Analysis of the physical origin of surface modes on finite-size photonic crystals

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The physical properties of the surface modes, which can exist on photonic crystals with limited extension in one direction, are investigated. We show that the dispersion relations of the modes present a continuous transition when crossing the edge of the band gap. Using the homogenization limit, we show that the periodic structure perpendicular to the crystal boundaries plays only a limited role in the phenomenon, namely that of confining the field close to the surface. It is also shown that the underlying physics of these surface modes can be understood using a very simple model where the guiding effect is due to a high index dielectric layer.

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I. INTRODUCTION

Substantial efforts have been done over the past decades to understand and then exploit the properties of photonic crystals. Their unique properties were highlighted in 1987 by two independent articles. The first, authored by John, was devoted to the use of a periodic dielectric structure to localize the light, that is the photonic counterpart of the Anderson localization of the electrons[1] while the second, by Yablonovitch, argued that such a periodic structure could be used to inhibit and more generally to control the spontaneous emission.[2] Then the subsequent pioneering works were mainly devoted to the quest for a structure exhibiting a full photonic bandgap, i.e., a frequency range in which the propagation of the electromagnetic waves is strictly forbidden, and to the study of the physical properties of these structures.

Nowadays the number of structures, physical phenomena and potential applications that have been proposed is so important that it has become impossible to review the field in an introduction and readers are therefore referred to a recent edited book on the subject.[3] The possible existence of surface modes on a finite size photonic crystal was discovered by Meade *et al.* only four years after the founding papers on the topic.[4] They also noted the practical importance of such modes on structures such as semiconductor lasers and the vital importance of the surface termination on their features. Several theoretical papers have been devoted to their study.[5–8] Their existence has been confirmed using a different approach (without supercell approximation) and the coupling between the surface modes on each side of a slab of 2D photonic crystal (a finite number of rods) has been observed.[5] It has also been shown that the position of the cut plane through the rods has a drastic influence on both the dispersion relations and the field confinement.[7] Recently, the local density of photonic states associated has been studied and their application for the enhancement of nonlinear effects envisaged.[8]

Few experimental papers can be found that demonstrate the existence and the effects of the surface modes. A prism coupler experiment has evidenced their presence on one-dimensional photonic crystal,[9] and a recent, elegant, experimental and theoretical work has shown their importance on the outcoupling of the light from a waveguide in 2D photonic crystals made of macroporous silicon.[10] It is possible thanks to the surface modes to achieve highly directional emission from photonic crystal waveguides of small width. This is, of course, the all-dielectric effect equivalent to the high directional emission of a subwavelength hole in a metallic film.[11]

Therefore, it appears from earlier studies that the surface modes on photonic crystals have both fundamental and practical important aspects. However, to the best of our knowledge, no paper has been devoted to the understanding of the physical nature of these modes. In this paper, we attempt to clarify the basic physics involved by these modes and we have found that for numerous aspects, the denomination surface mode could be misleading. Indeed, the mode supported by the structure is rather a guided mode in the dielectric layers than a real surface mode, such as, for example, a surface plasmon wave at the boundary between a metal and a dielectric. We would like to stress that our aim is not to be controversial, but only be precise to the exact nature of the modes. The denomination surface was of course the natural choice because when the parameters are suitably chosen, certain modes can be localized in thin layers at the vicinity of the surface.

We point out that the surface modes on photonic crystals can be seen as a photonic version of the Shockley surface states,[12] however, one must take care to the limits of such kind of analogy. A simple evidence of that is given by the strong dependence of the surface mode behavior on the polarization.

In this paper, a structure already studied in Ref. 7 will be considered. The aim is not to prove the existence of surface modes, which has already been done, but rather to understand their main features.

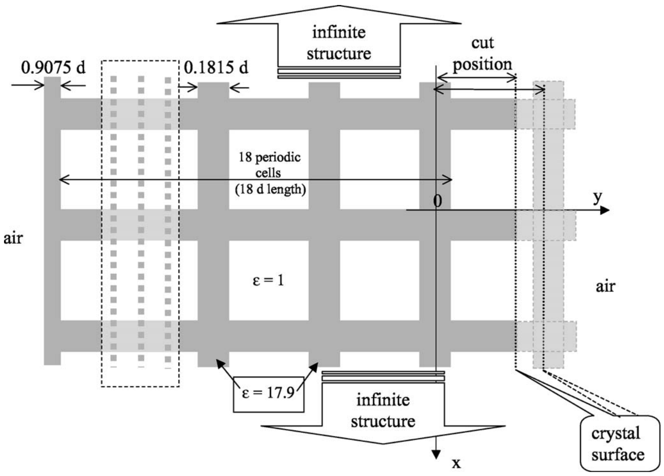

FIG. 1. Schematic representation and parameters of the studied photonic crystal structure. The permittivity of the dielectric is 17.9 and the square holes and surroundings are assumed to be vacuum.

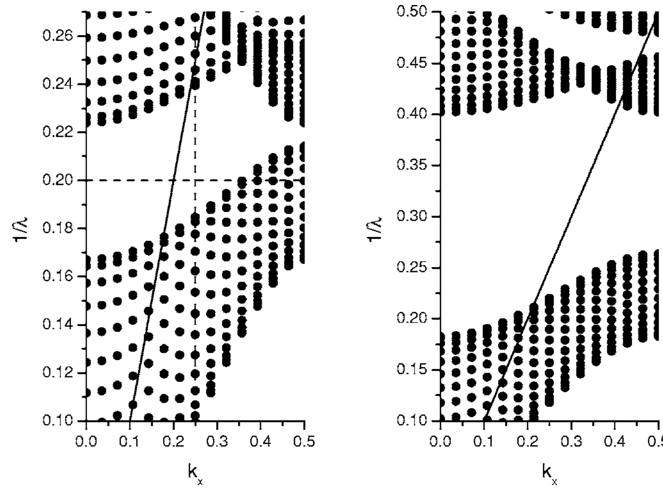

FIG. 2. Dispersion relation of Bloch modes in the infinite structure. Left: TE polarization. Right: TM polarization.

II. DEVICE UNDER STUDY AND BLOCH MODES DISPERSION RELATION

The structure studied is a two-dimensional photonic structure made of infinite square holes drilled into a dielectric substrate. The permittivity of the dielectric is 17.9 corresponding to the permittivity of a semiconductor in the near infrared wavelength domain. The structure is assumed to lie in vacuum. Figure 1 depicts the geometrical parameters of the photonic crystal. It has a square lattice, the periods of the structure are $d_x = d_y = d$, and the length of the edges of the square holes is 0.8185 d. The modeled structure is invariant along the z axis, infinite and periodic along the x axis, and finite along the y axis. The exact location of the truncation of the structure has been identified as a key parameter of the behavior of the surface modes.[7] When the cut position is nil, the whole thickness of the structure is 18 periods and the termination is at one half of the dielectric layer which separates two vacuum holes on both sides. When the cut position varies, only one side of the crystal is changed and the cut position is given by the fraction of the period added to or removed from the 18 periods.

The two-dimensional geometry of the problem (i.e., the structure and the electromagnetic fields are invariant along the z axis) implies that the problem can be divided into two fundamental cases of polarization. In the TE (TM) polarization case, the electric (magnetic) field is along the z axis. Figure 2 presents the dispersion relation of the Bloch modes in the infinite photonic crystal (along all the space directions). k_x is the normalized component of the wave vector defined by $k_x = d(\mathbf{k} \cdot \mathbf{e}_x)/(2\pi)$. The solid lines on the graphs represent the light line with the equation $\omega = ck$. The band structure has been obtained using the classic plane wave method.[13,14] In this method the Bloch modes are expressed using a plane wave basis and for the calculations presented in this paper the truncation of the plane wave basis has been checked to ensure a good accuracy of the results (2025 plane waves were used). The representation used shows the bands projected onto the x axis of the Bloch wave vector. This representation is useful in our context because when the crystal is truncated, the x component of this Bloch wave vector is conserved. The band structure possesses photonic bandgaps in both polarizations, but significantly larger in the case of TM polarization.

III. GUIDED MODES DISPERSION RELATION AND FIELD BEHAVIOR

The following numerical results have been computed with the rigorous coupled wave method for finite size structures. This method has been introduced for the modeling of diffraction gratings[15] and has been recently improved by two breakthroughs in the electromagnetic theory of gratings. The first one is the introduction by several authors of scattering matrix (S matrix) algorithm which has raised the problems related to evanescent growing and decaying waves in the numerical codes.[16] The second one is a more convergent calculation of Fourier components of a product of functions from the Fourier components of each of them.[17,18]

Although we will not describe in detail the method, we will briefly sketch its basic principles. As it is well known, the z component of the electric (TE) or magnetic (TM) field can be written below and above the structure (in homogeneous substrate and superstrate) as plane waves expansions, each of these plane waves corresponding to an order of the grating that can be propagative or evanescent. When the structure is enlightened by a plane wave, the diffracted field (total field minus the incident one) can be written as a discrete and infinite sum of plane waves. Moreover the diffracted field must satisfy the outgoing wave condition that is the equivalent to the usual Sommerfeld condition for gratings problems.[19]

The structure is then split in layers whose permittivity is invariant along the y axis. In each layer, it can be shown that the field can be described by a modal expansion

$$u(x,y) = \sum_{n=-\infty}^{+\infty} \phi_n(x)[u_n \exp(i\gamma_n y) + d_n \exp(-i\gamma_n y)]\exp(ik_x x) \quad (1)$$

with $k_x = \nu(\omega/c)\sin(\theta_{\text{inc}})$, ν is the optical index of the superstrate (medium where the incident plane wave propagates) and θ_{inc} is the angle of incidence of the incident plane wave. The modes $\phi_n(x)$ and their propagation constants γ_n are obtained thanks to an eigenvalue problem. In the rigorous coupled wave method this eigenvalue problem is written in the Fourier space, i.e., the modes are written as a plane wave sum. Then, to obtain a boundary value problem one must impose the continuity of the tangential components of the fields at the boundaries of each layer in addition to the outgoing wave condition satisfied by the diffracted field.

The guided modes in such structures are usually obtained by searching for the poles of the determinant of the scattering matrix.[20] In the problem under study we are interested in the surface modes on one side of the finite size crystal. Of course, each side of it can *a priori* support modes. If the structure is completely symmetric, the modes on each interface are identical with the modes propagating on the opposite side. Due to the tunnel effects through the crystal volume, these modes are mutually coupled, each couple forming two different modes. However, when the crystal is sufficiently thick, the coupling is weak enough and the modes propagating along each surface could be considered as mutually independent inside the bandgap region (this point has been carefully checked). From a numerical point of view, this leads to a singularity of the scattering matrix, which contains a double pole (for each of the two surfaces). One way to distinguish them is to look for the poles in the amplitude coefficient of the reflected wave with wave incident only on the one side of the photonic crystal. Similar to that, we introduce an asymmetry in the influence of each interface. Thus in all the presented results, the surface modes have been considered on one side only and the existing mode on the other side has been removed.

In order to understand the role of the position of the interface within a period, we have numerically studied how the surface mode evolves when the cut position changes. Figure 3 shows the normalized frequency of the mode when the cut position varies over a range equivalent to two entire periods. Thus, the structure has a total thickness varying from 17 to 19 periods. To obtain this figure, the x-component of the wave vector (i.e., of the propagation constant of the mode) has been kept constant and its normalized value k_x is 0.25 (shown in Fig. 2 by the vertical dashed line). First, we considered the case of TE polarization. The horizontal dashed lines indicate the positions of the light line (upper line) and of the lower and upper edges of the bandgap (lower lines). From this graph, it can easily be seen that the surface modes dispersion relation is quasi-periodic with respect to the thickness as expected for a periodic structure. It confirms that the important parameter is indeed the crystal termination. It is worth noticing that there is a continuous behavior of the mode when its frequency crosses the band edges. The presence of a bandgap therefore plays a role in the localization of

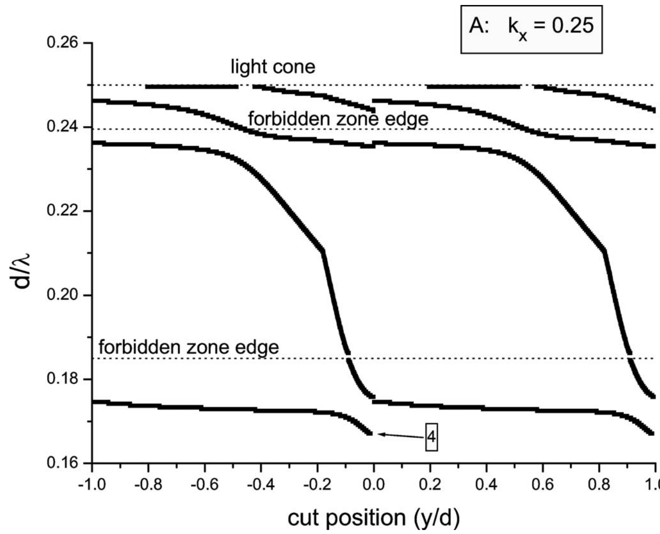

FIG. 3. Normalized frequency of the modes when the cut position varies, for $k_x = 0.25$. TE polarization.

the field at the vicinity of the interfaces (as will be discussed below) but does not determine its existence. Another important feature of the behavior observed is that a cutoff of the modes on the upper part of the graph corresponds to the light cone limit (i.e., the limit between propagative and evanescent waves).

Figure 4 shows a similar numerical study but here the normalized frequency has been kept constant and equal to 0.2 (see the horizontal dashed line in Fig. 2). Once again, the figure shows the normalized propagation constant when the cut position varies over a two-periods range and one observes again a cutoff which corresponds to the light cone limit and a continuous transition when the band edge is crossed.

For greater insight into the nature of the surface modes, we have plotted the electric field for several points indicated in Figs. 3 and 4. In Fig. 5 the modulus of the electric field is shown using a logarithmic scale for $d/\lambda = 0.2$ and $k_x = 0.268$

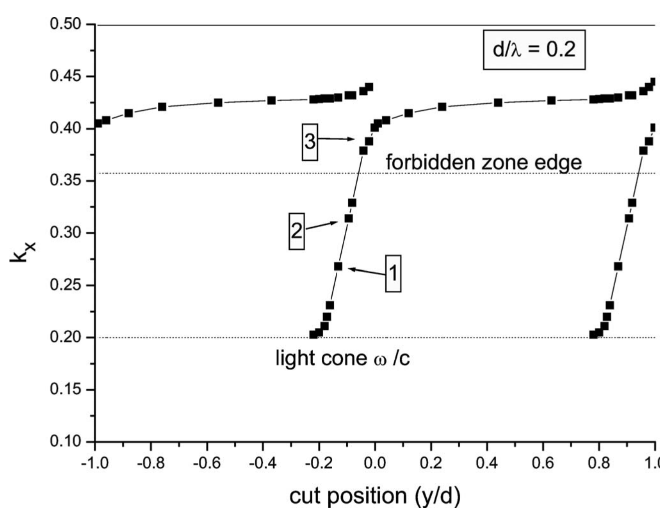

FIG. 4. Normalized propagation constant of the modes when the cut position varies, for $d/\lambda = 0.2$. TE polarization.

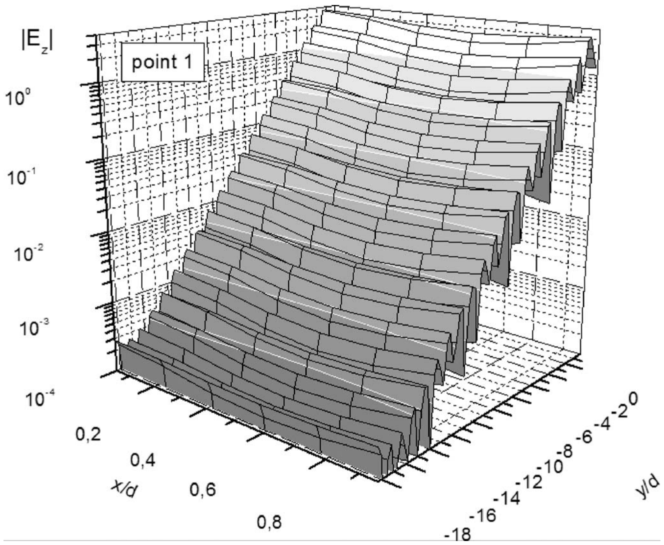

FIG. 5. Modulus of the electric field in the photonic crystal for $k_x=0.268$ and $d/\lambda=0.2$ (point 1 in Fig. 4). TE polarization.

corresponding to the point labeled 1 in Fig. 4. This point belongs to the bandgap and an exponentially decaying field can be expected in the photonic crystal. In this figure, we can observe only small variations of the field with respect to the x coordinate and the average exponential decay of the field with the y coordinate. Both features of the field are even more obvious in Fig. 6 where the modulus of the electric field with respect to the y-coordinate has been plotted for two different values of x (in between two square holes and across the middle of a hole). The field is of course necessarily decaying outside the crystal as the point has been chosen below the light cone. A closer look at the field reveals strong oscillations and only the field averaged on a period can be considered as exponentially decaying (see Fig. 6). When changing the cut position in order to reach a frequency closer to the edge of the bandgap, we expect to obtain a less important decay than for the previous example. It can be observed in Fig. 7, which has been obtained with $d/\lambda=0.2$ and $k_x=0.314$ (corresponding to the point labeled 2 in Fig. 4). In both cases, a weaker guiding effect close to the exit surface is observed as can be expected.

The position of point labeled 3 in Fig. 4 has been chosen to be outside of the bandgap region. The field modulus is plotted with respect to the y coordinate in Fig. 8 (top). The field is no longer really localized in the vicinity of the upper boundary of the crystal. This is even more obvious in Fig. 8 (bottom), which corresponds to the point 4 in Fig. 3. These modes are still guided modes as the fields are evanescent in vacuum (the point 4 is below the light line).

For the sake of completeness, Fig. 9 shows the normalized frequency when the cut position varies for the TM case of polarization. The results are similar to those in the case of TE polarization except that, given the width of the bandgap, the propagation constant reaches the light line before outgoing from the bandgap region.

IV. HOMOGENIZATION

With the aim to understand more precisely the physical processes involved, we have studied the homogenization limit of the structure. More precisely, all the dimensions along x are assumed to be shrunk and to tend towards zero with a constant filling factor. The theoretical limit has been known for years and is given by a homogeneous anisotropic layer whose permittivity tensor is given by[21]

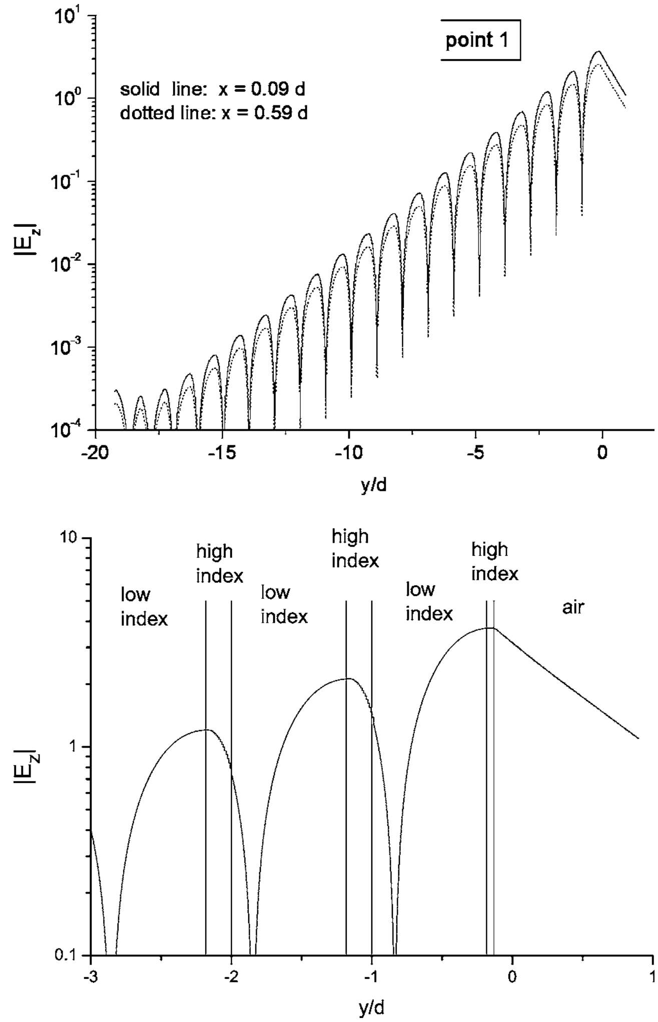

FIG. 6. Top: modulus of the electric field in the photonic crystal for $k_x=0.314$ and $d/\lambda=0.2$ and for two different values of the x coordinate. Bottom: zoom on the details of the oscillations of the electric field modulus, the vertical lines represent the position of the layers. TE polarization.

$$\varepsilon = \begin{bmatrix} \varepsilon_x & 0 & 0 \\ 0 & \varepsilon_y & 0 \\ 0 & 0 & \varepsilon_z \end{bmatrix}, \tag{2}$$

where

$$\varepsilon_y = \varepsilon_z = \frac{1}{d}\int_0^d \varepsilon(x)dx \tag{3}$$

and

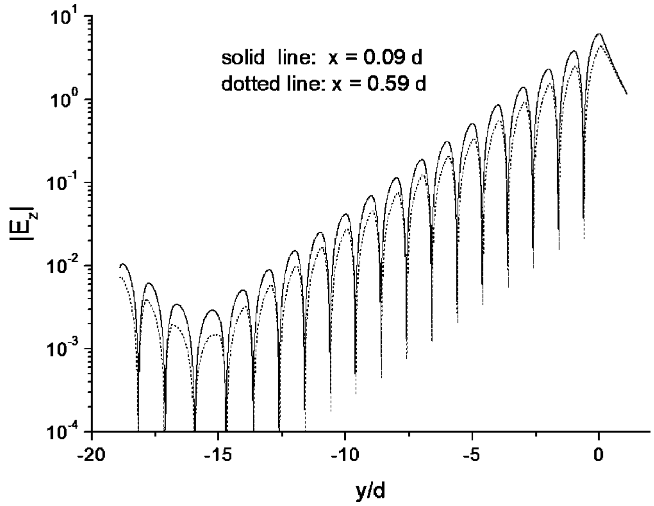

FIG. 7. Modulus of the electric field in the photonic crystal for $k_x=0.314$ and $d/\lambda=0.2$ (point 2 in Fig. 4). TE polarization.

$$\frac{1}{\varepsilon_x}=\frac{1}{d}\int_0^d \frac{1}{\varepsilon(x)}dx. \tag{4}$$

Note that the homogenized permittivity can be interpreted as an effective potential for the Helmoltz equation.

For the TE polarization case, the equivalent layer is isotropic with a permittivity ε_z. Thus, the homogenized structure is made of alternated homogeneous thin films whose permittivities are 17.9 and $\varepsilon_z=4.07$, with thickness equal to 0.1815 d and 0.8185 d, respectively. In Fig. 10, the evolution of the normalized propagation constant of the mode has been plotted starting from the value obtained for the point labeled 2 in Fig. 4 and making the period tend towards zero. The value corresponding to the homogenized structure ($d_x=0$) is also represented using Eq. (4). The relative variation of the normalized propagation constant of the mode is only approximately 10%. Subsequently, we expect to trace the main features of the surface modes on the homogenized structure. The direct comparison of the field modulus in both structures confirms the similarity of the modes (see Fig. 11). Thus, it has been shown in TE polarization that the lateral structure of the photonic crystal is not a determining factor in the existence and in the behavior of the surface modes on two-dimensional photonic crystals.

For the case of TM polarization, a stack of anisotropic homogenized layers must be considered where the relevant tensor components are $\varepsilon_x=1.21$ and $\varepsilon_y=4.07$ with a thickness of 0.8185 d and isotropic layers with a permittivity equal to 17.9 and a thickness equal to 0.1815 d. The square points in Fig. 9 show the dispersion relation for the homogenized structure and the curve obtained is surprisingly close to that obtained for the two-dimensional photonic crystal (solid line).

Note that even if the quantitative results are dependent on the chosen crystal, the conclusions based on qualitative aspects are not. Layer by layer homogenization has been proven to be efficient for different types of structures.[22] In the domain of grating theory, it has been shown that the homogenization procedure can give reliable results as long as only one diffracted order exists, requiring a period equal to the half of the wavelength.

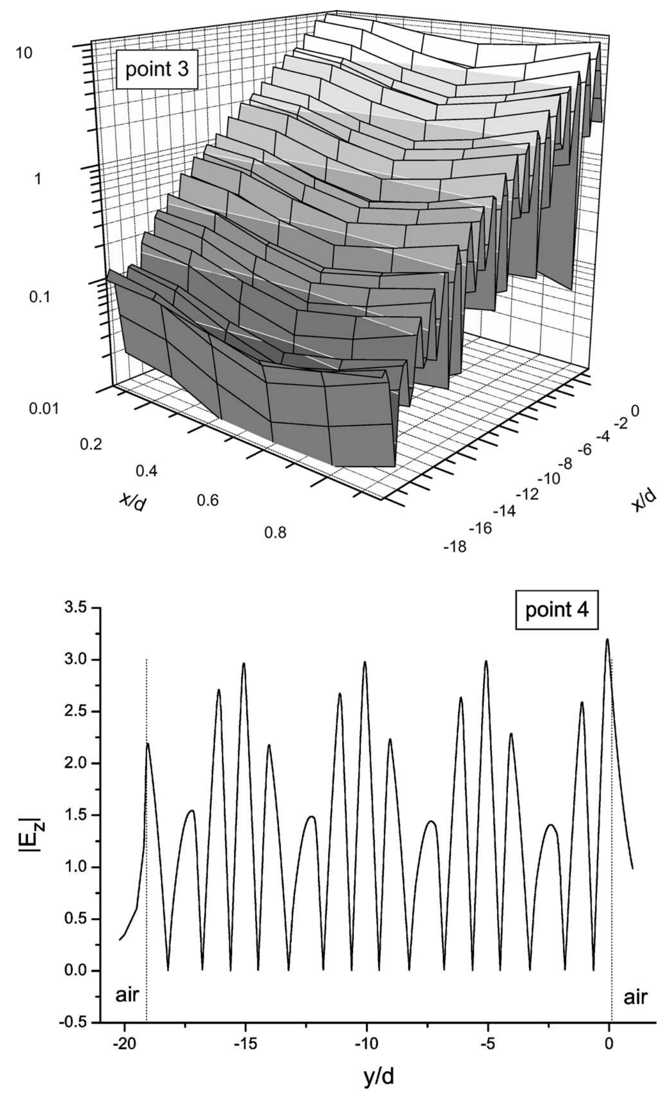

FIG. 8. Top: modulus of the electric field in the photonic crystal for $k_x=0.388$ and $d/\lambda=0.2$ (point 3 in Fig. 4). Bottom: modulus of the electric field in the photonic crystal for $k_x=0.25$ and $d/\lambda=0.167$ (point 4 in Fig. 3). TE polarization.

To understand the underlying physics of the surface modes on photonic crystals, the simplest model explaining the main observed features must be found. The homogenization presented above is the first step in that direction. Another way to approach the problem is to deduce an effective permittivity from the observation of the average exponential decay in the photonic crystal

$$\varepsilon_{\text{eff}}=\left(\frac{c}{\omega}\right)^2(k_x^2+k_y^2), \tag{5}$$

where the value of k_x is known and k_y is deduced from the exponential decay of the field in the structure. Note that k_y can also be obtained more conveniently using the eigenvalues of the transfer matrix associated with one period. It

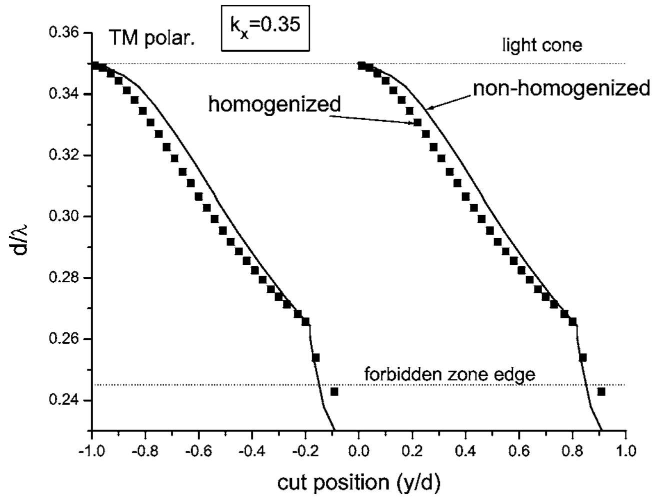

FIG. 9. Normalized frequency of the modes when the cut position varies, for $k_x=0.35$. Square dots: homogenized structure. TM polarization.

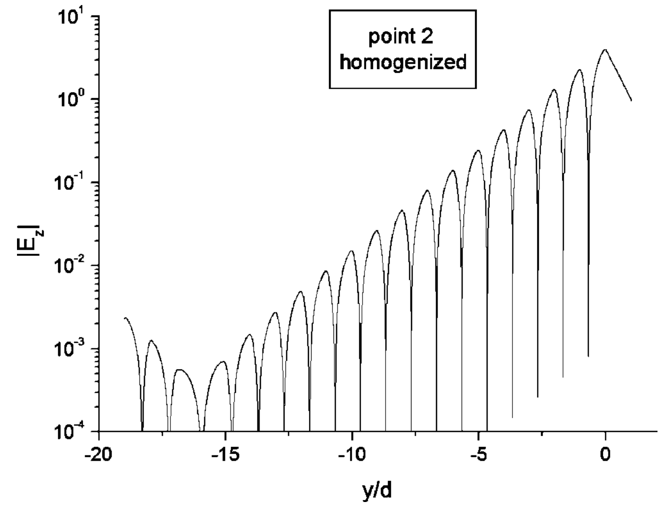

FIG. 11. Modulus of the electric field in the homogenized structure $k_x=0.314$ and $d/\lambda=0.2$. TE polarization.

should be recalled that the transfer matrix algorithm is unfortunately numerically unstable and more complex but stable algorithms must be used such as scattering matrix ones.[23]

In the studied cases, with the parameters of the crystal we use and for both polarizations, the obtained permittivity is always positive below the light line. Thus the idea of surface plasmonlike modes can immediately be ruled out even for TM polarization.

Given the positive permittivity we have obtained, obviously, no true surface modes can be found and necessarily dielectric layers must be included in the model to enable the support of guided modes. In order to illustrate this approach, we will focus on the structure corresponding to the point 1 in Fig. 4. The selected model thus consists in a substrate with a permittivity equal to $\varepsilon_{\text{eff}}=1.598$ covered with a dielectric layer. The parameters of this layer have been tuned in order to obtain the mode for the same values of d/λ and k_x. The permittivity of the guiding layer is equal to 9.3 and its thickness equal to 1.05 d. The comparison of the modulus of the electric field in the structures shows the relevance of the model (Fig. 12). The oscillations of the field in the crystal are of course absent in the homogeneous effective media, but the average exponential decay is identical. The effective media having been chosen in order to produce the same exponential attenuation, this result was not unexpected. More significant is the fact that the oscillations of the field in the first layer are also quasi-identical in both structures.

V. DISCUSSION AND CONCLUSION

The different results presented in this paper show that the main features of the surface modes supported by a photonic crystal can be explained by a simple model, which consists in a guiding homogeneous layer structure. It appears that the

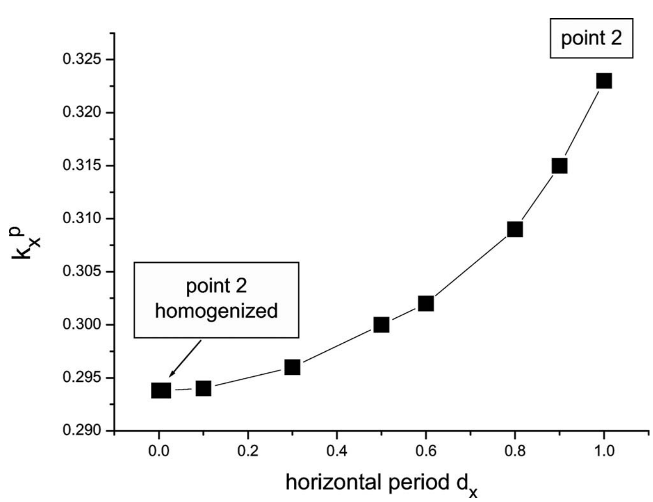

FIG. 10. Homogenization. Variations of the propagation constant of the mode when the lateral dimensions are shrunk. TE polarization.

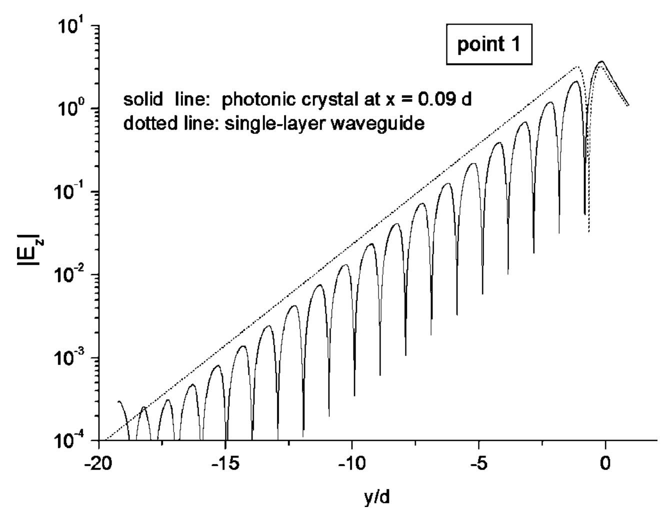

FIG. 12. Comparison between the fields in the photonic crystal structure and in the simple model that consists in one homogeneous guiding layer. TE polarization.

so-called surface modes should be considered rather as guided modes in dielectric layers than as real surface modes such as surface plasmons. A large part of the evidence is given by the similarity between the modes supported by both structures.

Let us now observe the similarities between the surface modes and guided modes in a high index dielectric layer. First, the existence of the modes is not really depending on the presence of a band gap and it has been shown that there is no cutoff corresponding to the edge of the band gap but rather a continuous transition from modes localized at the vicinity of the interface to modes that are delocalized in the whole structure. This behavior is fully consistent with the fact that in our model, the permittivity contrast will allow guiding in the thin dielectric layer only in the bandgap.

Second, the observed modes present a cutoff when the frequency reaches the light cone. This is again a characteristic of guided modes in a dielectric layer surrounded by lower optical index dielectric media. Thus, the physics of the surface modes supported by photonic crystals could be understood by using a very simple model of a dielectric guiding layer, and given their important role in the coupling (outcoupling) of light to (from) a photonic crystal, we believe that these attempts at clarifying the underlying physics are important.

ACKNOWLEDGMENT

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