Photonic bandgap optimization in inverted fcc photonic crystals

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We present results of photonic band-structure calculations for inverted photonic crystal structures. We consider a structure of air spheres in a dielectric background, arranged in an fcc lattice, with a cylindrical tunnel connecting each pair of neighboring spheres. We derive (semi)analytical expressions for the Fourier coefficients of the dielectric susceptibility, which are used as input in a standard plane-wave expansion method. We optimize the width of the photonic bandgap by applying a gradient search method and varying two geometrical parameters in the system: the ratios $R/a$ and $R_c/R$, where $a$ is the lattice constant, $R$ is the sphere radius, and $R_c$ is the cylinder radius. It follows from our calculations that the maximal gap width in this type of photonic-crystal structure with air spheres and cylinders in silicon is $\Delta \omega/\omega_0 = 9.59\%$. © 2000 Optical Society of America


1. INTRODUCTION

The effect that photonic crystals, i.e., materials with a spatially periodic dielectric function $\varepsilon(\mathbf{r})$, have on the propagation of electromagnetic radiation has been studied intensively over the past few decades. The dispersion relation $\omega(k)$ of these crystals is described by the photonic band structure, which consists of different photonic bands with gaps between them at the boundary of the Brillouin zone. The photonic bandgap is characterized by its central frequency $\omega_o$ and its spectral width $\Delta \omega$ and generally depends on the direction of wave propagation. It is well known that, for sufficient dielectric contrast, fcc photonic crystals may develop a full photonic bandgap, which overlaps the entire surface of the Brillouin zone, between the eighth and ninth bands of the band structure. Besides, a pseudogap develops between the fifth and sixth bands, which overlaps completely only a part of the Brillouin-zone surface.

One of the main motivations to produce dielectric structures that possess large photonic bandgaps is the desire to be able to control (i.e., to suppress or, in some cases, to enhance) the spontaneous emission of radiation from atoms. Other possibilities for practical applications of these photonic crystals include the realization of low-threshold lasers, high-quality resonant cavities, perfectly reflecting mirrors, and substrates for antennas.

In artificial photonic crystals, such as those created by Yablonovitch et al. and by Özbay et al., a complete photonic bandgap has been found for frequencies in the microwave regime. Until now, the smallest length scale at which artificial photonic crystals have been realized was of the order of the wavelength of infrared light. Much effort is taken nowadays to develop photonic crystals that have a complete photonic bandgap for frequencies of visible light.

A new type of photonic crystal is the inverted fcc crystal, which consists of a regular structure of spherical air holes in a dielectric medium. Such structures, with lattice constants of the order of several hundreds of nanometers, may be created by infiltration of dielectric material into the empty voids in fcc crystals that consist of colloidal spheres. The photonic properties of structures thus created have been studied by several groups of researchers. One obtains an inverted crystal if the original colloidal material is etched away after the infiltration process. Such crystals hold great promise for having complete bandgaps in the visible range.

Usually, the original colloidal crystal is closely packed (volume filling of 74%), so one would expect a closely packed inverted air-sphere crystal as final result. This does not happen, however, because during thermal annealing (sintering) of the colloidal crystal the colloidal particles become firmly attached, so the filling fraction increases above 74%. This effect may be modeled as the formation of cylindrical tunnels that connect neighboring spheres. In this spirit, the dependence of the photonic bandgap on the radius of the cylindrical air tunnels has been studied theoretically by Busch and John. These authors also studied the effect of incomplete infiltration of the opal. The fact that in these invertedopal structures both the dielectric region and the air region form a connected network (as a result of the air tunnels) is favorable for increasing the width of the photonic gap. However, a complete, omnidirectional bandgap has not been measured yet, because the materials used, such as titania, and carbon, have indices of refraction that are not sufficiently high.

Here we present results of the optimization of the calculated photonic bandgap in the fcc structure of air spheres with connecting air tunnels, surrounded by silicon.

The photonic band structures of these crystal structures were calculated by means of the plane-wave expansion method (Subsection 2.A below). A part of these calculations is the derivation of expressions for the Fourier coefficients of the dielectric susceptibility, which are used as input in a standard plane-wave expansion method.

2. METHOD

A. Plane-wave expansion

The calculation of the photonic band structure using plane-wave expansions requires the knowledge of the dielectric susceptibility $\varepsilon(k)$, which is given by

$$\varepsilon(k) = \varepsilon_{\text{IR}} - \nabla \cdot \mathbf{D}(\mathbf{k})$$

where $\varepsilon_{\text{IR}}$ is the static dielectric constant, $\mathbf{D}(\mathbf{k})$ is the electric displacement, and $\nabla$ is the gradient operator.

In practice, $\varepsilon(k)$ is approximated in terms of the realizable dielectric constants $\varepsilon_1$ and $\varepsilon_2$, as follows:

$$\varepsilon(k) = \varepsilon_1 - \nabla \cdot \mathbf{D}(\mathbf{k})$$

where $\varepsilon_1$ and $\varepsilon_2$ are functions of the real part of the dielectric constant $\varepsilon$.

In the case of a symmetric unit cell, the dielectric susceptibility can be expanded in terms of the translational symmetry of the crystal, namely, in terms of the left-hand and right-hand components of the electric field vector $\mathbf{E}(\mathbf{r},\omega)$ as follows:

$$\mathbf{E}(\mathbf{r},\omega) = H(\mathbf{r}) e^{i \mathbf{k} \cdot \mathbf{r}}$$

which satisfies the boundary condition of vanishing tangential field at any lateral surface of the crystal. The Bloch function $H(\mathbf{r})$, which represents the basis wave functions of the infinite periodic system, is found in the form of a plane wave with wave vector $\mathbf{k}$ and complex amplitude $E_\omega(\mathbf{k})$. Thus, the Bloch function is defined by

$$H(\mathbf{r}) = E_\omega(\mathbf{k}) e^{i \mathbf{k} \cdot \mathbf{r}}$$

This function is periodic in the crystal lattice, obeying the relation

$$H(\mathbf{r} + \mathbf{R}) = e^{i \mathbf{k} \cdot \mathbf{R}} H(\mathbf{r})$$

where $\mathbf{R}$ is a lattice vector.
2. METHOD OF CALCULATION

A. Plane-Wave Expansion Method

The calculations were performed by means of the classic plane-wave expansion method. The periodic dielectric structure is modeled by a Fourier series for the inverse dielectric function $\eta(r)$:

$$\eta(r) = \frac{1}{\varepsilon(r)} = \sum_m \eta_m \exp(-i\mathbf{g}_m \cdot r),$$

where $m$ labels the three-dimensional set of reciprocal-lattice vectors $\mathbf{g}_m$. In principle, the summation $\Sigma_m$ is carried out over all reciprocal-lattice vectors that exist in reciprocal space. The Fourier coefficients $\eta_m$ are given by

$$\eta_m = \frac{1}{\Omega} \int_{\Omega} \eta(r) \exp(i\mathbf{g}_m \cdot r) dr,$$

where the integration extends over the volume $\Omega$ of one unit cell in the direct lattice. Because of the inversion symmetry possessed by the unit cell and the fact that the dielectric function $\varepsilon(r)$ is assumed real, the Fourier coefficients $\eta_m$ are also real.

In photonic crystals, where $\varepsilon(r)$ is periodic and $\mu(r)$ is constant, Maxwell’s equations are solved preferentially in terms of the magnetic field $H$. The reason for this lies in the transversality of the magnetic field and in the Hermiticity of the operator, applied to the magnetic field in the left-hand side of the wave equation

$$\nabla \times [\eta(r) \nabla \times \mathbf{H}] = -\frac{1}{c^2} \frac{\partial^2 \mathbf{H}}{\partial t^2},$$

as explained by Joannopoulos et al.\(^1\)

The magnetic field is written as a Fourier series as well as

$$\mathbf{H}(r, t) = \exp(i\omega t) \sum_m \sum_k k^{m} \mathbf{h}_m(k) \hat{\mathbf{u}}_m \exp(-i\mathbf{k}_m \cdot r),$$

which is known as the Bloch-wave expansion. Here, for any label $m$, $(\hat{\mathbf{u}}_1, \hat{\mathbf{u}}_2, \hat{\mathbf{u}}_3)$ is a right-handed orthonormal basis for Euclidian space, chosen in such a way that

$$\hat{\mathbf{u}}_m \| \mathbf{k}_m.$$

Furthermore, $\mathbf{k}_m = \mathbf{k} + \mathbf{g}_m$, and the summation over $\mathbf{k}$ denotes the summation over all wave vectors within the first Brillouin zone. The length of the vector $\mathbf{k}_m$ will be denoted $\mathbf{k}_m$.

Substituting the Fourier expansions for $\eta(r)$ and $\mathbf{H}(r, t)$ into Maxwell’s equations, one arrives at the matrix equation

$$\sum_l k_l \mathbf{h}_m \eta_{m-l} \left[ \hat{\mathbf{u}}_m \cdot \hat{\mathbf{u}}_l \hat{\mathbf{u}}_m \cdot \hat{\mathbf{u}}_l \right] \mathbf{h}_l^T(k) = \left( \frac{\omega}{c} \right)^2 \mathbf{h}_m(k) \mathbf{h}_m^T(k).$$

Note that the $\lambda = 3$ components of the magnetic field vanish because $\nabla \cdot \mathbf{H} = 0$.

In practical cases, a finite number of $N$ reciprocal-lattice vectors is selected, and the set of fundamental equations (5) is commonly written as a $2N \times 2N$ matrix equation. Then the eigenvalues of the $2N \times 2N$ matrix $\mathcal{M}$ must be identified with $(\omega/c)^2$, which immediately gives us the photonic band structure. This $2N \times 2N$ matrix $\mathcal{M}$ is constructed in the following way: We regard the matrix $\mathcal{M}$ as an $N \times N$ matrix with elements $\mathcal{M}_{m,l}$, where each of the labels $m$ and $l$ corresponds to one of the reciprocal-lattice vectors $\mathbf{g}_m$ and $\mathbf{g}_l$ selected. In turn, each element $\mathcal{M}_{m,l}$ is a $2 \times 2$ matrix, assigned according to the following prescription:

$$\mathcal{M}_{m,l} = k_l k_m \eta_{m-l} \left[ \hat{\mathbf{u}}_m \cdot \hat{\mathbf{u}}_l \hat{\mathbf{u}}_m \cdot \hat{\mathbf{u}}_l \right].$$

Because of the inversion symmetry mentioned above and the assumption that the index of refraction of the material is a real quantity, matrix $\mathcal{M}$ is real and symmetric. Its eigenvalues are real-valued quantities, to be identified with $(\omega/c)^2$. Our calculations show that the eigenvalues are indeed nonnegative.

B. Including the Material Properties

In the plane-wave expansion method we need to substitute into Eq. (5) the Fourier coefficients $\eta_m$ of the inverse dielectric function $\eta(r)$. These coefficients may, of course, be calculated directly from Eq. (2). It turns out, however, that an indirect calculation by means of the Fourier coefficients $\epsilon_m$ of the dielectric function $\epsilon(r)$ leads to a more efficient band-structure calculation (see below). To this end, one first calculates the Fourier coefficients of the dielectric susceptibility $\chi(r)$ according to

$$\chi_m = \frac{1}{\Omega} \int_{\Omega} \chi(r) \exp(i\mathbf{g}_m \cdot r) dr,$$

[compare Eq. (2)] and obtains the Fourier coefficients $\epsilon_m$ as

$$\epsilon_m = \chi_{m,0} + \chi_m.$$

Next, one defines the Fourier coefficients matrix with matrix elements

$$\epsilon_{m,m'} = \epsilon_{m-m'}. $$

Inverting this matrix, one obtains the Fourier coefficient matrix that contains the desired coefficients $\eta_m$:
\[ \eta_{m,m'} = \eta_{m-m'} = \varepsilon_{m,m'}^{-1}. \]

Both \( \varepsilon_{m,m'} \) and \( \eta_{m,m'} \) are symmetric matrices.

We note that, strictly speaking, this method to obtain the coefficients \( \eta_m \) is incorrect, as it holds only in the limit of infinite matrix sizes \( (N \to \infty) \), whereas one is restricted to a finite matrix size in performing numerical computations. Yet it has been shown numerically that, with the above procedure (referred to in Ref. 30 as Ho’s method), the eigenvalues of \( \mathcal{M} \) converge to the correct values much faster for increasing \( N \) than if one used the direct approach (referred to in Ref. 30 as the slow method). This motivates us to use the matrix-inversion method. However, to our knowledge a convincing mathematical explanation for this artifact still does not exist.

Next we turn to the actual calculation of the coefficients \( \chi_m \). Motivated by their potential to exhibit large photonic bandgaps, we consider the inverted opals described in Section 1, consisting of air spheres and air tunnels surrounded by a dielectric. To be specific, we consider an fcc structure, with lattice constant \( a \), of nonoverlapping air spheres of radius \( R \), each of them connected to its 12 nearest neighbors by cylindrical air tunnels of radius \( R_c \). A three-dimensional visualization of this structure is shown in Fig. 1(a). The dimensions of lengths \( a \), \( R \), and \( R_c \) are indicated in Fig. 1(b).

For these crystals, evaluating the coefficients \( \chi_m \) according to Eq. (7) involves an integration over the dielectric regions that occur between the air spheres and the air tunnels. It is much more convenient, however, to perform integrations over the spheres and the cylinders themselves. To achieve this, we note that the band structure of a photonic crystal that is a composite of two dielectric materials \( (\varepsilon = \varepsilon_S \text{ for the spheres and } \varepsilon = \varepsilon_B \text{ for the background}) \) is determined not by the values of \( \varepsilon_S \) and \( \varepsilon_B \) independently but only by the dielectric contrast \( \varepsilon_S / \varepsilon_B \). The only way in which \( \varepsilon_B \) enters the band structure as a separate parameter is by a trivial rescaling of the frequency scale by a factor of \( \sqrt{\varepsilon_B} \).

Using the above values, we may consider the equivalent crystal with the effective dielectric constants

\[ \varepsilon_E = \frac{\varepsilon_S}{1 + \chi_S} = \frac{1 + \chi_S}{1 + \chi_B} = 1 + \chi_E \]

(8)

for the spheres and \( \varepsilon = 1 \) (i.e., \( \chi = 0 \)) for the background. From Eq. (8) we obtain the effective dielectric susceptibility of the spheres and cylinders in the equivalent crystal:

\[ \chi_E = \frac{\chi_S - \chi_B}{1 + \chi_B}. \]

Note that, for our case of air spheres and air cylinders in the original crystal, \( \chi_E < 0 \) (\( \chi_S = 0 \)). As the effective susceptibility for the regions between the spheres and the cylinders vanishes, the calculation of the Fourier coefficients for the equivalent crystal, according to Eq. (7), indeed involves only integrations over the spheres and the cylinders.

These integrations can be performed semianalytically, in close analogy to the calculations performed by Leung and Liu \( ^{31} \) for a different geometry, namely, that of an fcc lattice of overlapping spheres, where \( R/a > 1/4\sqrt{2} \). First we give the volume-filling fraction \( \phi \) of air in our (original) crystal:

\[ \phi = -\frac{80}{3} \pi (R/a)^3 + 12 \pi \sqrt{2} (R_c/a)^3 + 32 \pi \left( \frac{\sqrt{R^2 - R_c^2}}{a} \right)^3. \]

(10)

The condition for this expression to be valid is that \( R_c \leq R/2 \). For \( R_c = 0 \), Eq. (10) reduces to \( \phi = 16 \pi (R/a)^3/3 \).

Fig. 1. (a) Three-dimensional visualization of an fcc air-sphere crystal with nonoverlapping air spheres, each of them connected to all of its 12 nearest neighbors by cylindrical air tunnels. The particular structure shown here has geometrical parameters, which for a silicon background (gray) optimize the bandgap (see Section 3). (b) Schematic cross section of the structure in (a) with definitions of the lengths \( a \), \( R \), and \( R_c \) indicated.
Obviously, the zeroth Fourier coefficient of the equivalent crystal is given by 
\[ \chi_0 = \phi_XE. \]
For the derivation of the other coefficients \( \chi_m \) of the equivalent crystal we need to define six vectors \( \mathbf{Q}_m \), two of which have the following representations in cylindrical coordinates (\( \mathbf{Q}_{mp}, \mathbf{Q}_{mz} \)):
\[
\begin{align*}
\mathbf{Q}_{mp} &= \left[ g_{mz}^2 + \frac{1}{2}(g_{mx} - g_{my})^2 \right]^{1/2}, \\
\mathbf{Q}_{mz} &= \frac{1}{2}\sqrt{2}(g_{mx} - g_{my});
\end{align*}
\]
the remaining four are given by cyclic permutations of \( x, y, \) and \( z \). Then the analytical expression for \( \chi_m (m \neq 0) \) is given by
\[
\chi_m = X_E 16\pi R^3 \left[ \frac{a}{3}S(g_mR) + \sum_{\mathbf{Q}_m} \mathcal{Z} \left( \mathbf{Q}_m \right) \right]
\]
where
\[
S(x) = \frac{\sin x - x \cos x}{x^3}.
\]
The summation in Eq. (12) is over all six vectors \( \mathbf{Q}_m \) defined above, and the integral \( \mathcal{Z} \left( \mathbf{Q}_m \right) \) is given by
\[
\mathcal{Z} \left( \mathbf{Q}_m \right) = 8 \int_{\varphi=0}^{2\pi} \int_{\rho=0}^{\rho_{Q_{mp}}} \int_{z=\left[ (R/a)^2 - \rho^2 \right]^{1/2}} \rho \exp(i\rho Q_{mp}\cos \varphi) \cos(Q_{mz}z) d\rho dz d\varphi,
\]
which we can evaluate to
\[
\mathcal{Z} \left( \mathbf{Q}_m \right) = 16\pi \int_{0}^{\rho_{Q_{mp}}} \rho J_0(\rho Q_{mp}) \left\{ \frac{1}{4\sqrt{2}} - \left[\left(\frac{R}{a}\right)^2 - \rho^2 \right]^{1/2} \right\} d\rho
\]
for \( Q_{mz} = 0 \) and to
\[
\mathcal{Z} \left( \mathbf{Q}_m \right) = \frac{16\pi}{Q_{mz}} \int_{0}^{\rho_{Q_{mp}}} \rho J_0(\rho Q_{mp}) \left( \sin \left( \frac{Q_{mz}}{4\sqrt{2}} \right) - \sin \left( \frac{Q_{mz}}{2} \right) \right) d\rho
\]
for \( Q_{mz} \neq 0 \). The remaining integrals that appear in Eqs. (15) and (16) contain the Bessel function \( J_0 \) and have to be evaluated numerically.

3. RESULTS

In this section we discuss some characteristics of the photonic band structure of air-sphere crystals, which we calculated by the plane-wave expansion method as described in Section 2. The crystals under consideration are the inverted opals described in detail in subsection 2B (see Fig. 1). We shall take silicon [Si; \( n = 3.415 \) (Ref. 32)] as our choice for the dielectric that surrounds the air spheres and cylinders in this crystal. For explicitness, Fig. 2 shows the first Brillouin zone of the fcc lattice, in which the important symmetry points are indicated by the conventional symbols.

A typical band structure for a closely packed fcc crystal of air spheres in silicon (without the connecting cylinders) is shown in Fig. 3. Clearly seen are the pseudogap between the fifth and sixth bands and the full gap between the eighth and ninth bands. In what follows, we shall concentrate mainly on the full gap. One usually characterizes this gap by the quantity \( \Delta \omega/\omega_0 \), which is the relative width of the frequency range that is common to this bandgap in all directions in reciprocal space. The lower bound of this frequency range (\( \omega_- \)) is obtained at the point where the eighth band of the photonic band structure reaches its maximum, usually at point \( W \) of the Brillouin zone. The upper bound of this frequency range (\( \omega_+ \)) is obtained at the point where the ninth band reaches its minimum, usually at point \( X \) of the Brillouin zone. However, for some values of the geometrical parameters of the system, for instance in air-sphere crystals without the air cylinders, when the volume-filling fraction of the air spheres decreases below 67% it turns out that the lower and upper bounds of the full gap occur at different high-symmetry points. The relative gap width is given by
\[
\frac{\Delta \omega}{\omega_0} = 2 \frac{\omega_+ - \omega_-}{\omega_+ + \omega_-}.
\]

Our main interest is in the dependence of \( \Delta \omega/\omega_0 \) on the geometrical parameters \( R/a \) and \( R_c/a \). To this end, we have calculated band structures by varying these two parameters. In Fig. 4 we plot the relative bandgap thus ob-
tained as a function of the cylinder radius \( R_c/a \) for four different values of the sphere radius \( R/a \). These results were obtained for \( N = 339 \) plane waves. It is known that, for this type of crystal structure, one needs \( N \approx 10^3 \) plane waves to reach convergence of the band structure well below the 1% level.\(^{25}\) We used such high values for \( N \) only when we were optimizing the bandgap and calculating the density of states (see below). Comparison has taught us that the relative errors in the band structure depicted in Fig. 5.

In a first, crude approach toward the maximal gap, we used band-structure calculations with \( N = 339 \) plane waves, as before. We started at \( R/a = 0.3437 \) and \( R_c/R = 0.37 \), which yielded the maximal gap width as shown in Fig. 4, curve (a), and initially the adjustment of the parameters was a decrease of \( R/a \) of the order of 0.02 per step. Smaller step sizes were used as the value of \( \Delta \omega/\omega_0 \) decreased. Thus, following the prescribed by the gradient search method, using of the order of 15 steps, we finally reached \( R/a = 0.3220 \) and \( R_c/R = 0.398 \), for which \( \Delta \omega/\omega_0 \approx 0.744/c/a \). At all points along this path of steepest ascent, the width of the full photonic bandgap turned out to be determined by point \( W \) in hand eight and by point \( X \) band nine.

To obtain a more reliable value for the bandgap in this geometry, i.e., closer to convergence, we also calculated the gap width of the structure with \( R/a = 0.3200 \) and \( R_c/R = 0.398 \) using \( N = 1037 \) plane waves. The result

\[
\Delta \omega/\omega_0 = 0.398 c/a
\]

for certain values of \( R/a \) and \( R_c/R \) and adjusting \( R/a \) and \( R_c/R \) such that a step is taken in the direction of \( \nabla f \). Thus we reach the maximal value of \( f \) by following the path of steepest ascent.

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of this calculation is $\Delta \omega/\omega_0 = 9.59\%$. Further fine tuning of the optimum by applying the gradient search method once more, but now with $N = 1037$ plane waves are starting from the optimum obtained above, yield negligible changes: The maximally achievable gap width was found to be $\Delta \omega/\omega_0 = 0.95\%$ at $R/a = 0.3201$ and $R_c/R = 0.398$. The central frequency of the gap is $\omega_0/2\pi = 0.746c/a$. The photonic band structure for this geometry, calculated with $N = 1037$ plane waves, is shown in Fig. 5. The corresponding density of states, calculated by use of the Monkhorst–Park discretization scheme for the Brillouin zone, is shown in Fig. 6. This figure clearly demonstrates the existence of a full gap.

4. DISCUSSION AND CONCLUSIONS

We have studied the photonic band structure of inverted fcc photonic crystals, using the plane-wave expansion method. The crystals under consideration consist of an fcc structure of spherical air regions surrounded by a highly refractive material. The air spheres may be connected by cylindrical air tunnels. Recently such inverted fcc photonic crystals, with lattice dimensions at the length scale of the wavelengths of visible and near-infrared light, were created experimentally by Wijnhoven and Vos. Although the main purpose of the presence of the tunnels between neighboring air spheres in these inverted opal structures is to serve as passageways through which the original colloidal material is removed, it turns out from our calculations that these holes also have a positive influence on the width of the full photonic bandgap, provided that their radius is large enough.

Applying a gradient search method for these inverted opals, we optimized the relative width of the photonic bandgap by varying two parameters, $R/a$ and $R_c/R$. The optimal value that we obtained for the gap width is $\Delta \omega/\omega_0 = 9.59\%$ for a structure of air spheres in silicon, with sphere radius $R = 0.3201a$ and cylinder radius $R_c = 0.398R$. The central frequency of this bandgap is $\omega_0/2\pi = 0.746c/a$.

In general, the width of the photonic bandgap depends strongly on the dielectric contrast and on the volume-filling fraction. We point out that, for the optimized structure described above, the volume-filling fraction is only $33.7\%$; i.e., the optimal bandgap occurs in a rather empty structure [see Fig. 1(a)]. The controlled preparation and manipulation of such empty crystal geometries, calculated with $N = 1037$ plane waves, is a real challenge for material scientists and experimentalists. It will be worthwhile to investigate whether also for other classes of geometries such empty structures optimize the bandgap.

As is well known, the calculated band structures also depend significantly on the number $N$ of plane waves considered. It is accepted quite generally that, for $N \sim 10^9$, the error in the results for the lowest-lying photonic bands is well below 1% (for the type of crystal that we consider). Our calculations reveal that for $N = 239$ (which allows for much faster computing), the relative error in the bandgap is still of the order of 6%. At the same time, however, we have demonstrated that, even with this rather small number of plane waves, the dependence of the bandgap on the geometrical parameters can be studied with appreciable accuracy. In particular, we have shown that, using the gradient search method with $N = 339$ plane waves, one may determine the geometrical parameters that optimize the band gap quite accurately. By fine tuning these results, using $N = 1037$ plane waves, we found that the values of the optimal parameters change by only a small fraction, namely, less than 0.1% for the present case.

We note that the crystal structure considered by us formally belongs to the class of $A7$ structures discussed by Chan et al. The specific examples of this class considered by those authors consist of cylinders connecting neighboring lattice sites, for which they reported relative band gaps of up to 30% between the second and third bands. Our sphere–cylinder crystals would reduce to the specific case considered in Ref. 34 if $R < R_c$. This parameter range, however, lies outside the range considered by us (see below Eq. (10)) and also seems to be less relevant to the experimentally realized inverted opals.

We finally note that an alternative method for calculating photonic band structures is a photonic analog of the on-shell multiple scattering theory and the Korringa-Kohn-Rostoker method which was used by Moroz and Sommers. This method is known to yield convergence of the results much more rapidly than the plane-wave expansion method. However, it should be pointed out that, unlike the plane-wave expansion method that we use, the photonic Korringa–Kohn–Rostoker method is unsuitable for treating photonic crystals with either overlapping spheres or nonoverlapping spheres with cylindrical nearest-neighbor connections, as these correspond to the so-called non-muffin-tin potentials.

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