

Band structure and field distribution of 2D photonic crystals based on nanostructured porous silicon

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Porous silicon based two-dimensional photonic crystals were designed. These consist in nanometric porous silicon rods embedded into a silicon matrix arranged as to form a triangular lattice. The photonic band structure for the TM (magnetic field in-plane) and TE (electric field in-plane) modes was calculated as a function of the radius of the rods, finding a notable dependence on this parameter. In addition, the component of the magnetic field distribution perpendicular to the two-dimensional plane for the first eight TE bands was analyzed for increasing radius of the rods.

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1. Introduction

Photonic crystals can be defined as anisotropic optical media wherein the index of refraction is a periodic function on space [1,2,3]. Accordingly, these structures can allow or prohibit light propagation in a range of wavelengths. A photonic crystal affects the properties of photons in a similar way that a semiconductor affects the behavior of electrons. Consequently, photons in photonic crystals can have band structures, localized defect modes, surface modes, etc. [4]. In this respect, the possibility of controlling light propagation has led to the proposal of many novel devices [5]. Also, the dependence of the optical behavior of the photonic crystals on polarization can lead to the development of polarization-dependent optoelectronic devices.

Although three-dimensional (3D) photonic crystals show quite interesting properties, two-dimensional (2D) photonic crystals, which also provide functionality to steer and modify the flow of light in different manners, are much easier to fabricate since the procedure is similar to that used for planar electronic integrated circuits [6]. In addition, the development of 2D photonic band gap (PBG) structures overcame two main limitations associated to the use of dielectric filters (1D PBG structures) in the field of micro-optoelectronics [7]. Firstly, for an angle of incidence greater than a critical angle, light of frequency in the band gap of the 1D PBG structure can penetrate through the film. Secondly, there is no guidance of light, which lies energetically outside the photonic band gap or within a defect band.

Nanostructured porous silicon (PS) layers can be used for the development of 1D [8, 9, 10] and 2D photonic crystals [11,12]. By the use of PS, optically-active layers of selectable index of refraction (i.e., dielectric constant) and thickness can be grown, with values determined by the electrochemical fabrication parameters [13]. The precise control over the index of refraction of PS allows the development of tunable PBG structures, and consequently tunable optical response, entirely based on silicon. In

addition to the possibility of tuning the optical response of PS, there exists great interest on this material since its fabrication is based on standard semiconductor processes, thus allowing easy and inexpensive integration into the standard microelectronic fabrication processes and on nowadays micro-optoelectronic devices.

2. Porous silicon based 2d photonic structures

PS-based 2D photonic crystals consisting in PS rods embedded into a silicon matrix arranged as to form a triangular lattice were designed. A schematic representation is shown in Fig. 1. This structure was chosen since, despite the considerable amount of research undertaken on various lattice structures, the photonic band gap for a triangular lattice remains the largest both in the TM (magnetic field in-plane) modes with fields along (Hz, Ex, Ey) and TE (electric field in-plane) modes [14], with fields along (Ez, Hx, Hy). It is important to point out that macroporous silicon has been previously used for the development of photonic crystals, basically consisting on air holes with sizes in the range of a few microns embedded into a silicon matrix [15,16,17]. The structure proposed in the present work replaces the air holes with nanometric porous silicon, with characteristic sizes of the Si crystals in the range of 20 to 80 Å [18]. Thus, porous silicon can be considered a homogeneous medium for visible and infrared radiation [13].

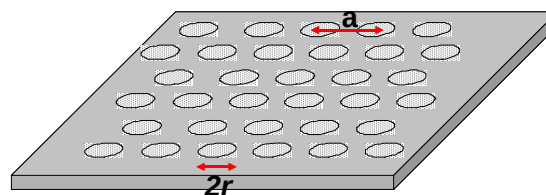


Fig. 1. Schematic of the designed PS-based 2D photonic crystals, consisting in PS rods embedded into a silicon matrix.

The experimental implementation of the designed structures can be performed by the use of a novel procedure developed in our laboratory [19]. In our experimental setup, we are able to independently vary the index of refraction of PS (n_{PS}), radius of the rods (r) and lattice parameter (a). In the present work, the photonic band structure of the designed PS-based 2D photonic crystals are calculated for PS rods of different radius, r ,

ranging from 0 to $0.5a$. Fig. 2 shows a cross-sectional view of the photonic crystals as a function of r . The height of the rods was taken to be infinity and the index of refraction of PS was kept constant ($n_{PS} = 1.4$) as to maximize the photonic band gap, based on our previous results on band structure calculations of PS/Si systems [12].

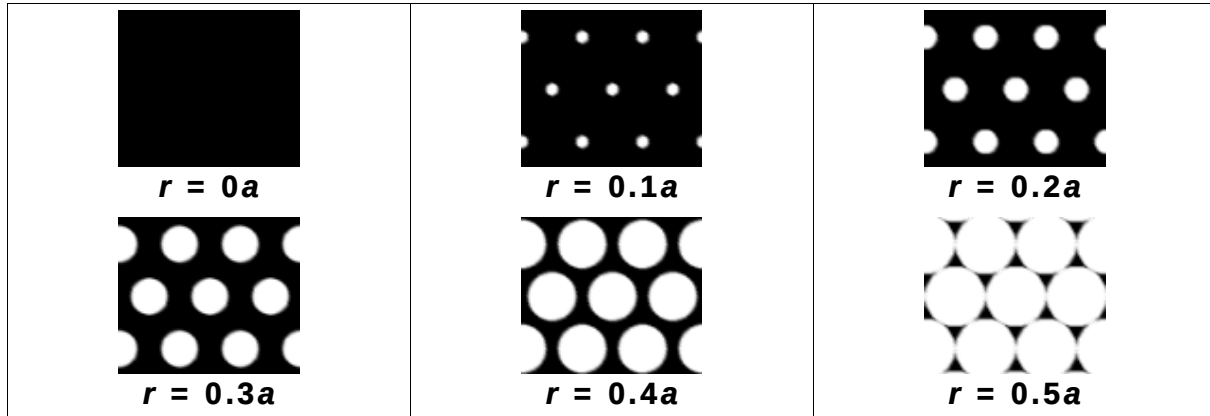


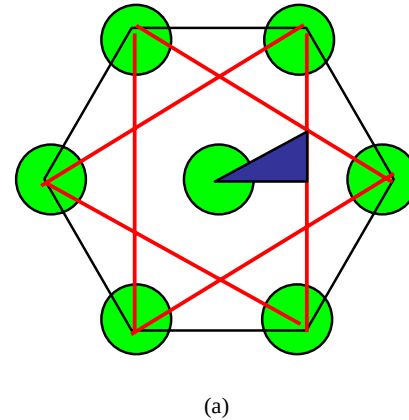
Fig. 2. Top cross-sectional view of the PS-based 2D photonic crystals for radius of the PS rods ranging from 0 to $0.5a$. Black areas correspond to Si and white to PS.

3. Computational method

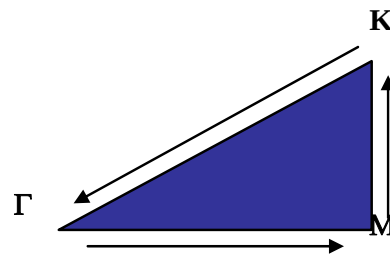
For the calculation of the photonic band structure of the PS-based 2-D photonic crystals, fully-vectorial eigenmodes of Maxwell's equations with periodic boundary conditions were computed by preconditioned conjugate-gradient minimization of the block Rayleigh quotient in a planewave basis [20,21,22]. By the use of this method it is possible to solve for interior eigenvalues without computing the many underlying eigenstates. It should be pointed out that this computational method has been previously tested on PS/Si photonic structures [12].

4. Band structure calculations (tm and te modes)

The band structure (including band gap where applicable) for the TM- and TE-like guided modes as a function of radius, r varying between 0 and $0.5a$, was calculated for the photonic crystals consisting in PS rods embedded into a silicon matrix. The values of the index of refraction of nanostructured porous silicon, n_{PS} , for the simulations were chosen based on our previous experience on its empirical determination from the optical spectra in the visible and near infrared ranges by using computational simulation techniques based on evolutionary algorithms [13]. Accordingly, n_{PS} was taken to be 1.4 since, as previously demonstrated, provides the highest band gap in the TE-like modes [12].



(a)



(b)

Fig. 3. (a) High-symmetry points within the two-dimensional Brillouin zone; and (b) irreducible Brillouin zone. The major symmetry points (Γ , M , K) are shown.

Because the TE and TM modes separate, the band structure for each polarization can be calculated independently as a function of the Brillouin zone points (Fig. 3). Thus, Figs. 4 to 8 show the calculated band structure (first eight bands) for the TM and TE modes for increasing radius of the PS rods, ranging from $r = 0.1a$ to $r = 0.5a$, being a the lattice parameter. In these plots, the normalized frequency (c/a , being c the speed of light in a vacuum) is represented versus the Brillouin zone points. From Figs. 4a to 8a no band gap is observed for the TM bands between the first and second bands. However, in some cases a band gap is found for very high frequency bands. Since these bands are usually above the light line, crystal implementation in a practical thin dielectric slab is generally impossible [2,23]. Thus, this study will mainly be focused on photonic crystals with band gap between the first two bands as to ensure that the band gap falls under the light line, enabling the fabrication of the crystal in a thin dielectric slab system.

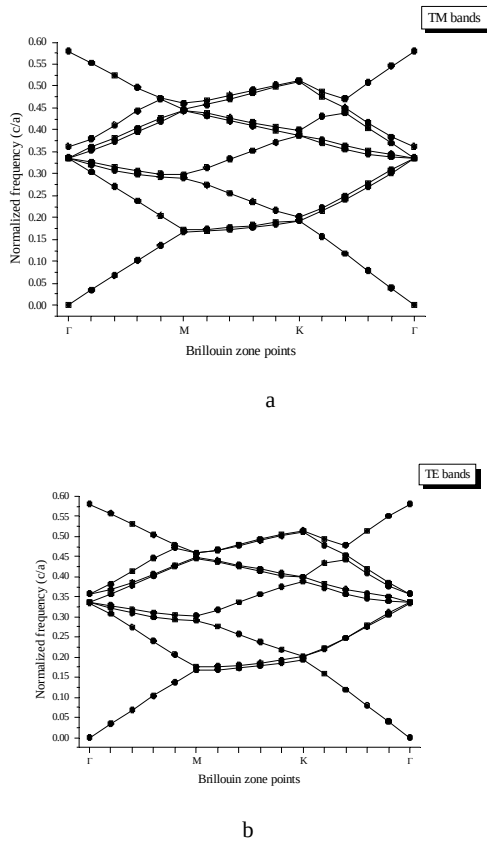


Fig. 4. (a) TM and (b) TE band structure for $n_{PS}=1.4$ and $r=0.1a$.

Calculations of the band structure for the TE bands are plotted in Figs. 4b to 8b. In the case of the TE bands, a band gap is observed from band 1 to band 2, in some cases (Figs. 6b and 7b). As expected, for $r = 0$ no band gap is observed, since in this case the structure just consists on a bulk Si macroscopic slab (see cross-sectional view, Fig. 2). It can also be noted that the value of the band gap rises for increasing radius until a maximum is reached. It

was calculated that the maximum TE band gap occurs around $r = 0.4a$ with gap size of 32 % in percentage of mid-gap frequency, and falls abruptly to 0% at $r = 0.5a$.

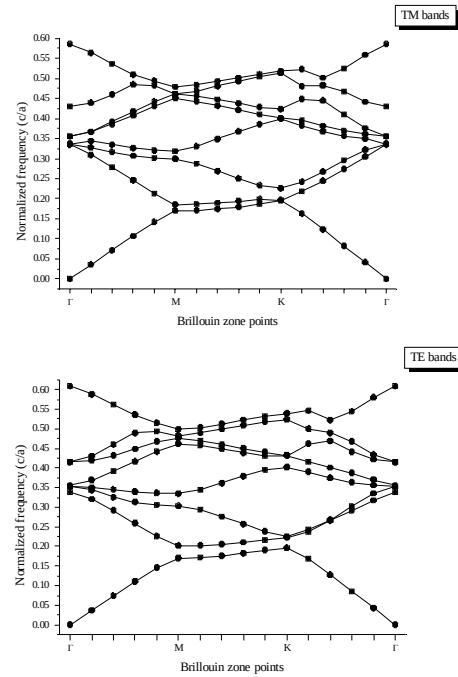


Fig. 5. (a) TM and (b) TE band structure for $n_{PS}=1.4$ and $r=0.2a$.

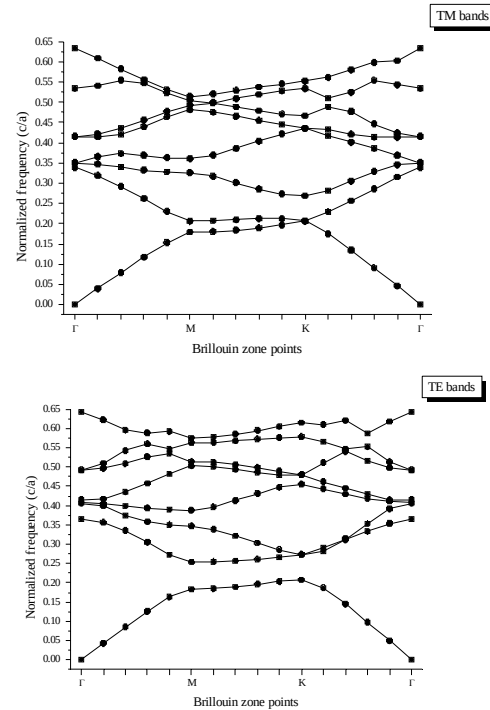


Fig. 6. (a) TM and (b) TE band structure for $n_{PS}=1.4$ and $r=0.3a$. A band-gap exist from band 1 to band 2 in the frequency range of $0.207c/a$ to $0.253c/a$ (20.12% in percentage of mid-gap frequency) for TE-like guided modes.

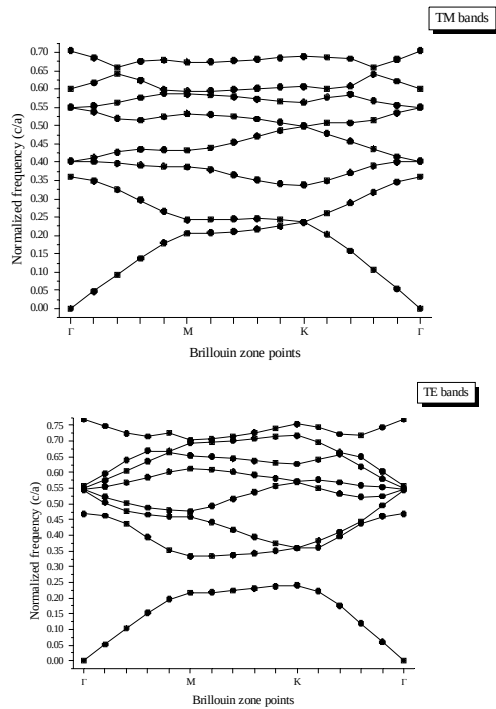


Fig. 7. (a) TM and (b) TE band structure for $n_{PS}=1.4$ and $r=0.4a$. A band-gap exist from band 1 to band 2 in the frequency range of $0.241c/a$ to $0.332c/a$ (32% in percentage of mid-gap frequency) for TE-like guided modes.

From the simulations it can be pointed out that the TE band gap could be made somewhat higher by making higher the dielectric constant contrast between the two materials, i.e. by the use of air rods rather than PS rods. However, by the use of PS one can take advantage of the tunability of n_{PS} as to control the optical response of the 2D photonic crystals for the further development of optoelectronic devices. It is also important to note that in all cases analyzed there are no complete (i.e. overlapping TE/TM) gaps.

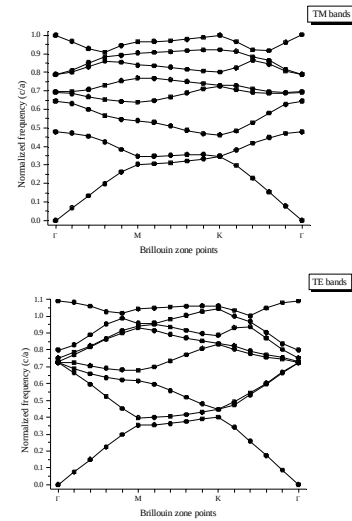


Fig. 8. (a) TM and (b) TE band structure for $n_{PS}=1.4$ and $r=0.5a$.

5. Magnetic field distributions

The field patterns will provide valuable information about the characters of the modes and provide some hints regarding the origin of the band gap. Thus, the magnetic field distribution was analyzed for increasing radius of the rods. Figs. 9 to 13 show the steady-state magnetic field distribution (H_z , real part of the z component of the magnetic field) for the first 8 TE bands at the K symmetry point for increasing radius of the rods. The H_z field component (perpendicular to the 2D plane) is shown in horizontal cross-section with blue/white/red indicating negative/zero/positive. It is apparent from Figs. 9 to 13 that in all cases the magnetic field is strongly concentrated in the rod regions (PS regions) for TE band 1, where maxima and minima for H_z are observed (red and blue tonality respectively). Accordingly, high magnetic field energy density is concentrated within the porous silicon rods, while high electric field energy density is found in the Si regions. The magnetic field distribution for the second and successive bands follows the criterion of orthogonality [23], leading to the shape shown in Figs. 9 to 13.

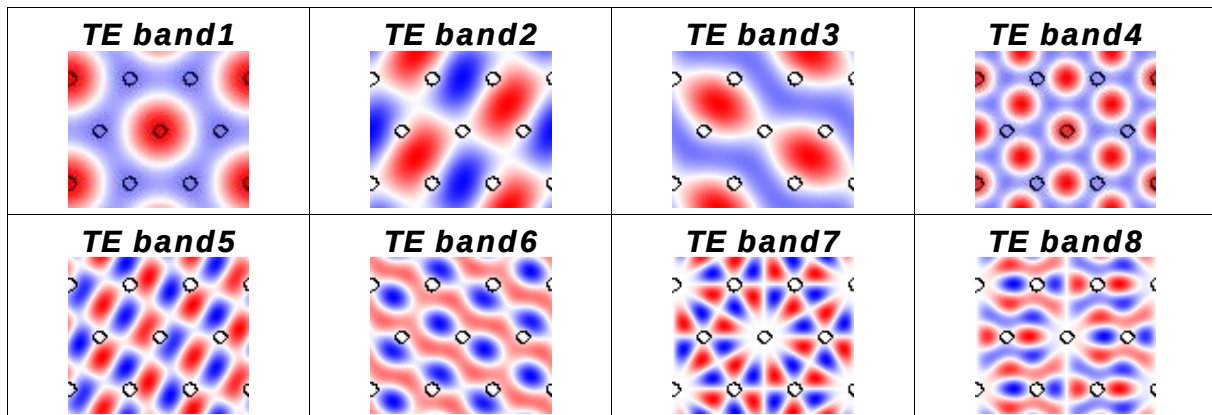


Fig. 9. Magnetic field distributions for the first eight bands at symmetry point K ($n_{PS}=1.4$ and $r=0.1a$). The H_z field component (perpendicular to the 2D plane) is shown in horizontal cross-section with blue/white/red indicating negative/zero/positive.

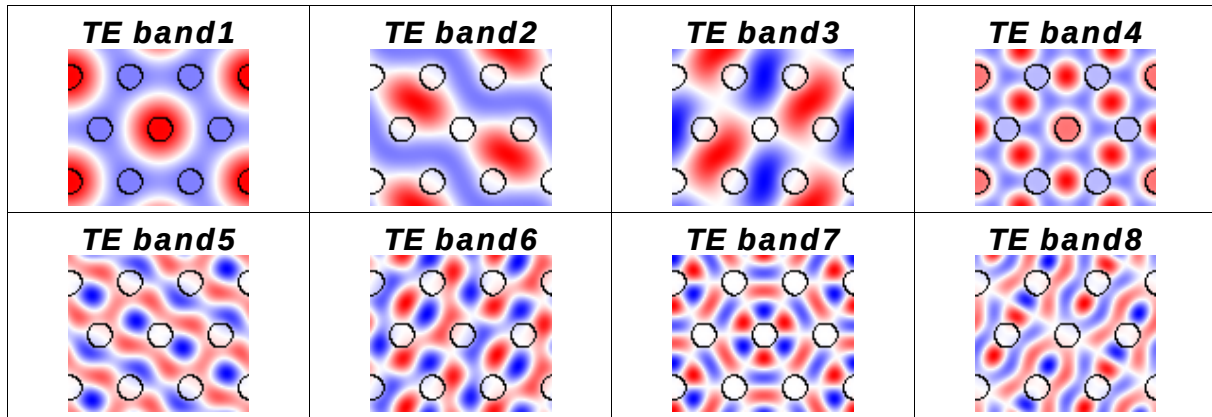


Fig. 10. Magnetic field distributions for the first eight bands at symmetry point K ($n_{PS}=1.4$ and $r=0.2a$). The H_z field component (perpendicular to the 2D plane) is shown in horizontal cross-section with blue/white/red indicating negative/zero/positive.

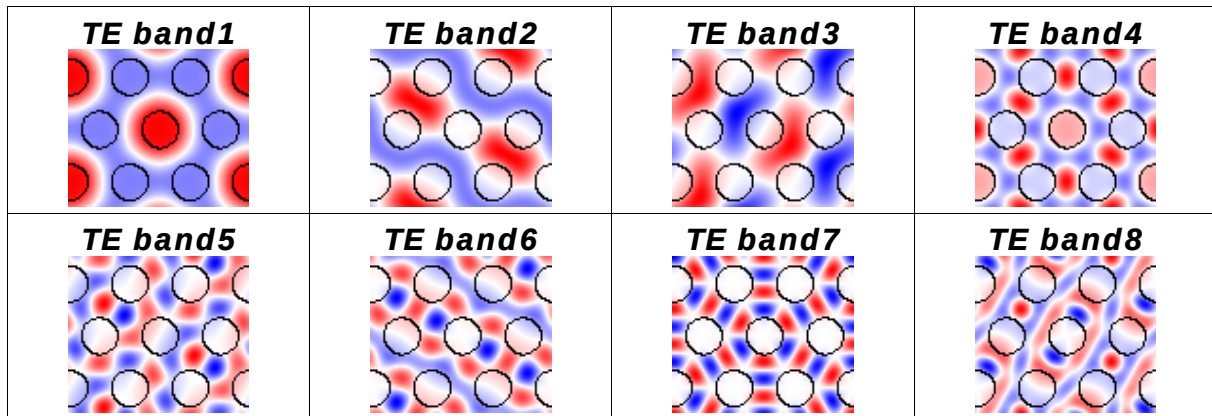


Fig. 11. Magnetic field distributions for the first eight bands at symmetry point K ($n_{PS}=1.4$ and $r=0.3a$). The H_z field component (perpendicular to the 2D plane) is shown in horizontal cross-section with blue/white/red indicating negative/zero/positive.

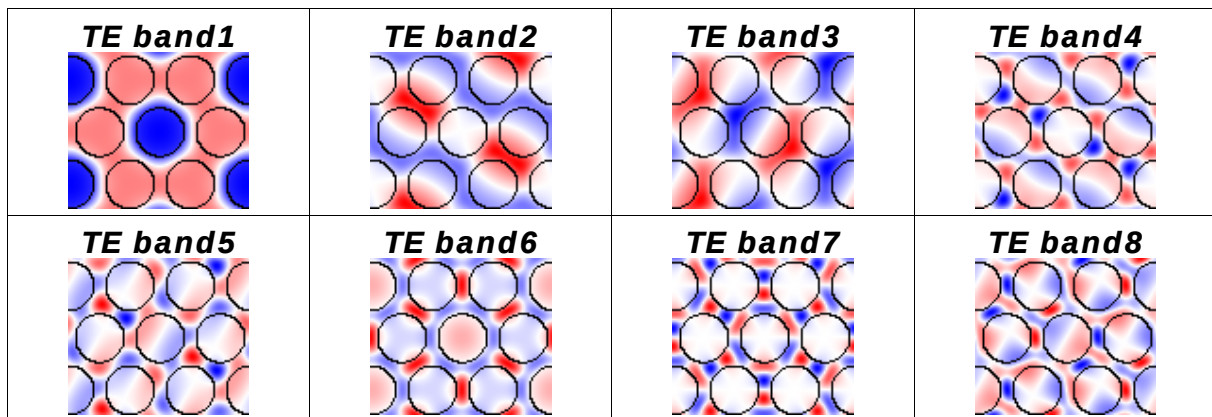


Fig. 12. Magnetic field distributions for the first eight bands at symmetry point K ($n_{PS}=1.4$ and $r=0.4a$). The H_z field component (perpendicular to the 2D plane) is shown in horizontal cross-section with blue/white/red indicating negative/zero/positive.

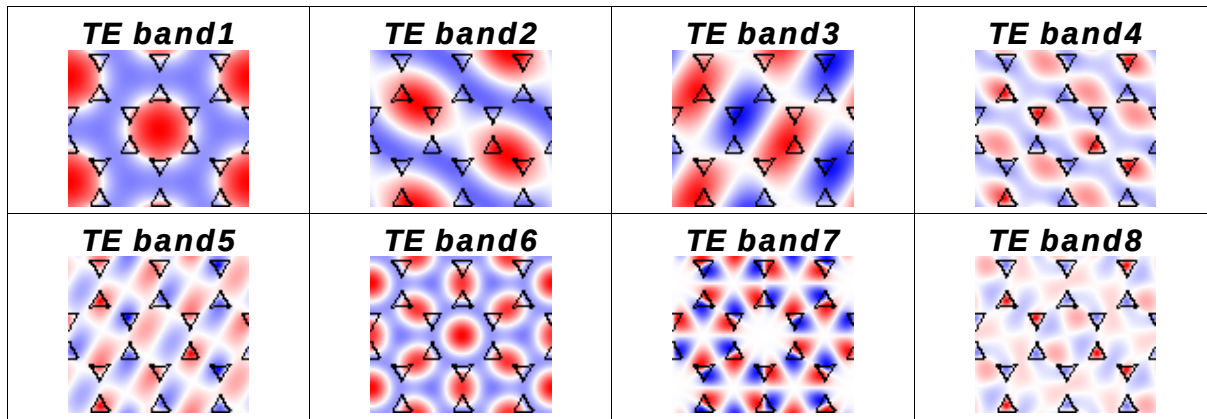


Fig. 13. Magnetic field distributions for the first eight bands at symmetry point K ($n_{PS}=1.4$ and $r=0.5a$). The H_z field component (perpendicular to the 2D plane) is shown in horizontal cross-section with blue/white/red indicating negative/zero/positive.

As expected, the low index PS rods are best suited to the formation of photonic band gap to TE light in which the electric field runs around the rods. Because the first TE band has most of its character in the PS regions while the second has most of its character in the Si regions, there is a large splitting between these bands, leading to the apparition of band gap regions. Since for higher TE bands there is a mixed behavior (Figs. 9 to 13), no band splitting is observed. Thus, in the case of TE polarization, it is the connectivity of the lattice that is crucial to yielding a photonic band gap [24]. On the other hand, the formation of Si rods embedded into a PS matrix would have favored the formation of photonic band gap to TM light.

6. Summary and conclusions

Nanometric porous silicon based photonic crystals, basically consisting on PS rods embedded into a silicon matrix arranged as to form a triangular lattice, were developed. The resulting photonic band structure for the TE and TM modes can be controlled by varying the radius of the PS rods. From band structure calculations it was found increasing band gap in the TE-like modes for increasing radius until a maximum is reached, which occurs at $r=0.4a$ with gap size of 32 % in percentage of mid-gap frequency (Fig. 7b). From this value the band gap falls abruptly to zero. Since no band gap in the TM-like modes was observed, there are no complete (i.e. overlapping TE/TM) gaps.

Connectivity within the two-dimensional plane was found to be important for the observation of band gaps in the TE polarization for the PS-based structures analyzed. Since concentrations of high dielectric constant materials are important to developing a photonic band gap for the TM polarization, this behavior might explain the absence of photonic band gap for this polarization in the structures studied in the present work.

Acknowledgements

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