'Hexagon-type' photonic crystal slabs based on SOI

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In this paper we discuss the design of a novel category of photonic crystal slabs (PCS) and as an example, we consider structures based on SOI wafers. Fabrication issues related to lithographic accuracy are addressed, too. The geometry consists in a triangular lattice of hexagons having their symmetry axes rotated with respect to the lattice. We show that the mirror-symmetric 'hexagon-type' PCS with air claddings can have an absolute (i.e. polarization independent) gap in guided modes with normalized width of approximately 10%. This gap, although reduced to about 4%, is still present in an asymmetric geometry, when the under-cladding is a silicon oxide layer with deeply etched holes.

Introduction

A photonic crystal slab (PCS) may support guided modes because of its finite thickness. If the slab has mirror-symmetry with respect to its horizontal middle plane, a gap between guided modes of certain symmetry can be opened [1]. For example, a PCS with triangular lattice of circular holes has a large gap in even modes. There are several reasons for which an absolute gap, independent of mode symmetry, would be a desirable feature. First, coupling between modes of opposite symmetry is possible in real structures, due to fabrication intrinsic imperfections. Second, a reasonable coupling efficiency between PCS and a ridge waveguide would need careful control over the polarization state. Third, the condition of mirror symmetry leads to an increase in the complexity of the fabrication process in certain cases. A PCS with a significant absolute gap in guided modes was discussed only recently [2]. The example considered in this reference is the familiar triangular lattice of air holes in a PCS with mirror symmetry.

In this paper we present two new structures based on silicon-on-insulator (SOI) substrates, having large, absolute gaps in guided modes. We present a design procedure and computations of dispersion diagrams. Fully-vectorial eigenmodes of Maxwell's equations with periodic boundary conditions were computed using a freely available software package [3]. Limits imposed by the lithographic accuracy are considered.

Two-dimensional photonic crystals

A PCS is obtained from its two-dimensional (2D) photonic crystal (PhC) counterpart by truncating the infinite thickness down to a fraction of the lattice constant. The modes of the PCS-structure have a lower effective index, resulting in a shift of its band diagrams towards higher frequencies. Then, if the initial 2D PhC has an absolute (i.e. polarization-independent) photonic band gap (PBG), this may be preserved in the PCS, depending on its thickness. On the other hand, one can infer that a 2D PhC that does not have a PBG in either TE or TM polarizations can be discarded for practical purposes, since the resulting PCS will not have a gap in guided modes. Therefore, calculations of 2D PhC's provide a good starting point in selecting promising structures for PCSs. Moreover, the calculation time is orders of magnitude shorter than that for 3D structures. Optimization of the PBG is

difficult, because it involves solving a multiparametric inverse problem. There are countless combinations of lattice symmetry, scattering object shape, filling factor and refractive index contrast, but it is impossible to say which one gives the largest absolute PBG. A systematic algorithm is still lacking, and the design is based on several *rules of thumb*. It is known that absolute PBG's are favored in PhC's that satisfy the following criteria: (a) the refractive index contrast is as high as possible, (b) the Brillouin zone is close to a circle, (c) the shape of scattering objects matches the symmetry of the Brillouin zone [4], and (d) the PhC is comprised of isolated dielectric islands connected by narrow veins, implying a high filling-factor for the low-index material.

Wang at al [4] recently performed a study on band diagrams of a broad range of 2D PhC's. They showed that an effective way of overlapping the TE and TM bands is by rotating noncircular 2D rods around their vertical (infinite) axis. The non-circular scattering objects introduce an additional degree of freedom (i.e. rotation angle), leading to an increased flexibility in the design, but also making the optimization even harder.

Calculations of band diagrams are presented in many papers [5-8]. Sometimes, the authors considered "exotic" materials (e.g tellurium [8]) or extreme filling factors. Both approaches pose serious challenges to the technology for PCS. In the design of a fabrication process for PCS's one usually starts from the available technology and high refractive index materials. Lithographic accuracy puts a lower boundary on the achievable thickness of the veins and this should be accounted for when performing calculations. Our 2D calculations are targeted to PCS design using SOI, having a PBG centered at the telecom wavelength of 1.55 μ m. Therefore, we consider only PhC's consisting of air holes etched vertically in a silicon slab ($n_{Si} = 3.45$). We now discuss the band diagrams of a triangular lattice of hexagonal holes (referred to briefly as 'hexagon-type'), a configuration potentially providing a large absolute PBG.

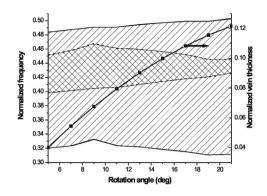
Band diagrams were studied as a function of two geometrical parameters: size of air rods and their angular orientation with respect to the lattice. The air holes filling factor should be high enough, leaving only a limited size range of interest for the holes. In our design procedure we fix the size and vary the rotation angle, aiming at maximizing the PBG. Optimum results were obtained for the hexagon's side R = 0.5a, where a is the lattice constant. This value will be assumed from now on in this paper.

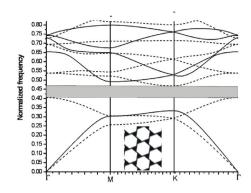
FIG. 1 shows the gaps for TE and TM polarizations and their overlap, as well as the veins' thickness, as function of rotation angle α , in hexagon-type geometry.

The veins' thickness x_{hex} is given by an analytical formula: $x_{\text{hex}} = a\sin(60^\circ + \alpha) - 2R\sin 60^\circ$. For $\alpha = 0^\circ$, the corners of nearest-neighbor hexagons touch one another. The gap for TE is very large, completely enclosing the TM gap, so that the PBG coincides with the gap for TM. It is apparent that the maximum PBG is reached for $\alpha = 9^\circ$. The band diagrams for this rotation angle are shown in FIG. 2. The PBG is between $(0.4045 \cdots 0.4679)(a/\lambda)$, with the center frequency $0.4362(a/\lambda)$ and normalized width of 14.5%.

Band diagrams of photonic crystal slabs

Up to now, the most studied PCS geometry has been the mirror-symmetric slab with a triangular lattice of circular air holes. This configuration is known to have a large gap in guided even modes and a smaller gap for odd guided modes. Under certain conditions⁴, these gaps can be made to overlap, leading to an absolute gap of about 8.5%. Here we show that large absolute gaps are achievable in both symmetric and asymmetric hexagon-type PCS's.





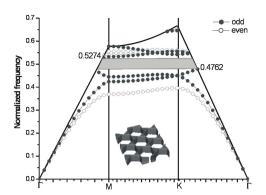
for air holes in a silicon background, hexagon side R = 0.5a; (hatched: gap for TE polarization; crosshatched: absolute band gap - coincides with gap for TM). Solid line: normalized vein thickness x_{hex}/a versus rotation angle.

FIG. 1. Gap overlap as a function of rotation angle FIG. 2. Band diagrams for hexagon-type 2D PhC (shown in inset), with hexagon side R = 0.5a and rotation angle $a = 9^{\circ}$; solid and dashed lines are bands for TE and TM polarizations, respectively; the PBG is shaded grey (width 14.5%).

The computational method requires a periodic cell. The PCS is patterned with a 2D periodic lattice and, in order to ensure 3D periodicity, we take a sequence of slabs periodical in the vertical direction (supercell) [1]. The period of the latter should be large enough so that the coupling among guided modes in adjacent slabs is negligible. The light cone divides the ω -k plane into two regions. Modes situated below the light-cone are confined in the slab and decay exponentially in the claddings. Modes above the light-cone are leaking into the claddings and they are interacting with one another; their frequencies calculated by the supercell method are false and we omit them from the graphical representation. During the numerical experiments we observed that, when slab thickness h is varied, the frequencies of odd modes are shifting at a higher rate than the frequencies of the even modes. Thus, h can be used for optimizing the absolute gap size.

We now proceed to calculating dispersion curves in PCS's, using the optimum geometry parameters (R, α) for the 2D structure of air holes in silicon, as obtained above. These optima might shift when moving from the purely 2D case to the slab geometry, possibly allowing further optimization, which has not been pursued in this work. Depicted in FIG. 3 (left panel) are band diagrams of guided modes in a hexagon-type symmetric PCS with air claddings and optimum thickness h = 0.59a. The absolute PBG is bounded by the second and third odd modes and the light cone and has 10.2% width. Tolerance of gap width with respect to h leads to the following conclusion: for $h = (0.575 \cdots 0.608) a$, the gap width is larger than 8%. Considering the midgap frequency for $\lambda = 1.55 \,\mu\text{m}$, we get $a = 777 \,\text{nm}$, $R = 388 \,\mathrm{nm}$, $h = 458 \,\mathrm{nm}$, $x_{\mathrm{hex}} = 52 \,\mathrm{nm}$.

For an asymmetric hexagon-type PCS, with air and SiO_2 ($n_{SiO_2} = 1.45$) upper and lower claddings respectively, the holes need to be etched through, deeply into the SiO₂ in order to maximize the bandgap. The resulting PBG for this case is reduced to 4.1%, as shown in FIG. 3. (right panel). This happens because the light cone is shifted towards lower frequencies, which are determined by the first TM band of the 2D PhC bottom cladding.



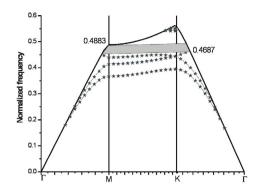


FIG. 3. Left panel: band diagrams of guided modes in a symmetric hexagon-type PCS with air claddings (central frequency of the absolute gap: $f_0 = 0.5018a$, gap width: 10.2%); Right panel: band diagrams of guided modes in an asymmetric hexagon-type PCS with air upper cladding and SiO₂ bottom cladding, both with thickness 4a; the air holes are penetrating the bottom-cladding; (central frequency of the absolute gap: $f_0 = 0.4785a$, gap width: 4.1%); geometrical parameters: R = 0.5a, $\alpha = 9^{\circ}$, h = 0.59a;

Conclusions

The hexagon-type PCS has some remarkable features: (a) its absolute gap is quite insensitive to variations of geometrical parameters; (b) the gap in even modes is very large, resulting in a high probability of obtaining an overlap with the gap for odd modes; and (c) the absolute gap is still present even in asymmetric PCS's. Especially the latter property, which does not hold for structures with circular holes, opens the possibility of reducing complexity of the technological process when using common SOI wafers, leading to devices that are both mechanically and thermally more stable.

The design presented here is the basis of a fabrication process that is currently under way. The experimental results will be presented in a following paper.

Acknowledgements

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