

Losses and transmission in two-dimensional slab photonic crystals

M. Kafesaki^{a)} and C. M. Soukoulis^{b)}

Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, P.O. Box 1527, 71110 Heraklion, Crete, Greece

M. Agio^{b)}

INFN-Dipartimento di Fisica "A. Volta," Università degli Studi di Pavia, via Bassi 6, I-27100 Pavia, Italy

(Received 9 February 2004; accepted 15 July 2004)

Using a three-dimensional finite-difference time-domain method, we present an extensive study of the losses in two-dimensional (2D) photonic crystals patterned in step-index waveguides. We examine the origin of these losses and their dependence on the various system parameters such as the filling ratio, the lattice constant, the shape of the holes, and the propagation direction. Furthermore, we examine the possibility of studying these losses using an approximate 2D model; the validity and limitations of such a model are discussed in detail. © 2004 American Institute of Physics. [DOI: 10.1063/1.1790068]

I. INTRODUCTION

Photonic crystals are periodic dielectric structures which exhibit in their spectrum band gaps, i.e., frequency regimes of forbidden electromagnetic (EM) wave propagation.¹⁻⁴ This property makes them excellent candidate structures in controlling the EM waves, giving them the ability to be used in a broad range of applications, such as e.g., in telecommunications for the construction of ultrasmall integrated circuits.

To have a full control of the EM wave propagation an omnidirectional band gap is required. This can be achieved only with a three-dimensional (3D) photonic crystal. However, the difficulty in the fabrication of such a crystal, especially at submicron length scales (required for applications in the telecommunications) has turned the attention of the community to an alternative approach. This is 2D-slab photonic crystals (PCs), i.e., 2D PCs combined with a vertical step-index waveguide.⁵⁻¹⁸ In most of the cases the PCs consist of airholes deeply etched in the waveguide structure (see Fig. 1). 2D-slab PCs offer 3D control of the EM waves without the presence of a 3D crystal; the control in the lateral direction is offered by the 2D PC while in the vertical direction by the classical step-index waveguide. Moreover, they have the great advantage that they can be easily fabricated, using existing microelectronics techniques, with full control over the fabrication. Thus they can offer ideal components for ultrathin photonic circuits.

For the 2D-slab systems, two possible designs have been studied, both theoretically and experimentally. One is a high-contrast (membrane) system, where the index contrast between the central/guiding layer and the claddings is high; the other is a low-contrast system, i.e., with low index contrast between core and claddings. A lot of effort has been devoted to the study of these systems and to the determination of which design is more suitable for applications in optoelec-

tronics. It was found that the high-contrast structures usually exhibit more losses at discontinuities (such as corners and interfaces) and they cannot be easily coupled with classical waveguiding structures;¹¹⁻¹⁴ they have though the great advantage that they can exhibit true (lossless) guided modes (modes below the light line of the claddings) for a large frequency-wave-vector regime. On the other hand, the low-contrast structures show better behavior (lower losses) (Refs.19 and 20) at discontinuities and they can be more easily coupled with classical structures. They do not exhibit though lossless guided modes. In low-contrast systems, an issue of central importance is the understanding of the mechanism responsible of losses and finding ways to minimize them, so the structures can be used in applications. Thus, it is very significant to carefully study the losses and their dependencies on the parameters of the system. The aim of this paper is to shed some light on this topic.

Before we proceed to the detailed presentation of our structures and results, we consider as useful to comment more on losses and to mention the sources of loss in slab systems. The losses here can be distinguished as intrinsic and nonintrinsic. The intrinsic losses are usually defined as the

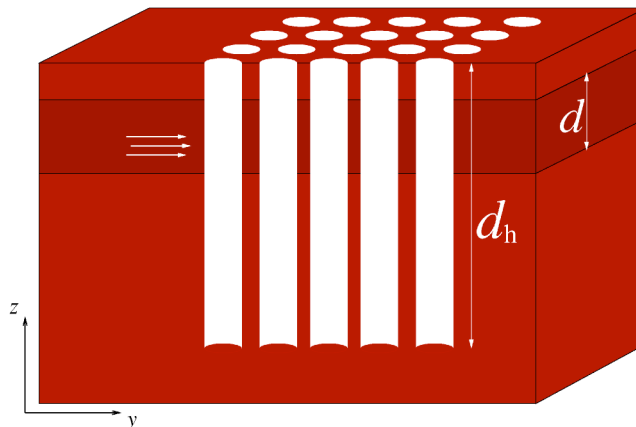


FIG. 1. A 2D-slab photonic crystal made of airholes patterned on a step-index dielectric waveguide.

^{a)}Electronic mail: kafesaki@iesl.forth.gr

^{b)}Also at Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa, 50011

losses for perfect, infinite, and infinitely deep PCs, and they originate from the lossy nature of the guided modes, which in a large ω - \mathbf{k} region lie above the light cone of the substrate. The nonintrinsic losses are either coupling losses, or “imperfection” losses. The coupling losses result from the mismatch between the mode of the unetched dielectric waveguide, which is usually the input system, and the mode of the perforated guide; they are usually expressed through back reflected waves. The imperfection losses, which are expressed mostly through coupling to the out-of-plane radiative modes, are due to deviations from the “perfect” design of the infinitely deep and perfect cylindrical holes; i.e., they come mainly from the insufficient etch depth (these losses usually scale with the vertical overlap of the guided mode with the missing hole part) and the imperfect hole shape. A theoretical analysis of the role of these two parameters can be found in Refs. 19, 21, and 22.

In this paper, restricted to low-contrast systems, and more specifically to systems of hexagonal PCs of airholes deeply etched in an InP/GaInAsP step-index waveguide, we study the dependence of the losses on various of the system parameters. The choice of this specific InP/GaInAsP combination is based on the fact that it has been already used in a large experimental effort. A lot of PC structures patterned on InP/GaInAsP combination have been already fabricated and characterized experimentally;^{21–23} their theoretical analysis though has been restricted to 2D approximate models.

Our study here is done mainly through transmission coefficient calculations and by the use of the finite difference time domain (FDTD) method in three dimensions. The use of the three-dimensional FDTD method is essential in slab PCs, as it can treat the system exactly, without the requirement of any adjustable or phenomenological parameters. Initially we consider deeply etched systems with either perfect cylindrical or conical holes and we study the transmission/losses dependence on the air filling ratio, the propagation direction, the lattice constant of the PC, and the conical hole shape. For the dependence on the waveguide profile and on the etch depth see Ref. 24. At a second step, we examine if and to what extent the study of losses in 2D-slab systems can be done using a 2D model, which treats a system of trenches etched in the step-index dielectric guide. The possibility of using a 2D calculation to describe 2D-slab structures is extremely important, as it provides an easy and fast optimization of the structures, without the requirement of the heavy and time consuming 3D calculations.

II. GEOMETRY AND METHOD OF CALCULATION

The structure studied here has the vertical profile shown in Fig. 1: a GaInAsP layer with $n=3.35$ and depth $d=434$ nm is surrounded by InP cladding ($n=3.17$). The top cladding has depth of 200 nm while the bottom one can extend up to 4 μm . (Analytic calculations show that a layered structure with this vertical profile is monomode in the vertical direction for a large frequency regime around 1.5 μm —the regime of our interest here.) In this three layer structure a PC (of lattice constant a) formed by a hexagonal array of airholes is created.

In almost all the calculations here we consider PCs of eight unit cells in the propagation direction and “infinite” in the perpendicular one (by imposing periodic boundary conditions at the related system boundaries). Moreover, in most of the cases the lattice constant is $a=420$ nm, and the total depth of the holes (d_h) is 3.834 μm . In the cases where different values are used it is written explicitly. The choice of the above parameters was dictated in a large degree from the fact that there is a large amount of experimental work carried out on structures with the above characteristics, thus we had the opportunity to validate our calculations by comparing directly with corresponding experimental data.²³ The use of periodic boundary conditions gave the chance to choose a source with a constant lateral profile (a source confined in the lateral direction would introduce one more parameter into the problem, obscuring thus the influence of the actual system parameters) avoiding simultaneously scattering effects due to the finite system size.

As it has been already mentioned, the study of losses here is done mainly through calculations of the transmission coefficient (T) and by employing the three-dimensional FDTD method.²⁵ The method and the calculation procedure (source choice, discretization, boundary conditions, and transmission calculation) are described in detail in Ref. 24. We just mention here, for completeness, that the transmission calculation procedure consists of sending a pulse, with vertical profile of the guided mode of the nonperforated structure, and calculating the electric and magnetic field components as functions of time, at many detection points after the PC. Using fast Fourier transform the frequency dependence of these fields is obtained and through it the Poynting vector. The transmission coefficient is calculated as the ratio of the transmitted to the incident Poynting vector, both averaged over the different detection points. (The incident Poynting vector is calculated without the presence of the PC.)

III. LOSSES VS SYSTEM PARAMETERS

In this section we discuss the dependence of the transmission T (and thus of the losses) on various system parameters. More specifically, we examine the influence on T of the air filling ratio, the conicity of the holes, the propagation direction, and the lattice constant.

A. Losses vs filling ratio

The scatterers’ filling ratio is one of the most important parameters for the propagation in 2D PCs, as it determines in a large degree the width of the 2D gap. In the case of “true” 2D hexagonal PCs of infinitely long airholes in InP host, the larger gap is obtained for filling ratios [$f=2\pi r^2/(a^2\sqrt{3})$] around 70%. Thus, as optimum f regime for applications, one could simply consider $f\approx 0.7$ also for PC-slab systems (based on InP structures). Unfortunately, when talking about slab systems the question of “best f ” does not have such a simple answer. The reason is that the change of f has also a considerable effect on the losses: increase of f results in increase of losses. A demonstration of this effect is given in Fig. 2, where we show the ΓM and ΓK transmission coefficient (T) for air filling ratios $f=0.22$ [panel (a)] and $f=0.5$

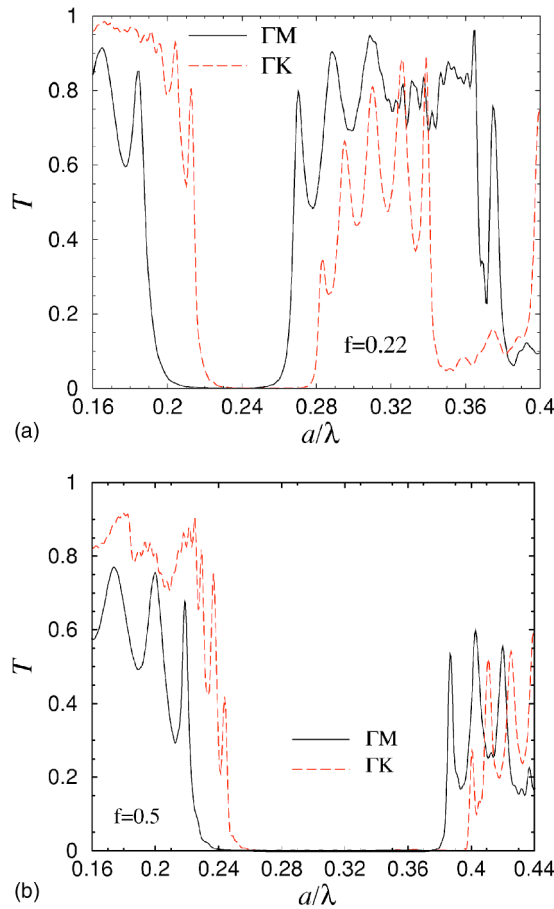


FIG. 2. (a) ΓM (solid line) and ΓK (dashed line) transmission vs dimensionless frequency (a/λ) for the 2D-slab system described in Sec. II. The air filling ratio is $f=0.22$. (b) The same as in (a) for $f=0.5$. a is the lattice constant and λ the free space wavelength.

[panel (b)]. One can clearly see that T decreases as f increases; i.e., the enlargement of the gap is followed by an increase of losses. These losses, as reflection calculations show, are mainly coupling losses, coming from an increase of the modal mismatch between the mode of the bare guide and the mode of the perforated guide. This increase of the mismatch is not unexpected, as increase of the air filling ratio can be considered as equivalent to decrease of the effective index of the mode, relatively to the index of the bare guide mode.

Taking into account the above, one can understand that the search for an optimum f regime, for a given application, depends strongly on the requirements of the specific problem/device. The relative importance of a large gap and lossless transmission for a given application is the key parameter.

B. Conicity of the holes

Another parameter that influences the transmission and is strongly related with the air filling ratio is the shape of the holes. Since in most samples the holes are not completely cylindrical but to a large degree conical (at least their bottom part), it is of considerable importance for the applications to examine the effect of conical hole shape. In Fig. 3 we show the ΓM transmission for the systems of Fig. 2 but for holes

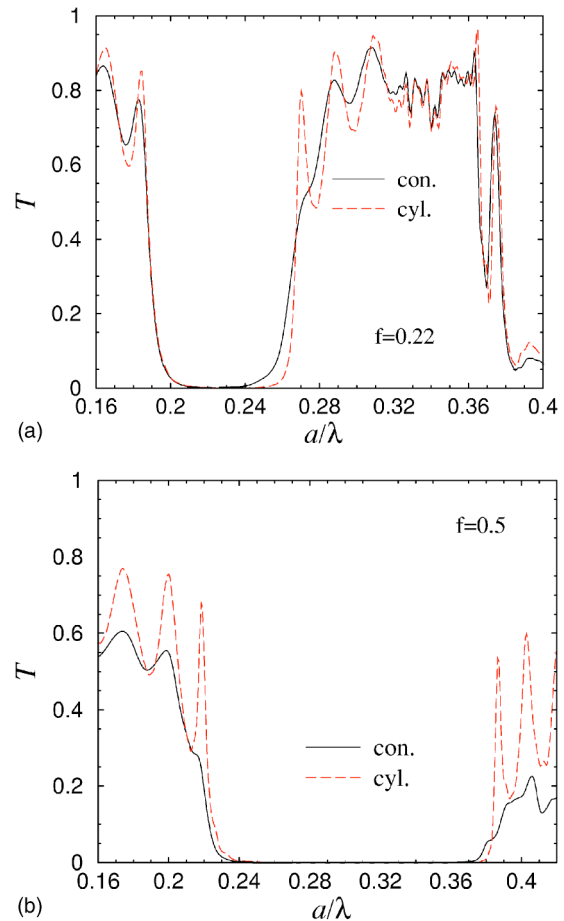


FIG. 3. (a) ΓM transmission vs frequency for the system of Fig. 1(a) for conical (solid line) and cylindrical (dashed line) holes. (b) The same as in (a), for the system of Fig. 2(b). The frequency is given in dimensionless units, a/λ , where a is the lattice constant and λ the free space wavelength.

with conical bottom part (the T for cylindrical holes is also shown here—see dashed lines—for easier comparison). The cone starts at about $1.5 \mu\text{m}$ below the guiding layer (i.e., the conical part has a height of $1.7 \mu\text{m}$ and it constitutes 53% of the part below the guiding layer depth of the holes), representing a “successful” experimental etching procedure. From Fig. 3 one can see that the conical shape at low filling ratios does not lead to a dramatic change of the transmission (compared to that for cylindrical shape). The same does not hold for large filling ratios, where the effect of the conical shape is much more pronounced.

Trying to examine in detail how the conical hole shape affects the propagation, we calculated the electric field all over the sample for both conical and cylindrical holes. A representative result is shown in Fig. 4; it shows the field $E=|\mathbf{E}|$ over a vertical y - z cross section (y is the propagation direction) of the system of Fig. 3(b), for cylindrical (a) and conical (b) holes. The incident wave is monochromatic, with frequency $a/\lambda=0.405$, and the propagation direction is ΓM . The source is launched at the left side of the system and the vertical lines show the “end” of the PC. One can see in Fig. 4(b) how the conical hole shape “destroys” the guided mode profile, increasing the coupling to out-of-plane radiative modes. The effect is the same also for small f but less pronounced.

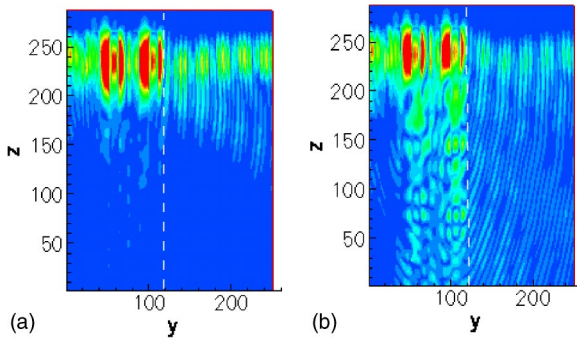


FIG. 4. (a) Field $|E|$ over a vertical y - z cross-section of the structure of Fig. 3(b), for cylindrical (a) and conical (b) holes (y is the propagation direction and z the direction vertical to the layers). The axes are in grid steps (gs), where 1 gs= $a/14$ in the horizontal axis and $a/28$ in the vertical one. The frequency is $a/\lambda=0.404$. The vertical line shows the "end" of the PC. For conical holes the conical region is between $z=9$ and $z=167$.

The influence of the conical hole shape has been already studied in the literature but not in connection with the filling ratio; it was the influence of the conical angle that has been mainly discussed, for both bulk PC-slabs^{21,22} and PC-slab waveguides,²⁶ as came out from that study, increase of the conical angle results in an increase of the out-of-plane losses. The increase of the losses for larger f that we note here is not though due to the resulting increase of the conical angle, as one could possibly argue (for constant hole depth, larger f corresponds to larger conical angle). Detailed calculations using 3D FDTD and an "equivalent" 2D model (see Sec. IV) showed that the main factor responsible for the larger losses at larger f is the f itself.

C. Losses vs propagation direction

Going back to Fig. 2 and comparing ΓK and ΓM transmission, one can see that at the dielectric band the ΓK transmission is larger than the ΓM one, while the case is opposite at the air-band edge. At the dielectric band, the relative reduction of the ΓM transmission in relation to ΓK one is due to an increase of the reflection. At the air-band edge, on the other hand, where stronger diffraction occurs, there is a considerable contribution to the losses coming from coupling to out-of-plane radiative modes. If one considers systems finite in the direction perpendicular to that of the propagation (replacing periodic boundary conditions by absorbing conditions), the reduction of T at the ΓK air-band edge, compared to T at the ΓM air-band edge, is more dramatic due to the presence of also lateral losses (confirmed by our calculations). This may be due to the strong diffraction combined with the fact that the ΓK air-band edge corresponds to ΓM propagation regime—in contrast to the ΓM air-band edge, which corresponds to ΓK gap and thus no lateral losses are allowed. We have to mention here that we found the above ΓK vs ΓM characteristics at all filling ratios that we examined. They have also been found experimentally²³ for a system of $f \approx 30\%$.

D. Lattice constant influence

Another parameter of the problem of propagation in PC-slab crystals is the lattice constant (a) of the PC. Changing

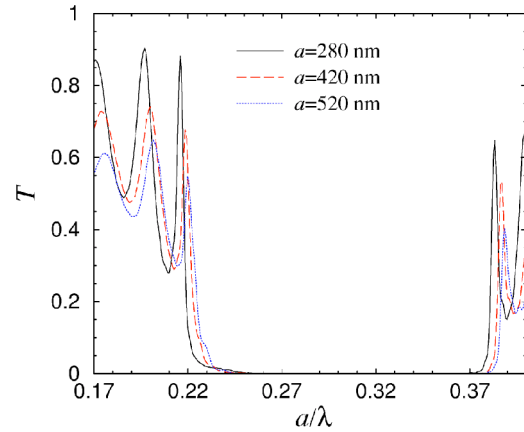


FIG. 5. ΓM transmission vs dimensionless frequency, for the system described in Sec. II, with $f=0.5$, for three different PC lattice constants: $a=280$ nm, $a=420$ nm, and $a=520$ nm.

the lattice constant one changes the working frequency regime (this is the way usually used in the experiments) and thus the vertical profile of the guided mode (the vertical profile depends on the ratio d/λ , where d is the depth of the guiding layer). Thus the results are not scalable in respect to lattice constant, as happens in pure 2D systems, and the requirement for a 3D calculation becomes essential. What is mainly influenced by the change of a in PC-slab crystals is the losses.

In Fig. 5 we show the ΓM transmission vs the dimensionless frequency a/λ for the system of Fig. 2(b), for three different lattice constants: $a=280$ nm, 420 nm, and 520 nm. One can see here that the smaller the a the better the transmission. This originates from the fact that for smaller a the near gap regime is at larger frequencies. At larger frequencies the guided mode is more confined vertically and thus less influenced by the finite hole depth and the conicity of the holes, if it exists. It means less out-of-plane losses. In our calculation though, since the holes are cylindrical and deep enough, out-of-plane losses do not constitute a significant loss component. Here the losses are mainly coupling losses, due to the modal mismatch between the guided mode of the bare guide and that of the perforated guide. A possible explanation for the larger mismatch at larger a may be the following: Since this mismatch is induced by the holes, when the guided mode is more extended vertically the hole volume that it "sees" becomes larger and thus the mismatch also becomes larger.

IV. 3D VERSUS 2D-VERTICAL CALCULATIONS

Since 3D FDTD calculations are very time and memory consuming (not allowing, thus treatment of large systems, complicated elements, and coupling to input/output devices), it is of considerable importance to replace them, where possible, with equivalent 2D calculations. For the study of losses in PC-slab crystals, the most reasonable choice of an "equivalent" 2D calculation concerns a system such as the one of Fig. 6, i.e., a system of trenches combined with the step-index guide of the actual PC-slab. In what follows, we try to study such a system (2D-vertical model) and to exam-

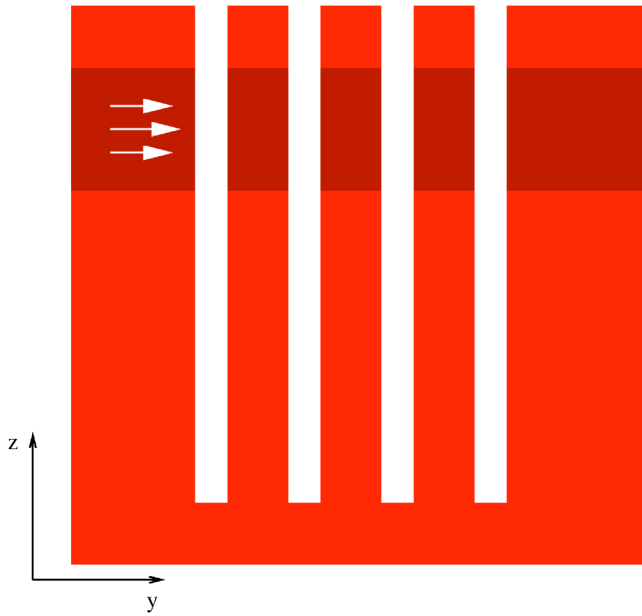


FIG. 6. The structure studied within the 2D-vertical model.

ine if and to what extent its study can replace the 3D study of the actual slab. This is done mainly by comparing corresponding 2D- vertical and 3D results.

A problem here is the choice of a “proper” air filling factor for the 2D-vertical system (f_{2D}); must it be that of the 3D system or should one choose a different value (e.g., trenches with width equal to the diameter of the holes of the 3D system)? Since there is not a straightforward answer, we consider the filling factor as one of the parameters of the problem and we examine various different f_{2D} values.

In an attempt to estimate the *quantitative* power of the 2D-vertical model we performed a variety of comparative 3D and 2D-vertical calculations. What we found is that it is not possible to reproduce both the gap width and the midgap position of the actual 3D system, with whatever choice of f_{2D} . Also, as it is apparent, one cannot reproduce any ΓK versus ΓM transmission features, since the model cannot distinguish between the two directions. Despite these disadvantages the quantitative power of such a model was found to be not negligible. Choosing $f_{2D}=f$, one can reproduce quite well the 3D ΓM transmission close to the air-band edge and around the dielectric band edge (see Fig. 7). Moreover, choosing $(r/a)_{2D}=r/a$ (r : hole or trench radius) one can obtain a midgap close to the average of ΓK and ΓM midgaps of the actual system (with a much larger gap width).

Although the quantitative power of the 2D-vertical model is somehow limited, the case is not the same for its *qualitative* power, which is really significant: it can reproduce extremely well the dependence of the losses on almost all the system parameters. A characteristic example showing the power of this model is given in Fig. 8. In Fig. 8(a) we show the 2D-vertical transmission for a system with $f_{2D}=0.3$, for cylindrical (i.e., rectangular) and conical (i.e., triangular) trenches (solid and dashed line, respectively). Figure 8(b) shows the same for $f_{2D}=0.6$. (In the conical case the cone starts immediately below the guiding layer.) Comparing Figs. 8(a) and 8(b) one can see the larger influence of the

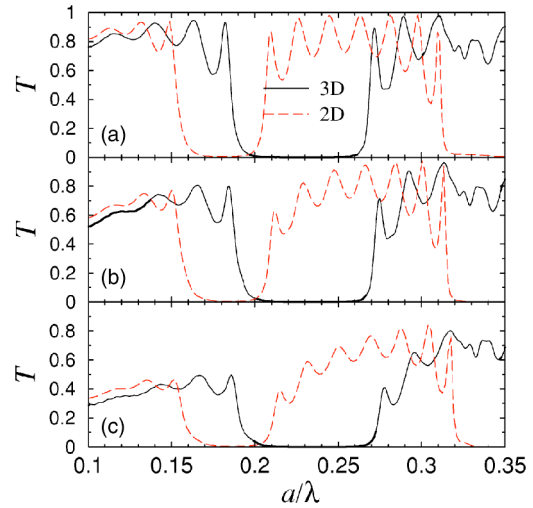


FIG. 7. Transmission (T) vs dimensionless frequency (a/λ) for a system with $f=f_{2D}=0.25$, for lattice constants $a=300$ nm (a), $a=420$ nm (b), and $a=600$ nm (c). The solid lines show the ΓM transmission produced by a full 3D calculation and the dashed lines the T obtained by the 2D-vertical model. The depth of the holes is $d_h=2.234 \mu\text{m}$.

conical shape at larger air filling ratios, which we discussed in the precoding section in connection with 3D calculations. The additional point here is that in changing the filling ratio we kept the conical angle (ϕ) constant, changing the depth of the trenches; nevertheless the relation “larger the f , larger the

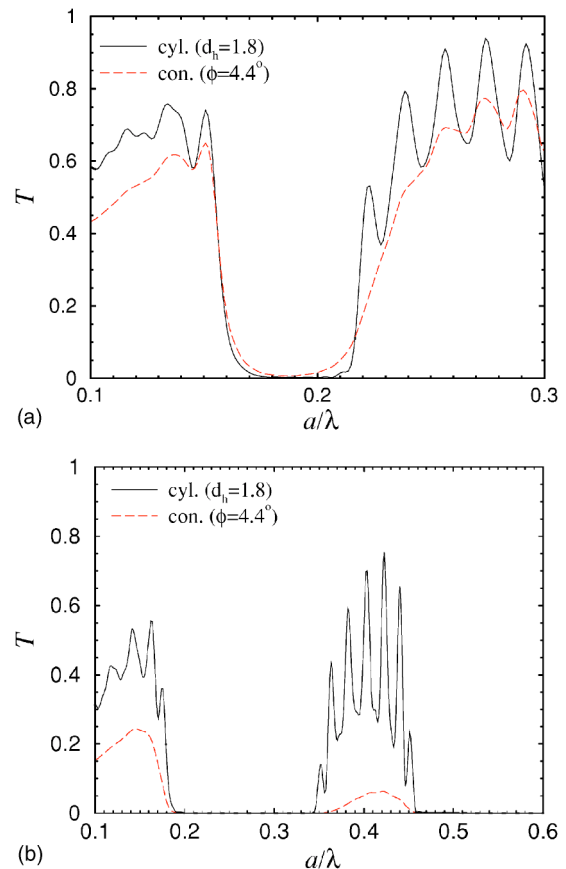


FIG. 8. 2D vertical T vs dimensionless frequency (a/λ) for a system with $f_{2D}=0.3$ (a) and $f_{2D}=0.6$ (b), for cylindrical (solid lines) and conical holes of conical angle $\phi=4.4^\circ$ (dashed lines). The depth of the holes (in μm) for the cylindrical case is mentioned on the graphs.

influence of the conical shape" still holds. This verifies that the parameter responsible for the larger influence of the conical shape at larger air filling ratios is the filling ratio itself and not any variation in the conical angle. Moreover, the filling ratio seems to have more dramatic influence than the conical angle on the conical holes' system transmission. Calculating the transmission for conical holes with $f_{2D}=0.6$ and depth equal to that of the cylindrical holes case, changing thus the conical angle (to $\approx 2\phi$), we found approximately the same transmission as in Fig. 8(b) shown by dashed line.

V. CONCLUSIONS

We studied systematically the transmission properties and the losses of hexagonal photonic crystal slabs, by the use of 3D FDTD method. The detailed 3D calculations led to a thorough investigation of the dependence of the losses on the filling ratio, the hole shape, and the lattice constant of the hexagonal PC. Our studies were concentrated in physically realizable low-contrast structures, consisting of a GaInAsP layer surrounded by InP claddings.

We found that, as the filling ratio of the air holes increases, the width of the gap increases but at the same time the absolute transmission decreases, and therefore the losses increase. Depending on the application one might need to have a big gap, but it is guaranteed that it will be associated with considerable losses. We also found that the shape of the holes plays an important role in accounting for losses, especially at large air filling ratios. Moreover we found that the losses depend on the propagation direction, as well as on the PC lattice constant; as the lattice constant is increased, losses are also increased. While in 2D studies the transmission is scalable with respect to the lattice constant, this is not the case for 2D finite PC-slabs. The reason is that the vertical profile of the propagating mode does not scale with the lattice constant, a , and therefore losses and transmission will depend on a . The width of the gap though of the finite PC-slabs remains the same as a is changed, since it scales with the lattice constant.

Finally, we compared our detailed 3D FDTD results with equivalent 2D results. We found out that a 2D system of trenches gives results with great qualitative agreement with the accurate 3D results.

Our detailed numerical studies can provide sufficient guidance in designing and fabrication of low-loss photonic crystal slab structures (PCs, PC waveguides,²⁷ combiners, splitters etc.). Simultaneous measurements of the transmission properties can be used to judge the quality of the fabricated structures.

ACKNOWLEDGEMENTS

The authors would like to thank H. Benisty and R. Ferrini for useful discussions. Ames Laboratory is operated by the U.S. Department of Energy by Iowa State University under Contract No. W-7405-Eng-82. This work was supported by the Director for Energy Research Office of Basic Science and European Union Information Societies Technology project PCIC (Photonic Crystal Integrated Circuits).

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