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Photonic Band-Gap Optimisation in Inverted FCC Photonic Crystals

Abstract

We present results of 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 cylindrical tunnels connecting each pair of neighbouring spheres. The width of the band gap is optimised by applying a gradient search method and varying two geometrical parameters: the ratios R/a and R_c/R, where a is the lattice constant, R the sphere radius and R_c the cylinder radius. We find that the maximal gap width in this type of photonic-crystal structure, with air spheres and cylinders in silicon, is $\Delta\omega/\omega_0 = 9.59\%$.

1 Introduction

Photonic crystals, and their effect on the propagation of electromagnetic waves, have been studied intensively over the past few decades. A photonic crystal is a material with a spatially periodic dielectric function $\varepsilon(\mathbf{r})$. Its dispersion relation $\omega(\mathbf{k})$, i.e. the photonic band structure, shows *photonic band gaps* between the bands, characterised by their central frequency ω_0 and spectral width $\Delta\omega$. The investigation of this type of dielectric structures, possessing large band gaps, is motivated e.g. by the desired ability to control spontaneous emission of radiation from atoms [1].

A new type of photonic crystal is the inverted FCC photonic crystal, consisting of a regular structure of spherical air holes in a dielectric medium [2, 3]. These air-sphere crystals are created using dried (polystyrene or silica) colloidal crystals, also known as artificial opals. Their structure is usually a close-packed ($\phi = 74\%$) stacking of colloidal spheres. At the stage of thermal annealing (sintering) of the artificial opal, the volume-filling fraction increases above 74%. This effect is modelled by means of cylindrical connections between each pair of neighbouring spheres. After sintering, the empty voids in the opal structure are infiltrated with titania (TiO_2). Then the original colloidal spheres are removed by chemical etching [2]. This air-sphere crystal, with a lattice constant matching the range of wavelengths of visible and near-infrared light, provides a good opportunity to establish a photonic band gap. However, a full photonic band gap has not been measured in these crystals yet, probably due to the use of materials like titania [2] or carbon [3], whose index of refraction n is not sufficiently high.

In this work we present results of the optimisation of the calculated photonic band gap in the FCC structure of air spheres with connecting air tunnels, surrounded by silicon. The photonic band structure of these crystal structures were calculated by means of the

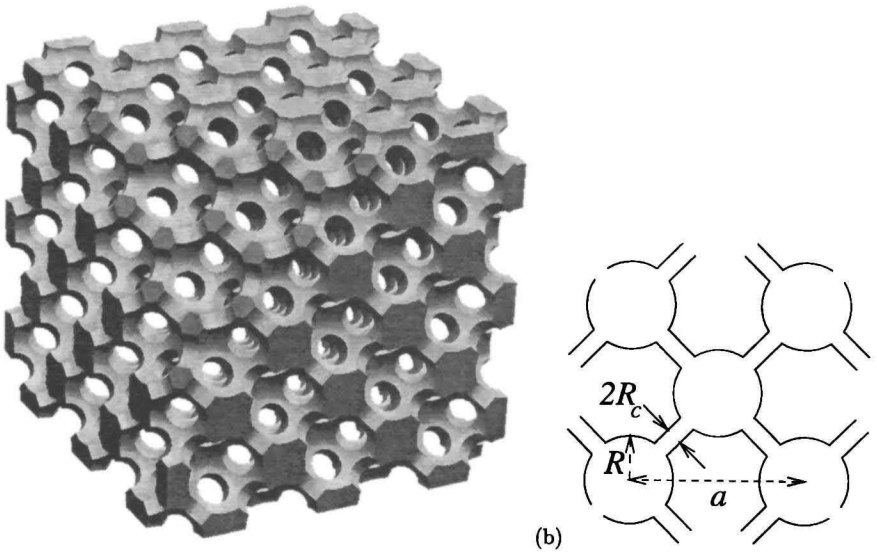

Figure 1: (a) Three-dimensional visualisation of an FCC air-sphere crystal with non-overlapping air spheres, each of them connected to all of its 12 nearest neighbours by cylindrical air tunnels. The particular structure shown here has geometrical parameters, which for a silicon background (grey) optimise the band gap (see section 3). (b) Schematic cross-section of the structure in Fig. 1(a) with the definition of the lengths a, R and R_c indicated.

plane-wave expansion method [4, 5]. Two parameters were varied in our band-structure calculations, namely the ratios R/a and R_c/R. Here R is the sphere radius, R_c is the cylinder radius and a is the lattice constant of the FCC lattice. The gap width increases substantially when the ratio R_c/R increases from zero to 0.4. By applying a gradient search method in combination with the variation of the two parameters mentioned above, we obtain the geometrical parameters for which the relative gap width $\Delta\omega/\omega_0$ reaches its maximum.

2 The method of calculation

We will consider the inverted opals described in the Introduction. We will use silicon (Si; $n = 3.415$) as our choice for the dielectric. To be specific, we consider an FCC structure, with lattice constant a, of non-overlapping air spheres of radius R, each of them connected to its twelve nearest neighbours by a cylindrical air tunnel of radius R_c. A three-dimensional visualisation of this structure is given in Fig. 1(a).

The crystal structure is represented by a Fourier series for the inverse dielectric function

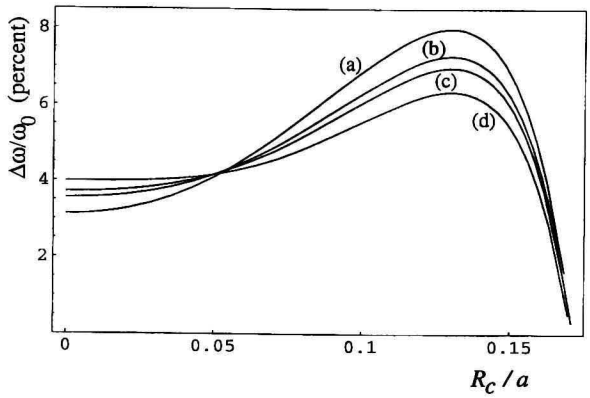

Figure 2: Relative width of the full photonic band gap between bands 8 and 9 in the FCC inverted opals, as a function of R_c/a. The background material is silicon (Si, $n = 3.415$). The number of plane waves used is $N = 339$. The four curves have been calculated for (a) $R/a = 0.3437$, (b) $R/a = 0.3486$, (c) $R/a = 0.3504$ and (d) $R/a = 0.3536$. For $R_c = 0$, this corresponds to $\phi = 68\%$, $\phi = 71\%$, $\phi = 72\%$ and $\phi = 74\%$, respectively.

$\eta(\mathbf{r})$:

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

where m labels the three-dimensional set of reciprocal-lattice vectors $\mathbf{g}_m$. We have derived analytical expressions for the coefficients η_m for the structure under consideration.

Also the magnetic field $\mathbf{H}$ is written as a Fourier series,

$$\mathbf{H}(\mathbf{r}, t) = \exp(i\omega t) \sum_m \sum_{\mathbf{k}} \sum_{\lambda=1}^{3} h_m^\lambda(\mathbf{k}) \hat{\mathbf{u}}_m^\lambda \exp(-i\mathbf{k}_m \cdot \mathbf{r}), \tag{2}$$

known as the Bloch-wave expansion. Here, for any label m, $\{\hat{\mathbf{u}}_m^1, \hat{\mathbf{u}}_m^2, \hat{\mathbf{u}}_m^3\}$ is a right-handed orthonormal basis for Euclidian space, chosen such that $\hat{\mathbf{u}}_m^3 \parallel \mathbf{k}_m$. 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.

Substitution of the Fourier expansions for $\eta(\mathbf{r})$ and $\mathbf{H}(\mathbf{r}, t)$ into Maxwell's equations yields the matrix equation

$$\sum_l k_l k_m \eta_{m-l} \begin{bmatrix} \hat{\mathbf{u}}_m^2 \cdot \hat{\mathbf{u}}_l^2 & -\hat{\mathbf{u}}_m^2 \cdot \hat{\mathbf{u}}_l^1 \\ -\hat{\mathbf{u}}_m^1 \cdot \hat{\mathbf{u}}_l^2 & \hat{\mathbf{u}}_m^1 \cdot \hat{\mathbf{u}}_l^1 \end{bmatrix} \begin{bmatrix} h_l^1(\mathbf{k}) \\ h_l^2(\mathbf{k}) \end{bmatrix} = \left(\frac{\omega}{c}\right)^2 \begin{bmatrix} h_m^1(\mathbf{k}) \\ h_m^2(\mathbf{k}) \end{bmatrix}, \quad k_m = |\mathbf{k}_m|. \tag{3}$$

The $\lambda = 3$ components of the magnetic field vanish because $\nabla \cdot \mathbf{H} = 0$. The eigenvalues of the matrix involved in this equation, are real-valued, non-negative quantities, to be identified with $(\omega/c)^2$.

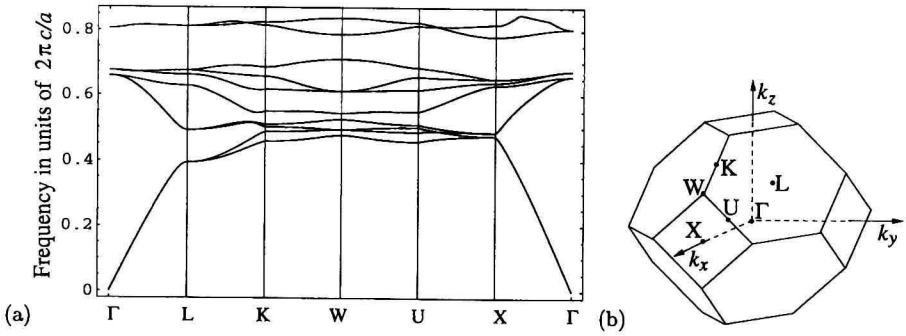

Figure 3: (a) Photonic band structure of an FCC inverted opal with silicon ($n = 3.415$) as dielectric medium and with the optimal parameters $R/a = 0.3201$ and $R_c/R = 0.398$. The optimal relative width of the full gap between the 8th and 9th bands is $\Delta\omega/\omega_0 = 9.59\%$ at $\omega_0/2\pi = 0.746c/a$. The volume-filling fraction of air spheres and cylinders in this structure is $\phi = 66.3\%$. The number of plane waves used is $N = 1037$. (b) The first Brillouin Zone for the FCC lattice (BCC in reciprocal space).

3 Results and discussion

Our main interest is the dependence of the relative width $\Delta\omega/\omega_0$ of the full photonic band gap between the 8th and 9th bands, on the parameters R/a and R_c/a. In Fig. 2, we plot the relative gap width as a function of R_c/a for four different values of R/a. These results were obtained using 339 plane waves. It is known that, for this type of crystal structure, one needs $N \sim 10^3$ plane waves in order to reach convergence of the band structure well below 1% [6]. We used such high values for N only when optimising the band gap and calculating the density of states (see below). The relative errors in the band gap at $N = 339$ appear to be in the order of 6%. Although this is by no means full convergence, it suffices to provide considerable insight in the behaviour of the band structure upon varying parameters, as we will see below.

From Fig. 2, we observe that at first, when the cylindrical air holes are very narrow, their effect on the gap width is rather small. While the main purpose of the tunnels between neighbouring air spheres in these inverted opal structures, is to serve as passageways through which the original colloidal material is removed, in addition these holes have a positive influence on the width of the band gap for larger values of R_c, as is observed in Fig. 2. For the crystal structure presently under consideration, the largest gap width is achieved around $R_c/R = 0.4$, and it tends to increase when the value of R/a decreases. Curve (d) in Fig. 2, which gives the dependence of the gap width on the cylinder radius for *close-packed* spheres, agrees well with the results of Busch and John [6]. A remarkable feature in Fig. 2 is the observation that the four curves nearly cross at one point for $R_c/a \approx 0.052$, where the gap width $\Delta\omega/\omega_0 \approx 4.2\%$. We were unable to establish whether this feature has any physical

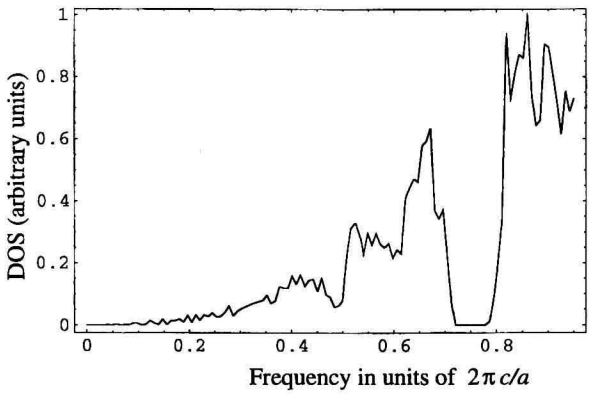

Figure 4: Density of states corresponding to the photonic band structure depicted in Fig. 3(a).

significance.

Now we turn to the optimisation of the relative width of the band gap, performing a two-parameter variation calculation, based on a gradient search method. This method consists of successively determining the gap width $f \equiv \Delta\omega/\omega_0$ and the gradient

$$\nabla f \equiv (\mathrm{d}f/\mathrm{d}(R/a), \mathrm{d}f/\mathrm{d}(R_c/R)),$$

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 ∇f. Thus we reach the maximal value of f by following the path of steepest ascent.

In a first "crude" approach towards the maximal gap, we used band-structure calculations with $N = 339$, as before. We started at $(R/a = 0.3437, R_c/R = 0.37)$, which yielded the maximal gap width as shown in Fig. 2, curve (a). Following the path of steepest ascent, we reached $(R/a = 0.3200, R_c/R = 0.398)$, for which $f = 9.3\%$ and $\nabla f \approx 0$. The central frequency of the gap obtained in this way, is $\omega_0/2\pi = 0.744c/a$. The error in this result is in the order of 6%.

The calculated band structures depend significantly on the number of plane waves considered. It is accepted quite generally that for $N \sim 10^3$, the error in the results for the lowest-lying photonic bands is well below 1% (for the type of crystals that we consider). Thus, a more reliable value for the gap width of our structure is obtained by doing the calculation using 1037 plane waves. This yields a value of $\Delta\omega/\omega_0 = 9.59\%$. Further fine-tuning of the optimum, using 1037 plane waves and starting from the optimum obtained above, yields negligible changes: $\Delta\omega/\omega_0 = 9.59\%$ at $(R/a = 0.3201, R_c/R = 0.398)$. We remark that with only 339 plane waves (which allows for much faster computing), the optimal parameters were determined very accurately, i.e. within a 0.1% margin.

The central frequency of the gap is $\omega_0/2\pi = 0.746c/a$. The photonic band structure for this geometry is shown in Fig. 3(a). The corresponding density of states is shown in Fig. 4.

This figure clearly demonstrates the existence of a full gap.

In general, the width of the photonic band gap depends strongly on the dielectric contrast and on the volume-filling fraction. We point out that for the optimised structure described above, the volume-filling fraction of silicon is only 33.7%, i.e., the optimal band gap occurs in a rather empty structure (see Fig. 1(a)). The controlled preparation and manipulation of such empty crystal structures will be a real challenge for material scientists and experimentalists. It will be worthwhile to investigate whether also for other classes of geometries such empty structures optimise the band gap.

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