Bandgap properties of two-dimensional low-index photonic crystals

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Abstract We study the bandgap properties of two-dimensional photonic crystals created by a lattice of rods or holes conformed in a symmetric or asymmetric triangular structure. Using the plane-wave analysis, we calculate a minimum value of the refractive index contrast for opening both partial and full two-dimensional spectral gaps for both TM and TE polarized waves. We also analyze the effect of ellipticity of rods and holes and their orientation on the threshold value and the relative size of the bandgap.

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1 Introduction

It is well established that three-dimensional periodic dielectric structures, called photonic crystals, possess one or many complete photonic band gaps in the transmission spectrum for propagation of electromagnetic waves [1]. Light-based technological applications have their roots in planar technology, which requires a knowledge of the bandgap properties of two-dimensional structures assumed an infinitely long extension in the third dimension. The theoretical study of photonic crystals in two dimensions is easier due to the fact that in this case the wave propagation can be analyzed separately for two different polarizations, thus the original vector problem is reduced to two scalar problems. These polarizations are Transverse Magnetic (TM), if the electric field is perpendicular to the plane defining the structure, and Transverse Electric (TE), if the same occurs for the magnetic field. When the bandgaps for two different polarizations overlap, they create a combined band gap known as an absolute (or full) photonic bandgap. Several structures are known to possess photonic band gaps for one of these polarizations and for both polarizations simultaneously, as examined comprehensively for high values of the refractive index ratio in the two-dimensional geometry [2].

One of the classical results in the theory of photonic crystals is the existence of the critical (minimum) value of the refractive index contrast to open a full spectral band gap in a three-dimensional geometry [1]. For example, as was first shown by Ho et al. [3], a diamond structure requires the minimum refractive index contrast larger than 2. Similarly, the threshold values of the refractive index appears in the theory of two-dimensional photonic crystals [4]. In particular, a triangular lattice of air holes in a dielectric material possesses a large band gap for TE polarized waves and a complete one for larger air holes.

Recently, several experimental groups demonstrated novel methods for fabricating photonic crystals in solid polymer materials. In particular, the group of Min Gu [5, 6] employed the generation of submicron-size void channels by tightly focused femtosecond-pulsed laser light; the technique is a one-step approach which does not require chemical postprocessing, and it allows to fabricate photonic crystals with a high degree of perfection. In addition, the studies of Zhou et al. [7] demonstrated two-dimensional triangular void channel photonic crystals fabricated by femtosecond laser drilling in a solid polymer material, and characterized their properties for TE and TM polarized illumination. Although complete photonic band gaps cannot exist in low-index contrast structures, two-dimensional band gaps are possible for specifically polarized electromagnetic modes, and such structures can be used for photonic-crystal optical devices such as superprisms or waveguides.

The purpose of this paper is twofold. First, we calculate the dependence of the spectral bandgaps on the refractive index contrast for the two most popular types of triangular lattices of two-dimensional photonic crystals. In particular, we find the critical value of the refractive index contrast for opening partial (for TM or TE polarized waves, respectively) as well as full two-dimensional spectral band gaps. Second, being motivated by the recent success in fabricating low-index photonic crystal
structures in solid polymers and chalcogenide glass, we explore further the concept of the partial bandgaps of two-dimensional photonic crystals and analyze the effect of ellipticity of rods and holes and their orientation on the critical value and the size of both partial and full spectral bandgaps.

As we assume that the materials we are working with are macroscopic and isotropic, we are able to define the refractive index as \( n = \epsilon^{1/2} \) keeping \( \mu = 1 \). In this paper, we also interchange between the \( \omega a/2\pi c \) form and the \( a/\lambda \) forms to show more clearly how the ratio increases with a decreasing refractive index, as shown by Li et al. \[8\].

The paper is organized as follows. In Sec. 2 we consider a two-dimensional photonic crystal created by a triangular lattice of dielectric rods in air. In this case, a partial gap appears first for the TM polarized waves, and it is shown to require a relatively low index contrast. In Sec. 3 we consider the same problem for a two-dimensional photonic crystal created by air holes drilled in a dielectric slab, where the bandgaps first appear for the TE polarized waves. And last, Sec. 4 concludes the paper.

2 Dielectric rods in air

First, we consider a two-dimensional photonic crystal created by a triangular lattice of circular or elliptic dielectric rods assuming an arbitrary rotation of the elliptic rod relative to the lattice symmetry axis. The photonic bandgap spectrum is calculated by solving Maxwell equations by means of the plane-wave expansion method \[9\] employing the well-known numerical algorithm \[10\].

An example of the photonic band-gap structure of such a two-dimensional photonic crystal is shown in Fig. 1 for the well-known case of a triangular lattice of circular rods. The rods have the electric permittivity \( \epsilon = 5.8 \) that corresponds to the values measured for planar waveguides made of chalcogenide glass \[11\]. In this case, the frequency spectrum of a lattice of circular rods display several gaps for the TM polarized waves, and two relatively large lower bandgaps with the relative size 27.15% and 14.61%, respectively.

As the next step, we verify a general concept of the bandgap spectrum of asymmetric lattices \[12\] and consider a triangular lattice made of elliptic rods with an arbitrary orientation. In particular, we study the effect of the hole rotation on the value of the partial and absolute bandgaps. These results can naturally be compared with the bandgap spectra of the two-dimensional structures created by circular holes (see below). In a full agreement with the previous studies \[13\] and recent fabricated devices \[14\], we observe that for the case of dielectric rods in air a deviation of the cylinders from a circular symmetry produces a reduction of the relative size of the bandgaps. The similar effect is produced by the rod rotation, so that larger values of the photonic band gap are observed for the ellipses with smaller or no rotation (dotted curve in Fig. 2), and the bandgap becomes maximum for the case of circular rods.

Finally, we study how the ellipticity of the dielectric rods in the triangular-lattice photonic crystal may change the size of the maximum TM bandgap at different values of the filling fraction. We assume that the dielectric rods are ellipses with the axes \( C_x \) and \( C_y \), and we vary the value of \( C_x \) for a fixed orientation, also changing the size of \( C_y \) in order to keep the filling fraction constant. Figure 3 summarizes some of our results for three values of the filling fraction, 44.5% (solid), 30% (dotted), and 22.5% (dashed). The main result is that the maximum value of bandgap is achieved for a triangular lattice of circular rods (here, at \( C_x = C_y = 0.575 \)) with the filling fraction 30%. This result is in agreement with

![Fig. 1](image)

**Fig. 1** Bandgap spectrum of TM (left) and TE (right) polarized waves for a triangular lattice of circular rods \( C_x = C_y = 0.575 \) at \( \epsilon = 5.8 \) which is the permittivity of the chalcogenide glass waveguides \[11\].

![Fig. 2](image)

**Fig. 2** (a,b) Relative size of the partial bandgaps for TM (left) and TE (right) polarized waves for a triangular lattice of circular (solid curve) and elliptic (other three curves) rods as a function of \( \epsilon \) for the filling factor 30%. Dotted, dashed, and dot-dashed curves show the results for the elliptic rods \( C_x = 0.65, C_y = 0.51 \) with 0°, 15°, and 30° rotation angle. The critical value for the TM bandgap is \( \epsilon = 1.73 \). Stars indicate the permittivity of polymer \[3\] (at \( \epsilon = 2.4 \)) and the permittivity of the chalcogenide glass waveguides \[11\] (at \( \epsilon = 5.8 \)). Note the significant difference in scale of the two graphs.
Fig. 3 Effect of varying rod ellipticity and filling fraction on the size of the TM bandgap. Shown is the relative size of the lower bandgap of the TM polarized waves (see Fig. 1) as a function of $C_x$, with $C_y$ varying to retain a constant filling fraction, at $\epsilon = 2$. Maximum bandgap is found for the circles ($C_x = C_y = 0.575$) with the filling fraction 30%.

all previous studies of triangular-lattice two-dimensional photonic crystals.

3 Air holes drilled in dielectric

Next, we consider the other important case when a two-dimensional photonic crystal is created by a triangular lattice of circular [see Fig. 4] or elliptic [see Fig. 5] holes drilled in a dielectric slab, assuming an arbitrary rotation of the elliptic hole relative to the lattice symmetry axis.

As opposed to the case of rods, air holes produce an extremely large bandgap in the TE spectrum of a photonic crystal, this is demonstrated experimentally in the work of Zhou et al. [4]. The key advantage to this system as opposed to rods is the frequency position of the bandgap, especially for the case shown in Fig. 4 which is the case of the refractive index corresponding to the chalcogenide glass waveguides [11]. When it is viewed as a wavelength using the simple conversion $\omega a / 2\pi c = a / \lambda$ we can see that with the bandgap around $a / \lambda = 1$, the wavelength of the confined light is equal to the size of the lattice giving us the ability to fabricate the planar structures on the scale of the wavelength of interest unlike the common $a / \lambda$ values of 0.3 to 0.5 which would lead to structures 1/3 to 1/2 of the lattice size in order to produce a bandgap for the same wavelength, a challenge for any fabrication method.

Another advantage is in the nature of the holes drilled in a dielectric structure such as physical resistance to a damage. Indeed, the rods which, when being fabricated with the large aspect ratios to exhibit bandgaps, are very sensitive to a physical damage, whereas the hole structure, which has a constant lattice of joined dielectric is far stronger and therefore more resistant to the rigors of the fabrication processes than free-standing rods.

For the photonic crystals fabricated in the chalcogenide glass waveguides [11], round holes, 1139nm in diameter, forming a trigonal lattice with a lattice spacing of 1550nm should provide a photonic bandgap at telecommunications wavelengths. This should also, as shown by the previous studies, be able to support different guided modes although the adaptation of the structure to the specific optical devices should be analyzed in more details.

As follows from Figs. 5(a,b), the tradeoff when optimizing the structures also applies to the hole photonic crystals. In this case, the effect of rotation is insignificant and the case of purely circular holes is optimal and produces a bandgap of over 40% at $\epsilon = 10$. When comparing Fig. 2 and Fig. 5 we can see that the TM bandgap for the rod structure starts at a lower value of the permittivity than the TE bandgap for holes, and it can be seen that the rod bandgap is larger than the hole bandgap until around $\epsilon = 2.8$ after which the hole
bandgap becomes significantly larger ($\approx 7\%$ at $\epsilon = 10$). This should be taken into consideration when choosing an appropriate structure for a given fabrication process.

Figure 6 shows, by a very steep drop-off on all curves, that ellipticity has a far greater effect in this system than on the system shown in Fig. 3. It should be remembered in these two graphs that after the system passes through the point corresponding to a circle it becomes an equivalent ellipse rotated by 30º. While this will prove a problem for fabrication the bandgaps are large enough that small errors in ellipticity will not lead to the removal of the bandgap completely. It can also be seen that an error towards larger holes, visualized as a lower filling fraction of dielectric, retains the bandgap size better than a reduction in the hole size.

Our results demonstrate that a threshold value of the permittivity to open a partial bandgap is 1.73 which equates to a refractive index of 1.31, and we therefore believe that it is safe to rule out attempts at producing photonic bandgap devices in any system with a refractive index contrast for opening partial (either for TM or TE polarized waves) and full two-dimensional spectral bandgaps. We have analyzed the effect of ellipticity of rods and holes and their orientation on the critical value and the size of the bandgaps. In particular, we have predicted that partial bandgaps may appear in the frequency spectrum for the index contrast as low as $\epsilon = 1.73$, in the case of rods (for the TM polarized waves), and $\epsilon = 2$, in the case of holes (for TE polarized waves). We have demonstrated also that, by reducing the refractive index from some large values (e.g. for Si) to lower value slightly above the threshold, we are able to obtain far more fabricable periodic structures for experiment due to an increase in the wavelength-to-period ratio. We believe that our results will be important for the current efforts in fabricating planar photonic-crystal structures based on dielectric materials with low refractive index such as solid polymers, polymer resin, and chalcogenide glasses.

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