A **235** 195
[19] Sprik R, van Tiggelen B A and Lagendijk A 1996 *Europhys. Lett.* **35** 265
Tip A 1997 *Phys. Rev.* A **56** 5022
Tip A 1998 *Phys. Rev.* A **56** 4818
[20] Faulkner J S 1979 *Phys. Rev.* B **19** 6186
[21] Yablonovitch E and Gmitter T J 1989 *Phys. Rev. Lett.* **63** 1950
[22] Wiersma D S, Bartolini P, Lagendijk A and Righini R 1997 *Nature* **390** 671
[23] Ashcroft N W and Mermin N D 1976 *Solid State Physics* (Philadelphia, PA: Saunders College) pp 73–5
[24] Koster G F 1957 *Space Groups and Their Representations (Solid State Physics vol 5)* ed F Seitz and D Turnbull (New York: Academic) p 173
[25] Ohtaka K and Tanabe Y 1996 *J. Phys. Soc. Japan* **65** 2670
Ohtaka K and Tanabe Y 1996 *J. Phys. Soc. Japan* **65** 3068
Sakoda K 1997 *Phys. Rev.* B **55** 15 345
[26] Monkhorst H J and Pack J D 1976 *Phys. Rev.* B **13** 5188
[27] Maxwell-Garnett J C 1904 *Phil. Trans. R. Soc.* **203** 385
[28] Datta S, Chan C T, Ho K M and Soukoulis C M 1993 *Phys. Rev.* B **48** 14 936
[29] Suzuki T and Yu P K 1995 *J. Opt. Soc. Am.* B **12** 583
Yannopapas V, Stefanou N and Modinos A 1997 *J. Phys.: Condens. Matter* **9** 10 261
[30] Moroz A 1999 *Phys. Rev.* B submitted
[31] Moroz A and Tip A 1999 *J. Phys.: Condens. Matter* submitted