Band gap atlas for photonic crystals having the symmetry of the kagomé and pyrochlore lattices

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Abstract. The interesting photonic band gap maps of two- and three-dimensional photonic crystals with the symmetry of the kagomé and pyrochlore lattices are reported. From large complete photonic band gaps in three dimensions to enormous partial gaps in two dimensions for certain polarizations occurring at feature sizes that make these lattices amenable to fabrication, the results described below make this family of photonic crystals very promising for potential applications and very interesting from the fundamental point of view.

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1. Introduction

Photonic crystals are engineered periodic structures made of two or more materials with very different dielectric constants. They have generated an ever-increasing interest in the last 20 years because of their potential to control the propagation of light to an unprecedented level [1]–[17]. When an electromagnetic (EM) wave propagates in such a structure whose period is comparable
to the wavelength of the wave, interesting phenomena occur. Among the most interesting are
the possibility of forming a complete photonic band gap (CPBG), that is, a frequency range
for which no photons having frequencies within that range can propagate through the photonic
crystal, to localize light by introducing several types of defects in the lattice, or enhancing certain
nonlinear phenomena due to small group velocity effects.

The problems one faces in order to implement these advantageous properties into
technological applications are mainly twofold: on the one hand, the scarcity of known three-
dimensional (3D) symmetries with a CPBG. It is important to stress the difference between
symmetry and topology for a given photonic crystal. Indeed, most of the known structures with
a CPBG are based on the face-centred cubic (fcc) or diamond symmetry.1 To cite an example,
structures such as the opals, the Yablonovite, or the layered structure recently identified by
Johnson and Joannopoulos [2, 18], are different topologies of the fcc symmetry. An especially
lucid discussion about the importance of symmetry and topology in the context of photonic band
gap materials can be found in [19]. It is thus quite remarkable that in more than two decades of
intensive research in this field, only two or three symmetries amenable to giving rise to a CPBG
had been identified. On the other hand, manufacturing these lattices requires working on sub-
micron length scales, so ingenious innovations were required in order to actually fabricate them
[20]–[24]. Also, this has resulted in a lot of effort being devoted to investigating photonic-crystal
slabs, i.e., dielectric structures that are periodic in two dimensions and use index guiding to
confine light in the third dimension [12, 15, 16]. Therefore, identifying new 2D and 3D photonic
crystal structures based on symmetries that are different from the standard ones is an important
task, both at the fundamental and technological levels.

The main purpose of this paper is to explore the photonic properties of various topologies
based on the kagomé and pyrochlore symmetries (see figure 1(a)). The kagomé and pyrochlore
lattices are well known to the magnetic properties practitioners because of their intriguing
properties, which include geometrical frustration and anomalous electronic behaviours [25–32].
The 2D kagomé lattice is a lattice of corner-sharing triangles with ‘atoms’ located at the corners
of the triangles. The 3D pyrochlore lattice is a lattice of corner-sharing tetrahedral with ‘atoms’
located at the corners of the tetrahedra. Two important characteristics of these lattices—with
regard to the photonic crystals field—are that they are based on triangular elementary units and
that they are very sparsely connected, which are known to favour the formation of photonic band
gaps [1]. The results reported below show that photonic crystals based on these symmetries are
very promising candidates for photonic applications and quite interesting from the fundamental
point of view.

2. Details of the calculations and results

For the present work, perfectly periodic infinite lattices were considered and the band structure
of the EM field propagating in these structures was calculated. To this end, the eigenmodes
of Maxwell’s equations with periodic boundary conditions were computed by preconditioned
conjugate-gradient minimization of the block Rayleigh quotient in a planewave basis, using

1 A notable exception to this rule is the scaffold lattice, which is based on a simple cubic lattice and still exhibits a
sizeable 7% CPBG for rods of Si in air.
Figure 1. A primer on the kagomé and pyrochlore lattices. (a) Pictorial representation of the kagomé (left) and pyrochlore (right) lattices. (b) Basis vectors ($a_1$ and $a_2$), atomic positions (green dots), and 1st Brillouin zone (BZ) (red hexagon) of the kagomé unit cell. The atomic positions are given by (0, 0), (1/2, 0), and (0, 1/2) in the ($a_1$, $a_2$) basis. The special symmetry points $\Gamma$, $M$ and $K$ delimit the irreducible part of the 1st BZ (shaded in brown). Because of symmetry arguments, only $k$-vectors in that triangle are necessary for the band calculations. (c) Basis vectors ($a_1$, $a_2$ and $a_3$) and atomic positions (green spheres) of the pyrochlore unit cell. The atomic positions in this basis are given by (1/2, 1/2, 1/2), (0, 1/2, 1/2), (1/2, 0, 1/2) and (1/2, 1/2, 0). (d) 1st BZ of the pyrochlore lattice. The red polyhedron defined by the special symmetry points $\Gamma$, $L$, $K$, $W$, $X$ and $U$ delimits the irreducible part of the 1st BZ. It is important to notice that neither the kagomé nor the pyrochlore lattice is Bravais lattice, as it is not possible to find a unit cell that contains a single atom.

The freely available software package MIT Photonic-Bands (MPB) [33]. Some of the main advantages of using this software package are that it is fully vectorial, which allows us to calculate the photonic band structure of arbitrary 3D photonic crystals for arbitrary Bloch wavevectors; supports arbitrary, anisotropic dielectric structures and non-orthogonal unit cells; parallel computations are supported by using MPI, it provides a flexible user interface (extensible and scriptable), and it has been extensively tested by numerous researchers during the last
Figure 2. Band gap map at selected values of $\varepsilon$ for the kagomé lattice of dielectric rods in air. (a) Pictorial representation of the lattice at $r/a = 0.19$ (radius of the dielectric cylinders at which the maximum BG is attained for $\varepsilon = 12$). (b) Band gap map for this structure. (c) Band structure and density of states at $r/a = 0.19$ for $\varepsilon = 12$. The blue stripe delimits the photonic band gap. 32 TM bands and 32 TE bands were used for all the band calculations. A $32 \times 32$ grid was used for discretizing the lattice. 200 $k$-vectors along the contour of the irreducible part of the 1st BZ (see figure 1) were used to compute the bands and 3000 $k$-vectors in the 1st BZ were randomly selected to calculate the density of photonic states.

years. Five different topologies with the symmetry of the kagomé or pyrochlore lattices were studied.

- In two dimensions, a kagomé lattice of dielectric rods in air (figure 2(a)) and a kagomé lattice of air rods in dielectric (figure 3(a)) were considered. The dielectric material was assumed to be linear, isotropic and non-magnetic. Unlike [34]–[36], the band structures for these lattices were calculated for different values of the dielectric constant ($\varepsilon$) ranging from 3 to 12 and for a wider range of frequencies of the incident EM wave. Also, the band structure was calculated for several values of the ratio $r/a$, where $r$ is the radius of the rod and $a$ is the lattice parameter (see figure 1(b)), ranging from 0.01 to 0.5, so that the band gap map for a given $\varepsilon$ could be constructed [1]. For these 2D calculations, the EM wave was assumed to propagate in the plane of the lattice. Details of the computations can be found in the caption of figure 2.

- In three dimensions, three different topologies were studied. The first one corresponds to a pyrochlore lattice of dielectric spheres in air (see figure 4(a)). The second one corresponds to the inverse structure of air spheres embedded in a dielectric material (see figure 5(a)). Air cylinders along the lines that join the atomic positions in the pyrochlore lattice form the third one (see figure 6(a)). This latter one is especially interesting from the manufacturing
Figure 3. Band gap map at selected values of $\varepsilon$ for the kagomé lattice of air rods in dielectric. (a) Pictorial representation of the lattice at $r/a = 0.24$ (radius of the air cylinders at which the maximum BG is attained for $\varepsilon = 12$). (b) Band gap map for this structure. (c) Band structure and density of states at $r/a = 0.24$ for $\varepsilon = 12$; the blue stripe delimits the photonic band gap. See the caption of figure 2 for the computational details.

point of view as it can be made by directly drilling the air veins in a dielectric material, in a similar fashion to the well-known Yablonovite structure [9], as explained below. The same computational scheme as for the 2D lattices was applied to the 3D ones (see figures 1(c) and (d), and the caption of figure 4) with two differences: arbitrary propagation directions of the EM wave were considered and the dielectric constant range spans only from 6 to 12, due to the longer simulation times required for 3D calculations.

It is worth saying something about the various quantities reported below. First of all, as it is customary, results are quoted in terms of the dimensionless frequency $\omega a/2\pi$, with $\omega$ the wavenumber of the EM field, $a$ the lattice parameter and $c$ the speed of light in vacuum. With regard to the band gap maps presented below, it should be stressed that this is an important quantity as it readily provides a visual feedback of the frequency ranges in which photon propagation is forbidden for given values of the dielectric constant and the size of the feature defining the lattice. For a given topology, the band gap map is simply obtained by plotting the locations of the photonic gaps found in the band structure (if any) as a function of one or more parameters ($\varepsilon$ and $r/a$ in our case). One obvious advantage of this type of visualization is that it is very easy to identify the optimal geometrical parameters of the lattice in order to maximize the width of the band gap. Also, if fabrication at the optimal value of $r/a$ is not feasible for any reason, it can be readily known from this map whether fabrication at a larger feature size will still give rise to a CPBG, even at the cost of a smaller gap. Regarding the size of the gap, it should be noted that it is expressed in terms of the midgap to band gap ratio, $\Delta\omega/\omega_m$, which is a quantity that does not change with the frequency of the EM field. Another interesting
Figure 4. Band gap map at selected values of $\varepsilon$ for the pyrochlore lattice of dielectric spheres in air. (a) Pictorial representation of the lattice at $r/a = 0.19$ (radius of the dielectric spheres at which the maximum PBG is attained for $\varepsilon = 12$). (b) Band gap map for this structure. (c) Band structure and density of states at $r/a = 0.19$ for $\varepsilon = 12$. 16 bands were computed for all the calculations. A $24 \times 24 \times 24$ grid was used for discretizing the lattice. 500 $k$-vectors along the contour of the irreducible part of the 1st BZ were used to compute the bands and 5000 $k$-vectors in the 1st BZ were randomly selected to calculate the density of photonic states.

A quantity that can be readily computed from the band structure is the density of photonic states. Some examples of this quantity are also given in the figures below. This quantity is obtained by randomly selecting a number of $k$-vectors in the 1st Brillouin zone (BZ) and calculating the corresponding eigenfrequencies. The density of states is then obtained by counting the number of modes with frequencies in the range from $\omega$ to $\omega + \Delta \omega$, where $\Delta \omega$ is the frequency spacing (typically 0.001 in our calculations).

Let us now review the main results for the topologies studied in this work, starting with the 2D lattices. A summary of the most interesting results and the values of some parameters important for fabrication can be found in table 1. Figure 2(b) shows the band gap map of the kagome lattice of dielectric rods in air for selected values of $\varepsilon$. As can be seen from that figure, this geometry displays a wealth of PBG for TM polarization (even for values of $\varepsilon$ as small as 3) and some smaller PBG for TE polarization. Moreover, there is a small overlap between TM
Figure 5. Band gap map at selected values of ε for the pyrochlore lattice of air spheres in dielectric. (a) Pictorial representation of the lattice at $r/a = 0.27$ (radius of the air sphere at which the maximum PBG is attained for $\varepsilon = 12$). (b) Band gap map for this structure. (c) Band structure and density of states at $r/a = 0.27$ for $\varepsilon = 12$. See the caption of figure 4 for the computational details.

and TE gaps that gives rise to a PBG for all polarizations$^2$ with a maximum at $r/a = 0.21$ for $\varepsilon = 12$ (dielectric rods made of Si). However, this gap is small ($\Delta \omega / \omega_m \sim 3\%$) and extends over a narrow range of the dielectric rod radii, so we cannot expect it to be very robust upon disorder always present in real systems. On the other hand, the gaps for TM polarization are large and well separated from the TE ones, which could make this structure very useful for polarization-dependent applications. In particular, the TM gap between TM bands 3 and 4 is huge (539 nm at $\lambda = 1.3 \mu m$ for $\varepsilon = 12$) and extends over a large $r/a$ interval. As an illustrative example, the band structure of this lattice for $\varepsilon = 12$ at the value of $r/a$ that maximizes the PBG for all polarizations and the corresponding density of states are depicted in figure 2(c). The band structure for this lattice shows some interesting features. For example, the extrema of the band are not always located at the zone boundaries. This is a direct consequence of the non-Bravais character of this lattice, i.e., having more than one atom per unit cell. Also, some of the bands are very flat in some directions (noticeably bands 3 and 9 for both TM and TE polarizations in the Γ’M

$^2$ It is important to strike that for the 2D structures, the EM field is assumed to propagate in the plane of the lattice. In this sense, a photonic gap in 2D is not really a CPBG, as a wave that possesses an out-of-plane wave vector will ‘feel’ a non-periodic medium in that direction, so no band gap can be formed.
Figure 6. Band gap map at selected values of $\varepsilon$ for the pyrochlore lattice of air rods in dielectric. (a) Pictorial representation of the lattice at $r/a = 0.10$. (b) Band gap map for this structure. (c) Band structure and density of states at $r/a = 0.24$ for $\varepsilon = 12$ the grey stripes delimit the photonic band gap. See the caption of figure 4 for the computational details.

direction and the second TM band in the MK direction for small values of $\omega$ and especially bands with a large band index), which will give rise to the small group velocity effect associated with the enhancement of certain processes such as the stimulated emission, sum-frequency generation, etc, as discussed in [14, 37].

The density of photonic states is also shown in figures 2(c) and 3(c) for comparison. At low frequencies, this quantity is linear with a slope that depends on $\varepsilon$, due to the fact that long-wavelength modes are ‘insensitive’ to the inhomogeneities of the structure. As the frequency is increased, this quantity follows a more complicated behaviour due to the multiple scattering by the inhomogeneous structure. It is also apparent the small PBG for all polarizations mentioned above. Also, the small velocity effects mentioned before clearly show up in this quantity as very narrow peaks occurring most noticeably for large values of $\omega$.

The band gap map for the kagomé lattice of air rods in dielectric shows even more interesting features than the previous geometry does. Results for this lattice are shown in figure 3(b) and some data are also summarized in table 1. There are again a large number of TM gaps. In particular, there is an enormous TM gap between the first and second TM bands (668 nm at $\lambda = 1.3 \mu m$ for $\varepsilon = 12$) that extends over a very wide $r/a$ range. However, in contrast with the previous
### Table 1. Various important physical parameters of the photonic crystals studied in this work for $\varepsilon = 12$

| Lattice type | Polarization | LB | UB | $\Delta \omega / \omega_m$ (%) | $\omega_m a / 2\pi c$ | $r/a$ (max) | $r/a$ (min) | $\Delta \omega_{\text{max}}$ (1.3 $\mu$m) | $a$ (1.3 $\mu$m) | $r$ (1.3 $\mu$m) |
|--------------|--------------|----|----|-----------------|-----------------|----------|----------|-----------------|---------------|---------------|
| KDR          | TE           | 1  | 2  | 23              | 0.25            | 0.25     | 0.19     | 0.35            | 305           | 0.32          | 0.08          |
|              | TE           | 3  | 4  | 5               | 0.56            | 0.20     | 0.14     | 0.23            | 63            | 0.72          | 0.14          |
|              | TM           | 3  | 4  | 40              | 0.58            | 0.12     | 0.03     | 0.26            | 539           | 0.76          | 0.09          |
|              | TM           | 10 | 11 | 12              | 1.13            | 0.12     | 0.08     | 0.16            | 156           | 1.47          | 0.18          |
|              | TM           | 19 | 20 | 9               | 1.33            | 0.15     | 0.13     | 0.18            | 120           | 1.72          | 0.27          |
|              | TE+TM        | 4  | 5  | 3               | 0.38            | 0.21     | 0.19     | 0.22            | 42            | 0.49          | 0.10          |
| KAR          | TE           | 6  | 7  | 18              | 0.69            | 0.23     | 0.13     | 0.25            | 240           | 0.89          | 0.20          |
|              | TE           | 9  | 10 | 5               | 0.95            | 0.20     | 0.16     | 0.25            | 97            | 1.10          | 0.22          |
|              | TM           | 1  | 2  | 48              | 0.40            | 0.34     | 0.17     | 0.46            | 668           | 0.52          | 0.18          |
|              | TM           | 4  | 5  | 6               | 1.04            | 0.41     | 0.21     | 0.33            | 72            | 1.35          | 0.55          |
|              | TM           | 12 | 13 | 7               | 0.95            | 0.25     | 0.21     | 0.27            | 89            | 1.23          | 0.31          |
|              | TE+TM        | 21 | 22 | 5               | 0.94            | 0.25     | 0.23     | 0.27            | 67            | 1.23          | 0.30          |
|              | TE+TM        | 24 | 25 | 2               | 0.98            | 0.24     | 0.24     | 0.25            | 23            | 1.28          | 0.31          |
| PDS          | n.a.         | 2  | 3  | 14              | 0.45            | 0.19     | 0.16     | 0.24            | 179           | 0.59          | 0.11          |
| PAS          | n.a.         | 2  | 3  | 26              | 0.59            | 0.27     | 0.18     | 0.32            | 344           | 0.76          | 0.21          |
| PAR          | n.a.         | 2  | 3  | 25              | 0.60            | 0.23     | 0.10     | 0.28            | 336           | 0.78          | 0.18          |

KDR, kagomé lattice of dielectric rods; KAR, kagomé lattice of air rods; PDS, pyrochlore lattice of dielectric spheres; PAS, pyrochlore lattice of air spheres; PAR, pyrochlore lattice of air rods; LB, lower band defining the PBG; UB, upper band defining the PBG; $r/a$ at which the maximum midgap to band gap ratio occurs; $r_{\text{min}}$ and $r_{\text{max}}$ are the minimum and maximum values of $r/a$ between which there is a band gap, respectively; $\Delta \omega_{\text{max}} (1.3 \mu$m) stands for the maximum value of the band gap (in nm) at $\lambda = 1.3 \mu$m; and $a$ and $r$ are the lattice parameter and radius of the feature (sphere, rod, ...) in $\mu$m at which that maximum occurs for $\lambda = 1.3 \mu$m, respectively.

Geometry, now there are also various large TE gaps. For example, the TE gap occurring between the sixth and seventh TE bands has a $\Delta \omega / \omega_m = 18\%$ (240 nm at $\lambda = 1.3 \mu$m for $\varepsilon = 12$). What is even more interesting is the appearance of two PBGs for all polarizations at large frequency values. The lower one, between bands 21 and 22, has a $\Delta \omega / \omega_m = 5\%$. The important point about this gap is that due to the large frequency value at which it appears ($\omega_m a / 2\pi c \sim 1$), the lattice spacing required for applications at 1.3 $\mu$m would be $a \sim 1.3 \mu$m and the diameter of the rods $r \sim 0.6 \mu$m, even larger than those for the honeycomb lattice [1]. The band structure for this lattice at the value of $r/a$ that maximizes the complete gap (figure 3(c)) shows even more interesting features than the previous geometry. Indeed, the group velocity anomaly is even more noticeable for various TE and TM bands (most noticeably TM bands 1, 6, 9 and 11, TE bands 2, 5, 9 and 10 in the MK direction, and other higher energy bands for both polarizations). Again, this effect is clearly seen in the density of states. This time, however, it occurs very markedly around the PG.

Let us now turn our attention to the results for the 3D pyrochlore lattices. The band gap maps in this case are much simpler than for the 2D lattices but, at the same time, more appealing from the applications point of view. The most interesting result is that the three topologies studied in this work exhibit a cPBG between bands 2 and 3 that extends over a relatively wide range...
of $r/a$ values. The lattice of dielectric spheres in air (see figure 4(b)) exhibits a nice size gap with $\Delta \omega / \omega_m \sim 14\%$ for $\varepsilon = 12$ (179 nm gap at $\lambda = 1.3 \, \mu m$) at $r/a = 0.19$. However, fabricating the corresponding photonic crystal would require making spheres of $\sim 0.2 \, \mu m$ diameter, which still constitutes a formidable task. On the other hand, the inverse lattice made of air spheres in dielectric (see figure 5(b)) exhibits a large gap comparable to that of the inverse diamond lattice (which to our knowledge is the lattice displaying the biggest photonic gap) with a band gap to midgap ratio $\sim 26\%$ for $\varepsilon = 12$ (344 nm gap at $\lambda = 1.3 \, \mu m$) at $r/a = 0.27$. In this latter case, the lattice spacing required for applications at $1.3 \, \mu m$ is $a \sim 0.76 \, \mu m$ and the diameter of the air spheres is $\sim 0.41 \, \mu m$. These figures are more favourable from the manufacturing point of view than for the direct lattice. The band gap map for the pyrochlore lattice of air rods in dielectric (see figure 6(b)) is quite similar to the previous one, though shifted towards smaller values of $r/a$. The maximum band gap to midgap ratio in this case is $25\%$ for $\varepsilon = 12$ (336 nm gap at $\lambda = 1.3 \, \mu m$) at $r/a = 0.23$. This implies drilling channels of diameter 0.36 $\mu m$ for applications at $\lambda = 1.3 \, \mu m$.

If we now take a look at the band structure for these lattices ((c) panel in figures 4–6), we can notice that they are not that different from each other and, in turn, they are not that different from the one for the diamond lattice either, especially for the lower bands. To further stress this point, I have depicted in figure 5(a) the band structure for a diamond lattice of air spheres in dielectric for the radius of these spheres that maximizes the photonic band gap of this lattice ($r/a = 0.325$). As can be noticed, the band structures for both the diamond and pyrochlore inverse lattices are almost identical except for the fact that diamond bands above the second are shifted towards higher frequencies (which leads to a larger CPBG). More significant differences have to be sought at even higher frequencies than those depicted in figure 5(a). There are various reasons why these band structures are so similar in spite of coming from lattices with different symmetry. On the one hand, both lattices are related to the fcc symmetry. The diamond lattice is formed by two interpenetrating fcc lattices shifted with respect to each other by a vector $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$, whereas the pyrochlore lattice is formed by four interpenetrating fcc lattices that define another fcc lattice. This has the obvious consequence that the first Bz of both the diamond and pyrochlore lattices are similar to that of the fcc lattice, that is, they are as spherical as possible, which is known to favour the formation of a CPBG. On the other hand, in the particular case of a pyrochlore lattice of air spheres in dielectric and for the sphere radius that maximizes the CPBG, the air spheres overlap in such a way that the remaining dielectric material resembles very much the analogous diamond lattice at the sphere radius that maximizes the CPBG in this latter case, as can be seen in figure 7, where both structures are depicted for the value of $r/a$ that maximizes the corresponding photonic band gap. In fact, if the dielectric vein marked with a red ellipse (and the equivalent ones by symmetry operations) were removed, both structures would possess the same symmetry. Moreover, it is precisely these extra dielectric veins in the pyrochlore lattice that cause this lattice to have a slightly large filling fraction (21%) when compared to the diamond lattice depicted in figure 7(a) (19%), which yields a larger CPBG in this latter case.

The density of photonic states for the 3D lattices depicted in figures 4(c)–6(c) provides again information in a very intuitive fashion: at low frequencies, we can observe the quadratic behaviour of this quantity, exactly as for EM waves propagating in a 3D homogeneous material, for the reasons explained above. At higher frequencies, the periodic character of the medium clearly shows up as non-trivial features of this quantity, including some peaks associated to flat bands and small group velocity, as explained before. For the pyrochlore lattice of air spheres in dielectric, it has also been depicted in figure 5(c) that the density of states for an diamond lattice...
Figure 7. (a) A diamond lattice of air spheres in dielectric at $r/a = 0.325$, which is the value of the $r/a$ ratio that maximizes the PBG of this structure for $\varepsilon = 12$. (b) A pyrochlore lattice of air spheres in dielectric at $r/a = 0.27$, which is the value of the $r/a$ ratio that maximizes the PBG of this structure for $\varepsilon = 12$. See text for an explanation of the ellipse surrounding the dielectric vein for the pyrochlore lattice of air spheres.

Figure 8. Evolution of the band gap-to-midgap ratio with $\varepsilon$ for the structures studied in this work. See the legend of table 1 for the notations used in the legend of this figure.

of air spheres in dielectric at the value of the radius that maximizes the corresponding CPBG in order to further stress the similarity between the photonic properties of these two lattices discussed in the previous paragraph.

A study of the evolution of the band gap size with varying $\varepsilon$ at the value of $r/a$ that maximizes the corresponding gap for $\varepsilon = 12$ has also been performed and the results are displayed in figure 8. For the 2D lattices, only the evolution of the largest gap occurring for each polarization and that of the total gap (see table 1) has been studied. As briefly mentioned before, the total gaps for the 2D kagomé lattices are very small and only exist above very large values of $\varepsilon$ ($\varepsilon \sim 10.5$...
for the kagomé lattice of dielectric rods and $\varepsilon \sim 9$ for the kagomé lattice of air rods in dielectric). Therefore, these gaps are not very robust and it is very likely that, in real systems, they do not show up because of the disorder always present in real structures that tends to destroy the gap. The partial gaps, however, exist down to $\varepsilon \sim 2-2.5$, except for the first TE gap in the kagomé lattice of air rods in dielectric, which shows a crossover to a linear $\varepsilon$ dependence for $\varepsilon < 4.5$ and disappears for $\varepsilon \sim 3.5$. Even though this is an interesting behaviour that deserves further study, we do not have an explanation for it at this point. With regard to the gaps for the 3D lattices, the one for the pyrochlore lattice of dielectric spheres subsists down to $\varepsilon \sim 4.4$, whereas the evolution of the gap size with $\varepsilon$ for both the pyrochlore lattices of air spheres and air rods in dielectric survive down to $\varepsilon \sim 4$ and, actually, the curves that describe their behaviours are almost identical.

Even though this is not the main topic of the present paper, the plausibility of fabricating the structures studied in this work has been commented. A more detailed discussion about this subject will be given elsewhere [38]. Regarding the 2D lattices, the feature size and lattice spacing required for applications at $\lambda = 1.3 \mu m$ (see table 1) are well in the reach of current technological capabilities. In some cases, these sizes are even more favourable than the corresponding ones for photonic crystals based on the triangular lattice, which are routinely made in the laboratory, especially for the kagomé lattice of air rods in dielectric. Therefore, it should not be too difficult to fabricate this structure by using currently available lithographic techniques [39] or sedimentation of a binary mixture of colloidal particles. Indeed, photonic crystals based on the kagomé lattice have been made by Velikov et al [40] and ultrabroad spectra have been generated in such a photonic crystal by Glas et al [41]. Fabrication of the 3D structures, however, it is very likely more complicated. Fortunately, there are some geometrical features of the pyrochlore lattice that could simplify this task. In particular, the pyrochlore lattice can be built by stacking alternating triangular and kagomé lattices in an ABAB... sequence [38]. Given the fact just mentioned that triangular layers are relatively easy to make and that kagomé layers have been made in the laboratory [40], it is likely that photonic crystals with topologies based on spheres and the symmetry of the pyrochlore lattice could be fabricated by using sedimentation of colloidal particles in a layer-by-layer fashion. On the other hand, the pyrochlore lattice of air rods is amenable of fabrication for applications in the microwave regime by a technique analogous to the one that allowed to make the well-known Yablonovite structure some years ago [9], namely, by drilling or etching the air channels in a block of dielectric. In the visible range, ion beams or holographic techniques could probably be used to drill the channels. One possible pathway that can be followed to create the channel structure of the right geometry is depicted in figure 9. It consists on using two masks containing a triangular pattern which are arranged perpendicular to each other as shown in the figure and with the common edge parallel to one of the edges of the dielectric block (the $X$-direction). The channels are then drilled perpendicularly to the masks. Later, the masks are oriented with the common edge parallel to the $Y$ and $Z$ directions and the drilling operation is repeated. Of course, the procedure is not as simple as for the Yablonovite structure, but the size of the gap that can be obtained in this way makes it worth trying.

3. Conclusions

In this work, the photonic band gap maps of photonic crystals based on the kagomé and pyrochlore lattices have been reported. These exhibit important photonic properties that make them relevant
from the applications point of view. Two structures have been investigated in two dimensions, a kagomé lattice of dielectric rods in air and the inverse lattice consisting on a kagomé lattice of air rods in a dielectric matrix. The band gap maps for different values of the $r/a$ ratio and index contrast for EM waves propagating in the plane of the lattice are very rich and exhibit numerous band gaps for TM and TE polarizations. In the direct lattice, these gaps do not overlap, which makes this structure a good candidate for polarization-dependent devices. However, the inverse lattice of air rods in dielectric exhibits a complete, albeit small, photonic gap at the dimensionless frequency $\omega a / 2\pi c \approx 1$, which implies an advantageous $a \approx \lambda$ lattice parameter for actual device fabrication. In three dimensions, three different topologies have been studied, a pyrochlore lattice of dielectric spheres in air, the inverse structure consisting on a pyrochlore lattice of air spheres in a dielectric matrix, and the structure formed by air cylinders that connect the centres of the ‘atomic positions’ in the pyrochlore lattice embedded in a dielectric medium. These three cases exhibit large complete band gaps in a wide range of the $r/a$ ratio and index contrast. Especially interesting is the case of air spheres in dielectric, which exhibits a complete band gap with a maximum band gap to midgap ratio of 26% for $\varepsilon = 12$. The similarities between the photonic band structure for this lattice and an inverse diamond lattice have been discussed on the basis of the similar geometry shared by both structures for the value of the $r/a$ ratio that maximizes the corresponding CPBG. The lattice made of air cylinders in dielectric, on the other hand, is very convenient from a fabrication point of view and also exhibits a complete band gap of the same size as the the previous topology. The lattice parameter and feature size required to fabricate devices based on these symmetries are also very convenient, especially for the pyrochlore lattice of air spheres in dielectric and the tubular structure of air rods in dielectric.

Of course, this is not a closed topic. There is a wealth of additional studies that could be performed in order to further assess the usefulness of these new symmetries for applications. For example, one could try to optimize the size of the gaps by using coated spheres or cylinders or using slightly different topologies. Additionally, it would be very interesting to study how robust the photonic gaps are against positional and/or compositional disorder that will always occur in
real systems. Also, it is crucial to consider how well these geometries could confine and guide light by introducing different kinds of organized defects such as channels or point defects.

Furthermore, it would be very important from a fundamental point of view to investigate why lattices based on triangular units (such as the triangular, honeycomb or kagomé lattices in 2D and the fcc, diamond and pyrochlore lattices in 3D) have such a propensity to form CPBGs. Qualitatively, it can be seen that this comes about because of the inability of these systems to reconcile both local and extended symmetry constraints at the same time; that is, due to the special geometry of these lattices, it is not possible to fulfil the global requirement of the orthogonality of the modes belonging to different eigenvalues while, at the same time, transforming according to the local symmetry group. Therefore, a gap appears in a certain energy range. This competition between local and extended degrees of freedom that leads to interesting new phenomenon is usually termed ‘geometrical frustration’ in other fields of physics [25, 27]. Therefore, it would be very interesting if one could bridge a link between the optical properties of photonic band gap materials and the concept of geometrical frustration. However, putting these facts into a formal mathematical basis is quite involved in the general case and this research programme is currently underway.

In conclusion, it is hoped that this work serves the purpose of stimulating other researchers in this field to further explore the properties of materials based on the kagomé and pyrochlore lattices for prospective photonic applications.

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References

[1] Joannopoulos J D, Meade R D and Winn J N 1999 Photonic Crystals: Molding the Flow of Light (Princeton, NJ: Princeton University Press)
[2] Johnson S G and Joannopoulos J D 2003 Photonic Crystals: The Road from Theory to Practice (London: Luwer Academic)
[3] John S 1987 Strong localization of photons in certain disordered dielectric superlattices Phys. Rev. Lett. 58 2486–9
[4] Yablonovitch E 1987 Inhibited spontaneous emission in solid-state physics and electronics Phys. Rev. Lett. 58 2059–62
[5] Yablonovitch E and Gmitter T J 1989 Photonic band structures: the face-centered cubic case Phys. Rev. Lett. 63 1950
[6] Ho K M, Chan C T and Soukoulis C M 1990 Existence of photonic gaps in periodic dielectric structures Phys. Rev. Lett. 65 3152–5
[7] Martorell J and Lawandy N M 1990 Observation of inhibited spontaneous emission in a periodic dielectric structure Phys. Rev. Lett. 65 1877
[8] Chan C T, Ho K M and Soukoulis C M 1991 Photonic band gaps in experimentally realizable periodic dielectric structures Europhys. Lett. 16 563
[9] Yablonovitch E, Gmitter T J and Leung K M 1991 Photonic band structures: the face-centered cubic case employing non-spherical atoms Phys. Rev. Lett. 67 2295
[10] Meade R D, Brommer K D, Rappe A M and Joannopoulos J D 1991 Electromagnetic Block waves at the surface of a photonic crystal Phys. Rev. B 44 10961
[11] Meade R D, Brommer K D, Rappe A M and Joannopoulos J D 1992 Existence of a photonic band gap in two dimensions Appl. Phys. Lett. 61 495
[12] Chow E et al 2000 Three-dimensional control of light in a two-dimensional photonic crystal slab Nature 407 983–6
[13] Joannopoulos J D 2001 Self-assembly lights up Nature 414 257–8
[14] Sakoda K 2001 Optical Properties of Photonic Crystals (Heidelberg: Springer)
[15] Fleischer J W, Segev M, Efremidis N K and Christodoulides D N 2003 Observation of two-dimensional discrete solitons in optically induced nonlinear photonic lattices Nature 422 147–50
[16] Akahane Y, Asano T, Song B S and Noda S 2003 High-Q photonic nanocavity in a two-dimensional photonic crystal Nature 425 944–7
[17] Soljacic M and Joannopoulos J D 2004 Enhancement of nonlinear effects using photonic crystals Nat. Mater. 3 211–9
[18] Maldovan M, Ullal C K, Carter W C and Thomas E L 2003 Exploring for 3D photonic bandgap structures in the 11 f.c.c. space groups Nat. Mater. 2 664–7
[19] Garcia-Santamaria F 2003 Photonic crystals based on silica microspheres PhD Thesis Universidad Autónoma de Madrid
[20] Blanco A et al 2000 Large-scale synthesis of a silicon photonic crystal with a complete three-dimensional bandgap near 1.5 micrometres Nature 405 437–40
[21] Toader O and John S 2001 Proposed square spiral microfabrication architecture for large three-dimensional photonic band gap crystals Science 292 1133–5
[22] Noda S, Tomoda K, Yamamoto N and Chutinan A 2000 Full three-dimensional photonic bandgap crystals at near-infrared wavelengths Science 289 604–6
[23] Fleming J G, Lin S Y, El-Kady I, Biswas R and Ho K M 2002 All-metallic three-dimensional photonic crystals with a large infrared bandgap Nature 417 52–5
[24] Qi M H 2004 A three-dimensional optical photonic crystal with designed point defects Nature 429 538–42
[25] Ramirez A P 2003 Geometric frustration: magic moments Nature 421 483
[26] Schiffer P 2002 Condensed-matter physics: magnetic frustration squeezed out Nature 420 35–8
[27] Garcia-Adeven A J and Huber D L 2000 Quantum tetrahedral mean field theory of the magnetic susceptibility for the pyrochlore lattice Phys. Rev. Lett. 85 4598–601
[28] Bramwell S T and Gingras M J P 2001 Spin ice state in frustrated magnetic pyrochlore materials Science 294 1495–501
[29] Shannon N 2002 Mixed valence on a pyrochlore lattice—LiV2O as a geometrically frustrated magnet Eur. Phys. J. B 27 527–40
[30] Taguchi Y, Oohara Y, Yoshizawa H, Nagaosa N and Tokura Y 2001 Spin chirality, Berry phase, and anomalous Hall effect in a frustrated ferromagnet Science 291 2573–6
[31] Lee W-L, Watauchi S, Miller V L, Cava R J and Ong N P 2004 Dissipationless anomalous Hall current in the ferromagnetic spinel CuCr2Se4−xBrx Science 303 1647–9
[32] Hermel M, Fisher M P A and Balents L 2004 Pyrochlore photons: the U(1) spin liquid in a S = 1/2 three-dimensional frustrated magnet Phys. Rev. B 69 6440401–21
[33] Johnson S G and Joannopoulos J D 2001 Block-iterative frequency-domain methods for Maxwell’s equations in a planewave basis Opt. Express 8 173–90. See also http://ab-initio.mit.edu/mpb/
[34] Nielsen J B, Sondergaard T, Barkou S E, Bjarklev A, Broeng J and Nielsen M B 1999 Two-dimensional kagomé structure, fundamental hexagonal photonic crystal configuration Electron. Lett. 35 1736–7
[35] Nielsen J B, Sondergaard T, Barkou S E, Bjarklev A and Broeng J 2000 Two-dimensional kagome photonic bandgap waveguide IEEE Photon. Technol. Lett. 12 630–2
[36] Susa N 2002 Large absolute and polarization-independent photonic band gaps for various lattice structures and rod shapes J. Appl. Phys. 91 3501–10
[37] Takeda H, Takashima T and Yoshino K 2004 Flat photonic bands in two-dimensional photonic crystals with kagome lattices J. Phys.: Condens. Matter 16 6317–24
[38] Garcia-Adeva A J, Balda R and Fernandez J 2005 The density of electromagnetic modes in photonic crystals based on the pyrochlore and kagomé lattices Opt. Mat. 27 1733–42
[39] Lópezc C 2003 Materials aspects of photonic crystals Adv. Mater. 15 1679
[40] Velikov K P, Christova C G, Dullens R P A and van Blaaderen A 2002 Layer-by-layer growth of binary colloidal crystals Science 296 106
[41] Glas P, Fischer D, Steinmeyer G, Husakou A, Herrmann J, Iliew R, Skibina N B, Beloglasov V I and Skibina Y S 2005 Supercontinuum generation in a two-dimensional photonic kagome crystal Appl. Phys. B 81 209