Surface states in photonic crystals

P. Vojtíšek^{1,2} and I. Richter²

¹Institute of Plasma Physics AS CR, v.v.i., Centre TOPTEC, Sobotecká 1660, Turnov 511-01, Czech Republic

²Czech Technical University in Prague, FNSPE, Department of Physical Electronics, Břehová 7, 115-19, Prague 1, Czech Republic

Abstract. Among many unusual and interesting physical properties of photonic crystals (PhC), in recent years, the propagation of surface electromagnetic waves along dielectric PhC boundaries have attracted considerable attention, also in connection to their possible applications. Such surfaces states, produced with the help of specialized defects on PhC boundaries, similarly to surfaces plasmons, are localized surfaces waves and, as such, can be used in various sensing applications. In this contribution, we present our recent studies on numerical modelling of surface states (SS) for all three cases of PhC dimensionality. Simulations of these states were carried out by the use of plane wave expansion (PWE) method via the MIT MPB package.

1 Introduction

Since their proposal in 1987 [1], photonic crystals (PhC) or photonic band gap (PBG) structures [1-4], still represent very interesting and promising structures of artificial origin. Their main characteristics are given by spatially periodic variations of dielectric constant enabling in a sense such physical properties for light interactions as are exhibited by electrons in semiconductors. These properties are mainly represented with such effects as photonic band gap (PBG) formation, prohibition of spontaneous emission and/or unusual laws of refraction / reflection,

Typically in theory, PhC are considered as ideal periodic crystals without presence of any defects, hence exhibiting corresponding Bloch modes. Contrary to this, realistically fabricated crystals usually exhibit some kind of defects which consequently alternate their properties. Figure 1 summarizes different types of defects which can be present in one-dimensional (1D), two-dimensional (2D) and three-dimensional (3D) PhC. Yet another type of defects can exist in ideal crystals, this defect is given by a finite size of a crystal and can, under some

conditions, lead to the excitation of a surface state (SS) propagating along the interface between a crystal and air (or more generally, background medium) [5-9], as a result of the interaction of PhC Bloch modes and outer plane wave modes. These surface states can exhibit very interesting properties leading to many potential applications in integrated photonics and optical sensing in particular [1], due to sharp resonant responses of these waves. Concerning the understanding of the physics of SS, however, there is still lack of theoretical background and proper analysis of such intriguing phenomena.

Hence, the purpose of this paper, as a continuation of our previous studies, is to present and discuss our recent results on theoretical simulations of surface states as localized waves at the interface of PhC and air. Following that aim, this paper is organized as follows. After this introductory section, section 2 briefly presents the basics of surface states in PhC. Next, in section 3, the paper concentrates further on our theoretical results, obtained via the plane wave expansion method (MIT MPB package) [10], of simulations of SS in 1D, 2D, and 3D cases, respectively. Finally, section 4 summarizes the results and concludes the paper.

Fig. 1. Schematic view of a) 1D PhC with corresponding structural defects, b) 2D PhC with point and linear defects, and c) 3D PhC with three types of defects (point, linear, plane).

2 Surface states at the boundary of PhC

Since surface states represent localized waves at the interface of two media, they are in a sense similar to surface plasmons (SP) [3] which exist at the interface of a dielectric and metal. In contrast, in our case of SS, instead of a metallic component, a periodic modulation of the dielectric constant is considered, and connected to that, some kind of a PhC termination is required. Clearly, such termination breaks strict periodicity of the crystal. In fact, surface states can be excited at the surface of PhC if two conditions are met – (1) PhC has to be such that it pronounces a full photonic band gap in the spectral region of interest (around this SS) and (2) light on the outer PhC side (air) has to be index-guided [1].

With respect to these two conditions one can divide surface states of light, which exist along the interface, into the two groups – (1) localized (decay, D) states, which exponentially decrease in an outer medium, and (2) extended (E) states, which propagate inside a medium. Further, one can specify four types of arrangements of these two states, which characterize possible states at both sides (and hence, along the boundary) of the interface simultaneously – EE, ED, DE, DD [2], where the first letter represents the state outside of a crystal and the second letter state inside a crystal. A proper surface state is the last one (i.e. DD), it is characterized by a decay of the fields on both sides of the interface. In other words, such DD surface states represent the Bloch states, and consequently, as such, do not couple to incoming / outgoing radiation.

Further, if one considers that a PhC already exhibits a full PBG in the spectral region of interest (this is mainly given by the periodicity and dielectric contrast), then we have to fulfil the condition for index-guiding of light outside of a crystal. Indeed, this condition can be met by appropriate modification of the last PhC period at the border with outside medium, i.e. via a change of inclination or a termination of this last period. Typically, the latter, i.e. the change in termination, is considered; it practically represents the elimination of some part of building blocks within the last period. Generally, a proper PhC termination is important for existence of a surface state, with no termination applied, there is no SS. Idea of a termination of 1D PhC is presented schematically in figure 2a) together with a corresponding idea of excited surface state intensity at the interface is shown in figure 2b).

Fig. 2. a) Idea of termination of 1D PhC and b) schematic distribution of a field intensity of a surface state along the boundary.

3 Theoretical analysis of surface states

In this section, we will present theoretical modelling and analysis of surface states at the interface of three different types (1D, 2D, and 3D) of a PhC and air. Simulations have been carried out by the use of PWE which was incorporated in the MPB package [9]. One, two and three dimensional simulations have been done to cover all three possible representations in which PhC is usually prepared.

Fig. 3. Projected dispersion diagram for 1D PhC with three SS for different values of the termination (1/4, 1/2, 3/4) of the last layer of a PhC structure. a denotes the period of a PhC. Materials used were Si (layer dimension $0.36a$) and SiO_2 ($0.64a$).

Fig. 4. Profile of 1D PhC (Si:SiO₂, 0.36a:0.64a) with 1/2 termination of the last layer indicated.

In the case of 1D PhC, which is represented with a simple thin film multilayer, we have made the calculations for a structure consisting of periodic repetition of Si ($\epsilon = 12.25$ [11]) and SiO_2 ($\epsilon = 3.9$). The width of a Si component (in fact, the thickness of a Si layer) was $0.36a$ and the width of SiO_2 $0.64a$, where a is the period of a structure. Figure 3 presents calculated projected dispersion diagram while figure 4 shows the corresponding profile of a dielectric constant with indicated interface, for the termination of 1/2 of the last layer. In figure 3, we can see three surface states for the three different types of termination (1/4, 1/2 and 3/4) and four areas within the dispersion diagram which correspond to different behaviour of light. Above the light line (red line), there are blue and turquoise coloured areas present which correspond to EE and ED states, respectively. Below the light line, we can see DE states (pink colour) and PBG (white colour) areas. From the

location of SS inside PBG, it is apparent that with a change of termination, the SS location is change as well.

In the case of 2D PhC, clearly, a spatial variability of possible structures is higher. For simulations, we have chosen two typical material PhC configurations – direct PhC and inverse PhC, both with a triangular lattice (see figure 5).

Fig. 5. Distribution of dielectric material for a) direct ($r = 0.2a$) and b) inverse ($r = 0.48a$) 2D PhC, a denotes the size of an elementary lattice vector.

In both cases, we have used as a base material Si (with $\epsilon = 12.25$) and air ($\epsilon = 1$) as a background material. For the direct PhC, the structure consisted of dielectric rods with radius of $r = 0.2a$, while for the inverse PhC, the radius of air rods was chosen to be $r = 0.48a$. The projected dispersion diagram (for TM polarization) is for a direct PhC shown in figure 6. Then, figure 7 presents the dispersion diagram for both TM and TE polarizations for the case of an inverse PhC. From each diagram (figures. 6 and 7), one can see that surface states can be indeed excited in such structures, for a properly chosen termination of the last period. In the case of an inverse PhC, next, we have attempted to answer the following interesting question: Does a chosen termination of a crystal exist which would physically allow the existence of SS for both polarizations simultaneously? From the diagram shown in figure 8, which represents the calculated dependence of the location of SS inside the PBG on the termination value chosen, it is apparent that, unfortunately, such termination does not exist, and, hence, SS for TM and TE polarization cannot be excited simultaneously for the same termination of a PhC boundary.

Fig. 6. Projected dispersion diagram of a direct 2D PhC with existing SS indicated, for different termination values.

Fig. 7. Projected dispersion diagrams of an inverse 2D PhC: a) TM and b) TE polarization. Also, on the right-hand side, corresponding terminations user are shown.

Finally, for the three dimensional type of PhC, we have chosen a simple opal FCC structure. On such an opaline based PhC, we have studied possible existence of surface states. Here, the dielectric contrast was chosen to be 13 and the radius of an elementary ball $r = 1/\sqrt{8}a$, where a is the size of an elementary lattice. Figure 9 shows that, for these 3D structures, there is a possibility, for the chosen termination, to excite two surfaces states simultaneously. Additionally, in figure 10, one can see the corresponding distribution of the density of energy of the electric field. As can be seen, while one of the two possible SS is localized more inside the PhC opal, the other has more of its energy distributed outside of the crystal.

Fig. 8. Dependence of the spectral position of SS for $k_x = 0.48(2\pi/a)$ with respect to the termination for TM and TE polarizations, a denotes the size of an elementary lattice vector.

Fig. 9. Projected dispersion diagram for opaline 3D PhC with two surface states present. Red dots denote position in k space where density of energy of electric field was computed (see figure 10).

Fig. 10 . a) Distribution of a dielectric constant for 3D opal PhC considered, b) and c) distributions of the density of the electric energy of two possible surface states (SS1 and SS2 respectively, see figure 9), d), e) and f) cross-section of a), b) and c) along the interface.

4 Conclusions

In summary, we have presented our new results on the theoretical simulations of surface states as localized states in the presence of a special defect at a PhC boundary, i.e. the termination of the last PhC period. Our simulation results were based on the plane wave expansion method (represented with the MPB simulation package). Through simulations, we confirmed the existence of surfaces states on interfaces between a PhC crystal and air, for all three spatial dimensions. It was shown that different terminations of the last PhC period lead to different positions of SS inside a PBG, and hence, through different terminations, a proper tuning of spectral position of SS can be performed. In particular, for 3D opaline PhC, two simultaneous surface states for the chosen termination were shown for the first time to exist. Although this existence was theoretically confirmed, practical realization of such samples can still be extremely difficult, clearly above the scope of simple self-assembled techniques efficiently used for the preparation of simple periodically arranged opaline PhC. To conclude, such surface states, especially those existing

for 2D PhC structures, can not only open up new possibilities for the design and operation of photonic structures in feeding / redistributing light applications, such as novel light couplers, emitters, etc., but also find their usage in sensing applications as interesting alternatives to surface plasmons.

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