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

Alexander Moroz\textsuperscript{1*} and Charles Sommers\textsuperscript{2†}

\textsuperscript{1} FOM-Instituut voor Atoom- en Moleculphysica, Kruislaan 407, 1098 SJ Amsterdam, The Netherlands
\textsuperscript{2} Laboratoire de Physique des Solides, Univ. Paris-Sud, Bâtiment 510, F-91405 Orsay Cedex, France

Abstract

We show that the photonic analogue of the Korringa-Kohn-Rostocker method is a viable alternative to the plane-wave method to analyze the spectrum of electromagnetic waves in a three-dimensional periodic dielectric lattice. Firstly, in the case of an fcc lattice of homogeneous dielectric spheres, we reproduce the main features 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 eights and ninth bands if the dielectric constant $\varepsilon_s$ of spheres is lower than the dielectric constant $\varepsilon_b$ 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 an fcc lattice of coated spheres, we demonstrate that a suitable coating can enhance gap widths by as much as 50\%.

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\textsuperscript{*}e-mail address : moroz@amolf.nl
\textsuperscript{†}e-mail address : root@classic.lps.u-psud.fr
1 Introduction

Under certain conditions, a gap can open in the spectrum of electromagnetic waves in a dielectric medium, independent 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 to study various atomic processes. Indeed, if a gap opens in the spectrum of electromagnetic waves, all parameters and characteristics of atom placed in such a medium, such as, for example, 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 $\mathbf{k}$. Energy (frequency) levels $\nu_n$ are continuous functions of the Bloch momentum $\mathbf{k}$ in the (first) Brillouin zone. We say that there is a full gap, or simply a gap between the $n$th and $(n+1)$th levels when $\nu_{n+1}(\mathbf{k}) > \nu_n(\mathbf{k}')$ for all $\mathbf{k}$ and $\mathbf{k}'$. We say that there is a direct gap between the $n$th and $(n+1)$th levels when $\nu_{n+1}(\mathbf{k}) > \nu_n(\mathbf{k})$ for all $\mathbf{k}$. 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 in two and higher dimensions. One can prove 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 [1]. If electromagnetic waves are considered, opening a gap in the spectrum is even more difficult and it took several years of intensive search to achieve it experimentally for microwaves [5]. Note that Maxwell’s equations enjoy scale invariance so that, in principle, by scaling all sizes of a given structure one can shift a gap theoretically to whatever frequency range.

So far, the plane-wave method [6, 7, 8, 9, 10] has been the main tool to calculate the spectrum of electromagnetic waves in three-dimensional dielectric lattices. However, the plane-wave method is numerically rather unstable for a setup considered in experiment, namely when the dielectric function is piece-wise constant and changes discontinuously [7, 11, 12]. The main culprit for this behaviour is the Gibbs instability - the dielectric constant is poorly estimated near its spatial discontinuities by a truncated Fourier series which wildly oscillates even if more than one thousand of plane waves is 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 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
In order to have an universal method which can deal with 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 principle on-shell multiple-scattering theory (MST) and of the Korringa-Kohn-Rostocker (KKR) method \cite{15}. The unique feature of the on-shell MST is that, for nonoverlapping (muffin-tin) scatterers \cite{17} (the present situation), it disentangles single-scattering and multiple-scattering effects (see \cite{18} for a recent discussion). The KKR method \cite{16} uses explicitly scattering matrices and Green’s function which are expanded in the basis of spherical harmonics and the spectrum is determined by zeroes of a determinant. For electrons on a Bravais lattice, inclusion of spherical waves with angular momentum up to $l_{\text{max}} = 2$ already gives result within a few per cent of the exact calculation \cite{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 which case scattering matrices are simply nondiagonal in the angular momentum indices \cite{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 decay of excited states of atoms and molecules embedded in the lattice \cite{19}. Also, the frequency dependence of the dielectric constant can be easily implemented 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 to calculate 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 and is slightly lower than 8.4 obtained by the plane-wave method \cite{11}. In Section 3 we discuss the case of coated spheres, i.e. spheres made out of several spherical shells with different dielectric constant. We demonstrate that already a suitable single coating can enhance some of the gap widths by as much as 50%. Our conclusions are summarized in Section 4.

## 2 Face-centered cubic lattice of dielectric spheres

In this section, we shall present the results of our numerical calculation for a face-centered 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 collodial crystals are used \cite{11,12,13}. Some of the structures were shown to exhibit the so-called
stop gap (gap in the spectrum at a fixed direction of the incident light) at optical frequencies \[11, 12\] and are the natural candidates to achieve a full photonic band gap \[12\].

At the same time, the case of fcc lattice of dielectric spheres has been controversial since the first experimental results were published \[21\]. Results for a sample consisting from polycrystalline \(Al_2O_3\) spheres, 6\(mm\) in diameter with a microwave refractive index of 3.06 in thermal-compression-molded 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 \[6, 7\] claimed 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, Söžüer, Haus, and Inguva \[8\] did find a full gap for the fcc lattice of dielectric spheres between the eights and ninth bands. The discrepancy between the results of \[6, 7\] and \[8\] follows from the fact that unlike to 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 Söžüer, 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 the presence of each other. The largest gap between atomic levels is 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 does not open 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 a gap opens 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 \(\mathbb{I}\), figure 2), which is a complex lattice). The very same is also expected to apply for the localization of light \[3, 22\].

### 2.1 Results

Söžüer, 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 constitutes 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 eights and ninth bands
- 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 frequency the higher \(l_{\text{max}}\) is to be taken. Taking \(l_{\text{max}} = 1\) is sufficient to account for the linear part of the band structure around the \(\Gamma\) point. The intermediate region requires then \(l_{\text{max}} = 3 \rightarrow 5\) and \(l_{\text{max}} = 6\) is needed to ensure good convergence in the range considered.

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 \(\nu\) is plotted in scale-invariant units \(c/\pi A\), where \(A\) is the lattice constant\(^1\) 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-Park 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 calculated weights using the symmetries of the lattice. The resulting DOS per primitive cell is plotted in figure \(2\).

\(^1\)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 \(3\).
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 setup 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 Tab. I we give the width $\Delta \nu_L$ of the stop gap at the $L$ point and the effective refractive index $n_{\text{eff}}$ for a close-packed fcc lattice of air spheres in background media with $n_b = 1.33, 1.37, 1.47, \text{ and } 1.6$ used in recent experiments [11, 12], together with the case $n_b = 3$ for which the band structure was calculated (see figure 1).

| TABLE I. The width $\Delta \nu_L$ of the stop gap at the $L$ point, effective refractive indices $n_{\text{eff}}$ and $n_{\text{eff}}^{\text{MG}}$, and strength parameters $\varepsilon_r$ and $\Psi$ for a close-packed fcc lattice of air spheres in different background media. |
|---|---|---|---|---|
| $n_b$ | $\Delta \nu_L$ | $n_{\text{eff}}$ | $n_{\text{eff}}^{\text{MG}}$ | $\varepsilon_r$ | $\Psi$ |
| 1.33 | 0.145 | 1.084 | 1.085 | 0.281 | -0.376 |
| 1.37 | 0.159 | 1.094 | 1.096 | 0.313 | -0.410 |
| 1.47 | 0.195 | 1.120 | 1.122 | 0.391 | -0.485 |
| 1.60 | 0.236 | 1.153 | 1.158 | 0.487 | -0.566 |
| 3.00 | 0.368 | 1.567 | 1.607 | 1.140 | -0.935 |

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

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

where $\omega$ is the angular frequency. In the third row of Tab. I, we show the refractive index $n_{\text{eff}}^{\text{MG}}$ calculated by the Maxwell-Garnett formula [27],

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

with $f = \frac{n_b}{n_b + 1}$. The effective refractive index $n_{\text{eff}}$ is determined as the inverse of the slope of the band structure around the $\Gamma$ point,
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), $n_{\text{eff}}^{\text{MG}}$ gives the upper bound on $n_{\text{eff}}$. For $\varepsilon_b < \varepsilon_s$ the situation is reversed and $n_{\text{eff}}^{\text{MG}}$ is expected to give the lower bound on $n_{\text{eff}}$ [28]. For completeness, we also show parameters

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

(3)
 introduced in [8], and

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

(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 is the threshold dielectric contrast $\varepsilon_{\text{max}}/\varepsilon_{\text{min}}$, where $\varepsilon_{\text{max}}$ ($\varepsilon_{\text{min}}$) is bigger (smaller) of the $\varepsilon_s$ and $\varepsilon_b$, for which a full gap opens in the spectrum. Obviously, this threshold value changes with the radius of spheres and also depends on whether the dielectric constant of spheres is larger or smaller than that of the background medium. The precise value of the threshold dielectric contrast has been out of reach of the plane-wave calculations [8]. 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, already at $f = 0.70$, and close to the threshold dielectric contrast, the gap width is completely determined by the band structure at the $W$ point. We determined the lowest threshold dielectric contrast $\varepsilon_b/\varepsilon_s$ for an 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 spheres is lowered, the threshold dielectric contrast is higher. The threshold dielectric contrast obtained by the photonic KKR method implies the threshold refractive index contrast 2.8506 which is significantly higher than the early theoretical estimate 1.21 by Yablonovitch [2] and 1.46 by John [3]. On the other hand, the threshold dielectric contrast is slightly lower than 2.9 obtained by the plane wave method [10].

The plot of the relative gap width, which is the gap width divided by the midgap frequency, as a function of the the refractive index contrast for different filling fractions is presented in figure 4. The maximal value of the relative gap width approaches 14% in the close-packed case and 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 Face-centered 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 to calculate a photonic band structure, we shall proceed by investigating the case of coated spheres. A coated sphere is a sphere with the dielectric constant \( \varepsilon_1 \) and the radius \( r_1 \) embedded in a larger sphere with the dielectric constant \( \varepsilon_2 \) and the radius \( r_2 > r_1 \), which in turn can be embedded in a larger sphere, etc. Let \( \varepsilon_b \) be, as above, the background dielectric constant. Our interest in this system comes from the fact that there is an intensive experimental activity to produce 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 full gap extending over all the Brillouin zone as long as an fcc lattice remains a simple lattice. Nevertheless, following a suggestion 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 is that experimental techniques make it possible to allow 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 \( \Delta_L \) of an fcc lattice. For the case of dense spheres such an understanding is missing. There is a 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 \( \varepsilon_{\text{eff}} \) 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 (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 \( \varepsilon \) and \( r_s \), respectively. Defining \( x = r_1^3/r_s^3 \),

\[
\alpha_1 = \frac{\varepsilon_1 - \varepsilon}{\varepsilon_1 + 2\varepsilon}, \quad \alpha_0 = \frac{\varepsilon - \varepsilon_b}{\varepsilon + 2\varepsilon_b}, \quad (5)
\]

the polarization factor \( \alpha_c \) of a coated sphere with a single coating is

\[
\alpha_c = \frac{\alpha_0 + x\alpha_1 (\varepsilon_b + 2\varepsilon)/(\varepsilon + 2\varepsilon_b)}{1 + 2x\alpha_1 \alpha_0}. \quad (6)
\]
Here $0 \leq x \leq 1$ and $0 \leq \alpha_j < 1$. The Maxwell-Garnett formula \([27]\) then gives

$$
\varepsilon_{\text{eff}}^c \approx \varepsilon_b \left(1 + 2 f \alpha_c \right) / \left(1 - f \alpha_c \right),
$$

(7)

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

$$
\alpha_c = \frac{\varepsilon_1 - \varepsilon_b}{\varepsilon_1 + 2 \varepsilon_b},
$$

(8)

i.e. one reproduces the polarization factor of a homogeneous sphere with the dielectric constant $\varepsilon_1$ in the host with the dielectric constant $\varepsilon_b$. The same result one also recovers in the special case $\varepsilon_1 = \varepsilon$. In the limit $x \to 0$, i.e. if the radius of the interior sphere shrinks to zero, $\alpha_c \to \alpha_0$, the polarization factor of a homogeneous sphere with the dielectric constant $\varepsilon$ in the host with the dielectric constant $\varepsilon_b$. It is important to realize that as a function of the parameter $x$, $\alpha_c(x)$ is a monotonic function continuously interpolating between $\alpha_0$ and $\alpha_1$. The latter follows from the fact that the first derivative of $d\alpha_c(x)/dx$ has a constant sign determined by the sign of $\varepsilon - \varepsilon_b$. Since

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

(9)

also the effective dielectric constant $\varepsilon_{\text{eff}}^c$ is a monotonic function of $x$ which smoothly interpolates between the two limiting cases of homogeneous spheres with the dielectric constants $\varepsilon_1$ and $\varepsilon$, respectively, in the background with the dielectric constant $\varepsilon_b$. Therefore, for any $x$ the effective dielectric constant $\varepsilon_{\text{eff}}^c$ for a lattice of coated spheres is always smaller than the largest of the effective dielectric constants obtained for the two limiting cases of a lattice of homogeneous spheres. Using a transfer matrix method to calculate the polarization factor $\alpha_c$ for a coated sphere with an arbitrary number of coatings, one can show that this restriction on the values of the effective dielectric constant $\varepsilon_{\text{eff}}^c$ 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 $\varepsilon_j$, $j = 1, \ldots, N$. Then

$$
\varepsilon_{\text{eff}}^c \leq \max_j \{\varepsilon_j\}
$$

(10)

where $\varepsilon_j$ is the effective dielectric constants of a lattice of homogeneous spheres with the dielectric constant $\varepsilon_j$ in the background $\varepsilon_b$. Therefore, one would naively expect that a coating has mere effect of interpolating between the limiting cases of homogeneous spheres.

Nevertheless, considerations based on the value of $\varepsilon_{\text{eff}}^c$ can be deceptive. In figure 5 we show a plot of the relative L-gap width $\Delta_L$ for a close-packed fcc lattice of coated spheres as a function of $r_1/r_s$, the ratio of the interior and whole sphere radii. The solid line corresponds to the case when the refractive
index of the core sphere is \( n_1 = 2 \) (ZnS) and that of the shell is \( n = 1.45 \) (silica). The dashed line shows the reversed case, i.e., \( n_1 = 1.45 < n = 2 \). Obviously, the cases \( r_1/r_s = 0 \) and 1 correspond to the limit of homogeneous spheres. Let us denote by \( \Delta_+ \) the larger relative L-gap width of the two limiting homogeneous spheres cases. Then in the first case \((n_1 > n)\) around \( r_1/r_s \approx 0.68 \) the relative L-gap width can be increased by as much as 50% with respect to \( \Delta_+ \). In the second case \((n_1 < n)\), the relative L-gap width remains smaller than \( \Delta_+ \) for all values of \( r_1/r_s \).

In the following, we tested the Maxwell-Garnett formula (7) against the exact value of the effective dielectric constant \( \varepsilon_{\text{eff}} \) (refractive index \( n_{\text{eff}} = \sqrt{\varepsilon_{\text{eff}}} \)) obtained directly from a band structure. In Table II we collected the effective refractive indices \( n_{\text{eff}} \) and \( n_{\text{eff}}^{MG} \) (the Maxwell-Garnett value) for those values of \( r_1/r_s \) which are nearby the maximum and minimum of the relative L-gap width \( \Delta_L \) (cf. figure 5). Here one expects the largest deviations of \( n_{\text{eff}}^{MG} \) from \( n_{\text{eff}} \) because \( n_{\text{eff}}^{MG} \) is a monotonic function of \( r_1/r_s \) and hence, it does not have local minima and maxima.

**TABLE II.** The effective refractive indices \( n_{\text{eff}} \) and \( n_{\text{eff}}^{MG} \) for a simple close-packed fcc lattice of coated spheres in air. First three columns are for \( n_1 = 2 \) and \( n = 1.45 \), the last three columns are for the reversed case \( n_1 = 1.45 \) and \( n = 2 \).

| \( r_1/r_s \) | 0.65 | 0.68 | 0.72 | 0.75 | 0.8 | 0.85 |
|--------------|------|------|------|------|-----|------|
| \( n_{\text{eff}} \) | 1.419 | 1.434 | 1.444 | 1.540 | 1.507 | 1.469 |
| \( n_{\text{eff}}^{MG} \) | 1.414 | 1.428 | 1.438 | 1.525 | 1.494 | 1.460 |

It is interesting to note that \( n_{\text{eff}}^{MG} \) continues to approximate the exact value \( n_{\text{eff}} \) very well. Similarly as for the case of homogeneous spheres in air [28], in the case of coated spheres in air the Maxwell-Garnett formula (8) slightly underestimates the exact value of the effective refractive index \( n_{\text{eff}} \) obtained from a band structure

\[
n_{\text{eff}}^{MG} < n_{\text{eff}}.
\] (11)

4 Conclusions

We showed that the photonic KKR method is a viable alternative to calculate 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, 9, 10]. We confirmed that for a sufficiently high dielectric contrast a full gap opens between the eights 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 in the frequency range considered, it was sufficient to retain multipole fields with the angular momentum up to $l_{\text{max}} = 6$. In general, the higher frequency the higher value of $l_{\text{max}}$ is needed. In order to reproduce the first band and the linear part of the spectrum, $l_{\text{max}} = 1$ is enough. The size of a secular equation is reduced by almost a factor 10 compared the plane-wave method [8-10] which customarily requires well above thousand plane waves. Precision of the elements of the secular equation is determined by the standard Ewald summation [16] which yields structure constants [15] up to 6 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 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. For readers interested in the role of Mie’s resonances in the formation of a band structure we refer to [31].

An open question remains what causes such a different behaviour of a lattice of dense spheres compared to that of air spheres. This can be partially attributed to the fact that, for a lattice of spheres, $\varepsilon_b$ no longer describes the dielectric constant of the surrounding medium, which is instead described by the effective dielectric constant $\varepsilon_{\text{eff}}$. Therefore, the bare dielectric contrast $\delta$ is renormalized to $\delta_{\text{eff}} = \max(\varepsilon_s/\varepsilon_{\text{eff}}, \varepsilon_{\text{eff}}/\varepsilon_s)$, where $1 < \varepsilon_{\text{eff}} < \delta$ for $\varepsilon_s \neq \varepsilon_b$. Given the bare dielectric contrast $\delta$, one finds that the renormalized dielectric contrast $\delta_{\text{eff}} = \varepsilon_s/\varepsilon_{\text{eff}}$ in the case of dense spheres is always smaller than the renormalized dielectric contrast $\delta_{\text{eff}} = \varepsilon_{\text{eff}}$ in the case of air spheres (see figure 3). 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

$$\delta_{\text{eff}}^d \sim \delta (1 - f)/(1 + 2f) < \delta_{\text{eff}}^a \sim \delta (1 - f)/(1 + f/2).$$

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

Such as in the case of homogeneous spheres in air, also in the case of a simple fcc lattice of coated spheres in air no full gap opens in the spectrum. However, we showed that already a single coating
can enhance the relative L-gap width $\triangle_L$ by as much as 50% with respect to $\triangle_+$, the larger relative L-gap width of the two limiting cases of 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 a simple fcc lattice, in the latter case a full gap does open in the spectrum [14]. In general, $\triangle_L$ 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 (3) provides a very good approximation to the exact value of the effective refractive index $n_{eff}$ also for coated spheres. Similarly to 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 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 L-midgap angular frequency $\omega_c$ [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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Figure 1: 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 centered at $\nu = 2.796$. 

The DOS for a close-packed fcc lattice
($l_{\text{max}}=8, \, \varepsilon_b=9, \, \varepsilon_a=1$)
Figure 3: Photonic band structure for a close-packed fcc lattice of air spheres in a background dielectric medium with $\varepsilon_b = 2.1609$ ($n_b = 1.47$) - experimental setup reported in [11].
Figure 4: Relative band-gap width, which is the band gap width divided by the midgap frequency, as a function of the refractive index contrast for different filling fractions $f$. 
Figure 5: The relative L-gap width for a simple closed packed fcc lattice of coated spheres as a function of the ratio $r_1/r_s$ of the interior and whole sphere radii. The solid line corresponds to the case when the refractive index of the core sphere is $n_1 = 2$ (ZnS) and that of the shell is $n = 1.45$ (silica). The dashed line shows the reversed case, i.e., $n_1 = 1.45$ 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 $r_1/r_s = 0$ and 1 correspond to the limiting case of homogeneous spheres.
Figure 6: In a medium with finite density of scattering spheres, such as for spheres on a lattice, the bare refractive index contrast gets renormalized. This may give a partial explanation of the fact why the band structure of an fcc lattice of the dense and air spheres shows such a different behaviour. 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 line). Note that the latter is always smaller than the former. This plot was made for filling fraction $f = 0.4$. The Maxwell-Garnett overestimates $\varepsilon_{\text{eff}}$ for the case of air spheres and underestimates $\varepsilon_{\text{eff}}$ for the case of dielectric spheres in air. As the result, the exact curves are rotated slightly to the right with respect to the case when the Maxwell-Garnett value is taken for $\varepsilon_{\text{eff}}$. 