Guiding and reflecting light by boundary material

A. Huttunen\textsuperscript{a,*}, K. Varis\textsuperscript{b} K. Kataja\textsuperscript{c}, J. Aikio\textsuperscript{c}, P. Törmä\textsuperscript{d}

\textsuperscript{a}Department of Electrical and Communications Engineering, Laboratory of Computational Engineering, Helsinki University of Technology, FIN-02015 HUT, Finland

\textsuperscript{b}Department of Electrical and Communications Engineering, Optoelectronics Laboratory, Helsinki University of Technology, FIN-02015 HUT, Finland

\textsuperscript{c}VTT Electronics, FIN-90571 Oulu, Finland

\textsuperscript{d}Department of Physics, Nanoscience Center, FIN-40014 University of Jyväskylä, Finland

Abstract

We study effects of finite height and surrounding material on photonic crystal slabs of one- and two-dimensional photonic crystals with a pseudo-spectral method and finite difference time domain simulation methods. The band gap is shown to be strongly modified by the boundary material. As an application we suggest reflection and guiding of light by patterning the material on top/below the slab.

Key words: Photonic band gap materials, Photonic crystal slabs, Optical waveguides

PACS: 42.70.Qs, 42.82.Et

Photonic crystals are periodic dielectric structures that exhibit a photonic band gap, which can be utilized to control and confine light [1]. Photonic crystal slabs are planar structures, i.e., they are periodic in a plane, but have finite thicknesses in the third dimension. The slab acts as a planar waveguide, if the average refractive index of the slab is higher than that of the surroundings. Thus light can be controlled three-dimensionally, when the slab is patterned to form a two-dimensional photonic crystal [2,3]. Two-dimensional photonic crystal slabs are considerably easier to fabricate than three-dimensional photonic crystals. Analogously, light can be controlled two-dimensionally with

\* Corresponding author. Tel: +358 9 451 5730; Fax: +358 9 451 4830; Email: anu.huttunen@hut.fi
one-dimensional photonic crystal slabs [4,6,7]. The characteristics of photonic crystal slabs are notably different from the corresponding infinite photonic crystals and thus miniaturized photonic crystal components for, i.e., integrated optics cannot be designed based on the features of infinite structures.

Waveguides are basic components of an integrated optical circuit. Waveguides in two-dimensional photonic crystal slabs are formed by introducing line defects to the periodic structure [8,9,10,12,13,14,15,16,17]. Light with a frequency in the band gap of the photonic crystal cannot propagate in the periodic structure and thus follows the line defect. We are proposing a new way to guide light using the influence that the material surrounding the photonic crystal slab has on the band gap. The photonic crystal slab has a band gap for different frequencies depending on the material that is on top/below the slab.

We consider photonic crystal slabs of heights $h$ of the order of the period $P$. We calculate the band structures of two-dimensional photonic crystal slabs using a pseudo-spectral method [18]. Here, we show calculations for a specific geometry to illustrate the effects of different types of boundary materials above and below a photonic crystal slab. With boundary material we refer to the half-spaces above and below the slab. We show that varying the boundary material results in large changes in the band structures. We suggest to use this effect for guiding of light by patterning the boundary material — an alternative way for light guiding along crystal defects. The idea is the following (also explained in Fig. 2): planar two-dimensional photonic crystal would be fabricated with no defects and the waveguide would be realized by covering a channel (or leaving a channel uncovered) in otherwise uncovered (covered) slab. The difference of the band structures in covered/uncovered areas confines light in the waveguide. We demonstrate the idea with three-dimensional finite difference time domain (FDTD) simulations. For one-dimensional photonic crystal slabs the same effect can be used for reflecting light traveling along a one-dimensional photonic crystal slab by changing the boundary material abruptly. We demonstrate this with a two-dimensional FDTD method. The FDTD methods are described in Ref. [19].

To demonstrate that boundary material affects the band structure, we calculated band structures of two-dimensional photonic crystal slabs using a pseudo-spectral method [18]. The band structures for a triangular lattice photonic crystal slab with boundary materials air and a dielectric, with a dielectric constant $\varepsilon_b = 3$, are shown in Fig. 1. It can be seen that when the boundary material is air, the frequencies around $\omega P/(2\pi c) = 0.3$ fall into the band gap for even modes in the M-direction [Fig. 1 (a)]. However, when the boundary material has $\varepsilon_b = 3$, there is an even mode at $\omega P/(2\pi c) = 0.2937$ at the M-point [Fig. 1 (b)]. Thus a waveguide can be made for this frequency in the
M-direction by covering the photonic crystal slab in the waveguide region and leaving it otherwise uncovered. Light will follow the covered region where an allowed mode exists.

We performed three-dimensional FDTD calculations to study this type of waveguiding using the boundary material. The structures are shown in Fig. 2. We simulated the propagation of a Gaussian pulse with wavelength $\lambda = 1500$ nm. The period of the photonic crystal lattice was $P = 450$ nm, so that $P/\lambda = 0.3$. The spectral full width at half maximum (FWHM) of the pulse was $\Delta \omega P/(2\pi c) = 0.1$, so that the main frequencies of the pulse fit into the band gap of Fig. 1 (a). First we calculated the transmission of the pulse along a defect waveguide made by removing holes from the photonic crystal slab [Fig. 2 (a)]. Then we calculated the transmission for a photonic crystal slab with no defects [Fig. 2 (b)] which was covered by strips of dielectric with $\varepsilon_{wg} = 3$ [Fig. 2 (c)]. The width of the strips was $2P$. The transmission of a Gaussian pulse for the guiding by boundary material [Figs. 2 (b) and 2 (c)] was 40% larger than in the traditional defect waveguide case [Fig. 2 (a)].

We studied also 60° and 90° turns in the hexagonal lattice. For the 60° turn (see Fig. 4), it was found that 51-55% of the light follows the waveguide turn. (Throughput of 51% is reached for FWHM $\Delta \omega P/(2\pi c) = 0.1$ and 55% for FWHM $\Delta \omega P/(2\pi c) = 0.056$. The width of the band gap is $\Delta \omega P/(2\pi c) = 0.066$.) In contrast, only a small fraction (about 10%) of the light followed the 90° turn because there is no solution in the K-direction for the used wavelength in the covered photonic crystal ($P/\lambda = 0.3$). We repeated the simulations for a system where the photonic crystal was replaced by a material with a refractive index corresponding to the average index of the photonic crystal material ($n = 2.9493$): the amount of guided light was similar. Therefore, for this geometry and material, the effect of the photonic crystal reduces to an average refractive index material in a conventional ridge waveguide configuration. Finally, we repeated the simulations of the 60° and 90° turns for photonic crystal defect waveguides, and the guiding efficiency was considerably smaller (of the order of few percents). Note that the geometries and the coupling into the waveguides were not optimized, thus the results could probably be improved by optimizing the parameters. Furthermore, the comparison to ridge and defect waveguides refers to this specific example and should not be generalized without further study. However, the results demonstrate the in-principle usability of the idea.

The one-dimensional photonic crystal slab is a periodic stack of dielectric rectangular rods which have different dielectric constants. The considered geometry is shown schematically in Fig. 5. Parameters needed to define the structure are explained in the figure caption. Light traverses the structure ($y$-direction in Fig. 5), it reflects from each layer and interferes resulting in a band structure. We consider a polarization with field components $H_x$, $E_y$, and $E_z$. As
discussed above, the band gap of a photonic crystal slab depends on the dielectric constant of the boundary material. In structures with periodicity in one dimension only, it can be utilized for reflecting light by changing the boundary material abruptly. For the considered structure, light with frequency around $\omega P/(2\pi c) = 0.3$ has a solution in the photonic crystal when the slab is in air, but falls into the band gap when the slab is sandwiched between dielectric $\varepsilon_b = 13$. We can see from the two-dimensional FDTD simulations that light reflects at the point where the boundary material changes [see Fig. 6(a)]. Part of the light is diffracted to the boundary material that has a high dielectric constant. To estimate the efficiency of the reflection, we calculated the energy density of the light that was reflected back along the photonic crystal slab relative to the energy density of the incident pulse. This is illustrated in Fig. 6(b), where the energy density of the reflected pulse is shown as a function of the dielectric constant of the boundary material. It was calculated using the two-dimensional FDTD method. We can see that with increasing dielectric constant of the boundary material more light is reflected along the photonic crystal slab (indicating that for a totally reflecting boundary material such as metal the effect would be optimal). This and other properties of the crystal and its boundaries can be used to optimize the reflection. We have also studied a slab with a refractive index that is the average of that of the photonic crystal slab ($n = \sqrt{13 \cdot 0.2 + 1 \cdot 0.8}$). The considered boundary materials were dielectric with $\varepsilon_b = 13$ and metal (Au) with $n = 0.053 + 7.249i$. In these cases only a small fraction of the light is reflected back along the waveguide. This shows that, for this geometry and choice of materials, the effect of the photonic crystal cannot be reduced to a homogeneous material with a corresponding average refractive index.

Our studies show that in some cases (the 2D periodic structure considered here) the guiding of light by patterning the surrounding material of a photonic crystal slab seems to reduce to the use of a conventional ridge waveguide. However, in other cases (the 1D example), the effect of the photonic crystal clearly cannot be reduced to a homogeneous material with the average refractive index. The situation somewhat resembles the case of microstructured fibers: there, in some cases the guiding can be explained by a conventional step index fiber structure with an effective refractive index, whereas in other cases the guiding is a genuine photonic band gap effect. In both cases, the fibers have turned out to provide interesting applications.

The advantages of the guiding scheme proposed here depend on the type of guiding it actually provides. In all cases (even when the guiding is effectively equivalent to guiding by a homogeneous material ridge waveguide), the advantage over using a ridge waveguide is the integrability with photonic crystal components, e.g. active elements (one may even imagine realizing microcavities by the effect) and additional degrees of freedom in designing the mode properties. The advantage over defect waveguides may be better guiding in
some cases (as demonstrated here), easier fabrication or better integrability. In addition to these advantages, when the guiding is a genuine photonic band gap effect, one should be able to realize, for suitable crystal symmetries, sharp bends that are not possible with ridge waveguides. For the hexagonal lattice considered here, it was unfortunately not possible to demonstrate this since the frequencies of the band gaps as well as the frequency of the guided mode differ considerably in the K- and M-directions.

In summary, we have studied the effect of boundary materials and finite height of one- and two-dimensional photonic crystals to the band gap of the photonic crystal. We used a pseudo-spectral method and a finite difference time domain method. The band gap shows dependency on the boundary material. The strong effect of the boundary material on the band structures can be used for novel type of guiding of light in two-dimensional photonic crystals: the channel would be realized by covering a part (having the shape of the channel) in otherwise uncovered slab. We tested the idea by FDTD simulations of pulse propagation in a two-dimensional photonic crystal, and the proposed guiding by boundary material provided twice as effective transmission as the traditional guiding by a defect, for the (unoptimized) parameters used. Whether or not the guiding can be understood by replacing the photonic crystal by a homogenous material with the average refractive index was shown to depend on the choice of geometry and materials.

**Acknowledgements**

We thank the Academy of Finland for support (Project Nos. 48845, 53903, 205454). Jerome Moloney and Aramais Zakharian (Arizona Center for Mathematical Sciences, University of Arizona) are acknowledged for providing the original 3D FDTD code and Juuso Olkkonen (VTT Electronics, Finland and Optical Sciences Center, University of Arizona) for development and support of the 3D FDTD code.
References

[1] J. D. Joannopoulos, R. D. Meade, and J. N. Winn, Photonic Crystals, Princeton University Press, New Jersey, 1995.

[2] S. G. Johnson, S. Fan, P. R. Villeneuve, J. D. Joannopoulos, and L. A. Kolodziejski, Phys. Rev. B 60 (1999) 5751–5758.

[3] E. Chow, S. Y. Lin, S. G. Johnson, P. R. Villeneuve, J. D. Joannopoulos, J. R. Wendt, G. A. Vawter, W. Zubrzycki, H. Hou, and A. Alleman, Nature 407 (2000) 983–986.

[4] S. Fan, J. N. Winn, A. Devenyi, J. C. Chen, R. D. Meade, and J. D. Joannopoulos, J. Opt. Soc. Am. B 12 (1995) 1267–1272.

[5] D. M. Atkin, P. St. J. Russell, T. A. Birks, and P. J. Roberts, J. Mod. Opt. 43 (1996) 1035–1053.

[6] M. Patrini, M. Galli, F. Marabelli, M. Agio, L. C. Andreani, D. Peyrade, and Y. Chen, IEEE J. Quantum Electron. 38 (2002) 885–890.

[7] K. Koshino, Phys. Rev. B 67 (2003) 165213/1–165213/8.

[8] S. Kuchinsky, D. C. Allan, N. F. Borrelli, and J.-C. Cotteverte, Opt. Commun. 175 (2000) 147–152.

[9] M. Loncar, T. Doll, J. Vuckovic, and A. Scherer, J. Lightwave Technol. 18 (2000) 1402–1411.

[10] S. Y. Lin, E. Chow, S. G. Johnson, and J. D. Joannopoulos, Opt. Lett. 25 (2000) 1297–1299.

[11] S. G. Johnson, P. R. Villeneuve, S. Fan, and J. D. Joannopoulos, Phys. Rev. B 62 (2000) 8212–8222.

[12] M. Loncar, D. Nedeljkovic, T. Doll, J. Vuckovic, A. Scherer, and T. P. Pearsall, Appl. Phys. Lett. 77 (2000) 1937–1939.

[13] C. J. M. Smith, H. Benisty, S. Olivier, C. Weisbuch, T. F. Krauss, R. M. De La Rue, R. Houdre, and U. Oesterle, Appl. Phys. Lett. 77 (2000) 2813–2815.

[14] E. Chow, S. Y. Lin, J. R. Wendt, S. G. Johnson, and J. D. Joannopoulos, Opt. Lett. 26 (2001) 286–288.

[15] T. Baba, N. Fukaya, and A. Motegi, Electronics Lett. 37 (2001) 761–762.

[16] M. Notomi, K. Yamada, A. Shinya, J. Takahashi, C. Takahashi, and I. Yokohama, Phys. Rev. Lett. 87 (2001) 253902/1–253902/4.

[17] A. Chutinan, M. Okano, and S. Noda, Appl. Phys. Lett. 80 (2002) 1698–1700.

[18] K. Varis and A. R. Baghai-Wadji, ACES Journal 19 (2004) 101–111.

[19] A. Taflove and S. C. Hagness, Computational Electrodynamics: The Finite-Difference Time-Domain Method, Artech House, Boston, 2000.
Fig. 1. Band structures of a two-dimensional photonic crystal slab with triangular lattice of air holes. The dielectric constant of the slab is $\varepsilon = 12$. The boundary material on top/below the slab is air $\varepsilon_b = 1$ in (a) and dielectric $\varepsilon_b = 3$ in (b). The lattice parameters are radii of the holes $r/P = 0.24$ and the height of the slab $h/P = 0.3$ with respect to the period $P$. Solid curves are even modes, dashed curves are odd modes and black areas are above the light lines for the boundary material in question.
Fig. 2. Geometries for the 3D FDTD simulation of wave guiding in two-dimensional photonic crystal slabs. (a) Conventional photonic crystal waveguide: guiding along a line defect of missing air holes. (b) Slab of triangular lattice. (c) Guiding by boundary material: the slab with the geometry shown in (b) is drawn in black. Stripes of material with dielectric constant $\varepsilon_{wg} = 3$ are placed on top and below the slab (drawn in gray). The parameters of the lattice are as in Fig. 1.
Fig. 3. The energy density of the Gaussian pulse propagating in the waveguide with the geometry shown in Fig. 2 (b)-(c). In (a), the pulse is propagating in the $y$-direction. The energy density is integrated over the waveguide height in the $z$-direction. The cross section of the energy density at the plane denoted by a line is presented in (b). The waveguide width ($2P$) is denoted in both figures.
Fig. 4. (a) Geometry of a $60^\circ$ turn in the hexagonal lattice photonic crystal. The black waveguide areas are realized by placing waveguide strips on top/below the photonic crystal slab with no embedded defects. The geometry parameters are the same as in Figs. 1 and 2. (b) The energy density of the Gaussian pulse after propagating through the turn. The energy density is integrated over the waveguide height in $z$-direction and the shown area in $xy$-plane is marked with a white box in (a). The spectral full width at half maximum (FWHM) of the pulse was $\Delta \omega P/(2\pi c) = 0.056$. 
Fig. 5. Geometry of a one-dimensional photonic crystal slab. The rods, which are infinitely long in the $x$-direction and have a finite thickness $h$ in the $z$-direction, are periodically replicated in the $y$-direction. The parameters are thickness of one layer $l/P = 0.2$ and height of the slab $h/P = 0.5$, relative to the period $P$, and dielectric constants of the materials. Here, the other material in the periodic stack has dielectric constant $\varepsilon = 13$ and the other material is air. The dielectric constants of the boundary material $\varepsilon_b$ above ($z > h$) and below ($z < 0$) the slab are varied in the simulations.
Fig. 6. (a) Energy density profiles of a Gaussian pulse in a one-dimensional photonic crystal slab at different times. The profile is taken in the middle of the photonic crystal. Photonic crystal geometry is shown in the upmost part of the figure. The black areas denote GaAs and white ones air. The pulse has a scaled frequency $\omega P/(2\pi c) = 0.3$. Light with this frequency can propagate in the photonic crystal when the boundary material is air, but falls into the band gap when the boundary material is GaAs. This can be seen from the intensity profile as the pulse is reflected. (b) The fraction of the energy density of a Gaussian pulse that is reflected inside the slab from the point where the boundary material above and below the photonic crystal slab changes from air to a material with dielectric constant $\varepsilon_b$. The rest of the energy of the pulse is diffracted into the boundary material. Solid line indicates dielectric boundary materials and dots indicate metals: gold, silver, and aluminum for which the refractive indices are $n_{Au} = 0.053 + 7.249i$, $n_{Ag} = 0.078 + 7.249i$, and $n_{Al} = 0.384 + 11.88i$, respectively.