

Introduction of 3D Photonic Crystal Waveguide Structure by Calculating Effective Refractive Index

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Abstract

We analyze two- and three-dimensional Photonic Crystal Slabs by calculating effective refractive index and out of plane losses. According to the physical properties of the photonic crystal such as lattice constant, structure, material and the holes radius, versus wavelength; we analyze the transmission in the slabs. In addition, in 2D photonic crystal slabs, the incident light will be controlled in third dimension by interior reflection; therefore, we simulate a photonic crystal waveguide by using Finite Element Method as a special method to solve physical problems mathematically. We decline dimension of our simulation in two-dimension and calculate its effective refractive index. In addition, we will add this index in 3D photonic crystal simulation as a waveguide like experimental samples and calculate effective refractive index of other layers again. Then, we set these effective refractive indexes in 3D photonic crystal waveguide and introduce an optimized model to validate our model transmission versus wavelength is plotted two and three dimension photonic crystal waveguide and the results of these two models are comprised and have a good agreement in 2 and 3 dimension. Therefore, it will be effective in construction of optoelectronic devices.

Keywords: Effective Refractive Index, Finite Element Method, Light Emitting Diodes, 3D Photonic Crystal, Waveguide

1. Introduction

According to electronic limitation to reduce the size of device, enhance the speed of data entertainment in modern industry, scientists tried to find a solution like using photon instead of electron¹. Therefore, in the last few decades, researchers concentrate their attention on Photonic Crystals (PhC) in Nano-scale to reach superior speed and capacity. This kind of PhCs due to their particular attribute and high potential in optoelectronic, are lead to integrated optics applications in telecommunication, information technology, medicine, military industry and etc^{1,2}.

Uppermost, 2D and 3D periodic structures are called Photonic Crystals which Yablonovitch introduced in 1950 for the first time^{3,4}. Nowadays, one of the most important use of these crystals observed in the industry of Light Emitting Diodes (LED) which are one of the best choices

to save energy in order to their brilliance of solid state materials. Furthermore, LEDs are a kind of the important devices due to their ability to convert electricity to light directly. First time, Benisty and his coworkers studied two-dimensional PhC with triangular array air holes that drilled as a laser waveguide, achieved out of plane losses in different ways and introduced role and significance of these losses as well as effect of hole depth to enhance the quality and efficiency of LEDs⁵⁻⁷. Since, to have higher efficiency in LEDs is a challenging issue, extensive investigation is being conducted to increase the optical efficiency of LEDs. PhCs exactly can be one of appropriate options for achieving efficient LEDs.

LEDs are one of the prominent sources to extract light. Given the wane of available energy sources and try to save energy; they appropriate a special position in business in the last years. On the one hand, according to the high expense of manufacturing PhC devices, we should

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design them by numerical solutions and on the other hand, dearth of suitable computer sources as well as high volume calculations in 3D simulations impossible to do by personal computers, we should solve our problem in two-dimension, albeit we may lose few information. There are different ways to build PhC slabs and there are different ways to reduce losses in third dimension, hence, we are selected localization of refractive index among plane waveguide that induce radiate models around by coupling guide modes and cause out of plane losses in third dimension^{8,9}. In this paper, we selected finite element method to simulate a PhC waveguide and perturbation analytical method to be used losses⁷. Firstly, we will introduce a PhC waveguides and its physical structures; next, we will calculate the effective refractive index and simulate a model by finite element method, and finally we will compare two and three-dimensional PhC slabs in order to achieve optimum PhC waveguide transmission in 2 and 3 dimension.

2. Photonic Crystal

Photonic crystals are periodic structures of dielectrics with different refractive index. According to their periodicity in one, two and three dimension are called one, two and three-dimension photonic crystal which use to design devices like mirrors, waveguides, cavities, Light Emitting Diodes (LEDs) and so on. In addition, it is possible to employ light control and guiding by combination of these devices⁵. Furthermore, by considering dimensions and lattice constant, gaps are producing in the PhC band structure which light propagation in certain directions is forbidden. However, when there is a defect in PhC in certain frequency, light is allowed to propagate. Line defect by removing one or several rows of rods is created in order to propagate light through it, which allows us to design a PhC waveguide and control the band gap to spread certain frequency. In spite of 3D PhC, which has a complete band gap, 2D PhC slab easier to fabricate with conventional semiconductor processing technology. However, light is diffracted and leaked away in 2D structures, which are localized by total interior reflection in third dimension¹¹. Therefore, light has to be bound in the plane of PhC, which sandwiched between two slabs. In vertical direction, light is bound to the slab waveguide by layers with the higher refractive index and the core. In fact, PhC slabs consist of air holes etching through the bottom cladding in semiconductor PhC waveguide,

which results losses inside the PhC waveguide. Taking account these losses could allow us to treat 2D PhC slabs as a 2D problem in simulation space.

Light will be controlled by PhC or propagate into line defect; by combining PhC and slab in parallel direction of waveguide layer, considering different shape and depth of air holes as well as calculating effective refractive index can allow us to introduce the optimized structure of waveguide more effective and functional if the model would be close to real structure. Since the Figure of perfectly cylindrical holes with a flat bottom does not correspond to reality as it is shown in Figure 1⁹, and we cannot manufacture this ideal model, we have to take into account different more realistic hole shapes such as cone and cone tail clipping and compare their losses⁸. This method introduced as a useful simulation tool for optimizing etching techniques for the fabrication of PhC structures as a potent structure to demonstrate optoelectronic devices. In addition, according to both high expense of PhC production and effort of artisans to construct high quality applicants, such simulations in order to save cash and means beside improve grade of devices, would be valuable and useful because they can prevent increasing application prices and try enhancing satisfaction customers.

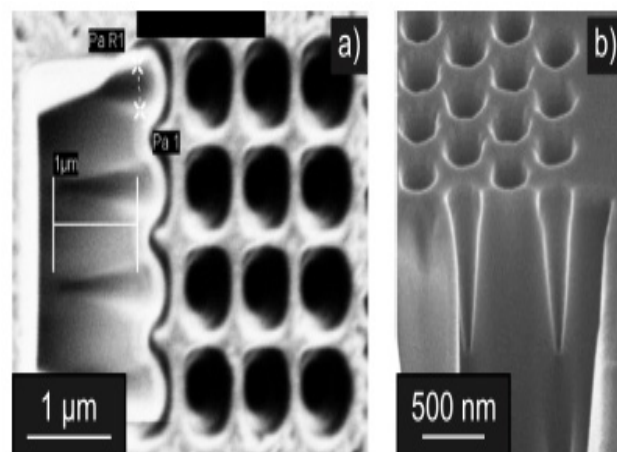


Figure 1. Experimental sample of drilled holes⁹.

3. Effective Refractive Index and Out of Plane Losses

However general format of 3D PhC as shown Figure 2, in this paper we consider 2D PhC models which is simple and fast to simulate and allow us to model in personal

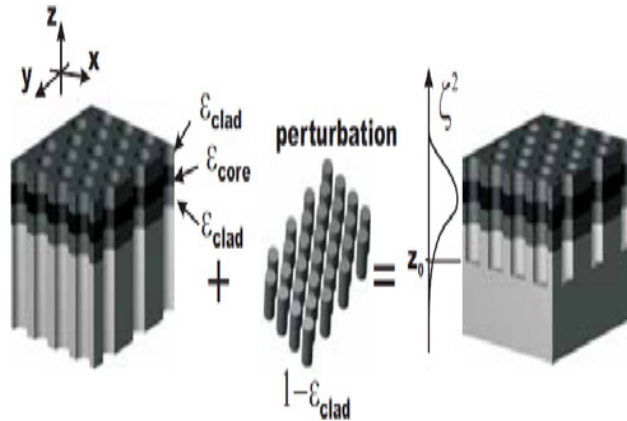


Figure 2. Structure of PhC with certain hole depth, dielectric adds as perturbation in uncertain structure.

computer but we must consider third dimension effects in the crystal structure. Furthermore, we should optimize different related parameter in order to close the result of our simulation to the expected result of experimental data, since the obvious contrasts between them are transmission versus frequency. First one occurs because of transmission differences in 2D PhC with context effective refractive index and 3D crystal structure with three parallel semiconductor layer and second one occurs due to out of plane losses in vertical direction created by certain length of holes depth. For analyzing losses due to holes depth, we will consider 2D PhC structure that etched through a semiconductor waveguide and calculate its effective refractive index. Then we will set it in the 3D model a refractive index of its core. Differences in transmission and frequency displacement in 2D and 3D PhC allow us to estimate total effective refractive index of the waveguide and introduce the optimum structure. Besides, these compares help us to improve total effective refractive index of photonic applications and calculate out of plane losses due to hole certain depth. In general, PhC Structure consists of a core as a guiding layer in order to bound and control light in vertical direction with refractive index $\epsilon^2 = n_2^2$, a top cladding and a bottom cladding which sandwich core with lower refractive index $\epsilon_1 = n_1^2$. Drilling the waveguide slab into the cladding in third dimension causes destructing vertical localization and out of plane losses. Etching these air holes lead to losses through air and bottom layers. H. Benisty et al. has developed a model for calculation of intrinsic losses based on

perturbation approach and its relation to effective refractive index⁹.

Out of plane losses can be split into the intrinsic loss and losses due to the hole characteristics (hole depth, hole shape, hole surface rugosity):

$$\epsilon'' = \epsilon''_{\text{int}} + \epsilon''_{\text{hole}}$$

It is shown that ϵ''_{int} values refer to the xy plane and has first order of magnitude lower than the ϵ'' values. Thus, ϵ''_{hole} is the main factor that sets the loss level and refer to the z direction. In analysis of ϵ'' , an imaginary dielectric constant in air holes is introduced in order to taking account scattering losses. As it is shown in Figure 3, PhC structure is considered as the sum of the indefinite plugs with dielectric constant $\tilde{\epsilon} = 1 - \epsilon_1$. According to the perturbation method selected in this paper, we assume layer are closed to the core and the electric field is neglected by $\Delta\epsilon$ disorder; therefore, we can analyze it in z direction and xy plane:



Figure 3. Model of drilled hole in this simulation and location of Z_{eq} .

$$E(x, y, z) = \psi(x, y)\zeta(z)$$

Since perturbation is taken only in the bottom cladding, a special mode as $\zeta(z)$ has the exponential decay toward the substrate. Then, the partial confinement factor $\Gamma(z_0)$ will be calculated by the overlap integral of $\zeta(z)^2 = e^{-2kz}$ with the missing air column region:

$$\Gamma(z_0) = \frac{\int_{-\infty}^{z_0} \zeta^2}{\int_{-\infty}^{+\infty} \zeta^2}$$

This factor calculated in different depth in Relation between depth hole and confinement factor (Table 1):

Table 1. Relation between depth hole and confinement factor

590	610	650	Etched depth(nm)
0.03	0.02	0.01	$(z_0)\Gamma$

Z_0 is the location where the end of ideal cylindrical hole is drilled into the substrate¹¹. Unfortunately the model of drilled hole in this simulation and location of Z_{eq} figure does not correspond to reality and holes penetrate into substrate conical shape. Whereas its base is located at $z_b = z_a + \Delta z$, z_b is the location where the cylindrical part ends and Δz is the cone height as it is shown in mentioned figure. Moreover, By replacing z_0 in $\Gamma(z_0)$ by z_{eq} that allows us to take into account different hole shapes and compare their losses, we will calculate this factor for our model. This method introduced as a useful simulation tool for optimizing etching techniques for the fabrication of PhC structures as depicted in model of drilled hole in this simulation and location of Z_{eq} .

$$K = (2\pi / \lambda) (n_{eff}^2 - n_1^2)^{1/2}$$

n_{eff} is guided effective refractive index. Here we introduce a quantity named L_{decay} as the decay length of the exponential decay of $\zeta(z)$ into the bottom cladding and it is equals to $1/k$. By comparing total dipole radiation power with dissipated power, we find out:

$$\mathcal{E}_{eff} = \tilde{\mathcal{E}}^2 \left((8\pi^2) / (3\lambda^8) \right) n_1 L_{decay} S_{hole} \Gamma(z_{eq})$$

S_{hole} is holes sectional area using effective hole radius compute using problem data such as filling factor (f) and lattice constant (a), regarding to the $D = a\sqrt{(2f/3)/\pi}$ that allows us to set required data in ϵ_{eff} and finally calculate the effective dielectric constant.

Losses and effective refractive index inherently are analyzed in three dimensions but Requiring of more computation sources make the simulation of PhC in three dimension more complex, therefore it needs too much time and computer resources and in some occasions simulation is impossible. Whereas, achieved result of 2D PhC simulation and experimental data matched with a good approximation, 3D models here can be taken into account in 2D models, which, is easy and fast to simulate, and allow us to model in personal computer. Plus, comparing 2D and 3D models and simulations can help us to introduce optimum structure of the waveguide with highest quality factor.

4. Analysis of Results

In this paper, we will simulate 2D PhC structure which etched through a semiconductor waveguide, calculate its effective refractive index and set in the 3D PhC structure. Then, we will calculate this index for two other layer of three-layer waveguide, which we called them bottom and lower clad. We will start this section by introduction of finite element method as our method to simulate the PhC waveguide. Next, given the certain parameters of the structure, we will describe simulation steps and calculation of total effective refractive index. Hence, we consider it in the three-layer and introduce the perfectly optimized model.

4.1 Finite Element Method

Finite Element Method can solve the problem as a mathematical (in form of equations) and physical (choosing the physical model) equation and the difference is concealed in the possibility of usage of physical and material systems and units. The advantage of this method is, solving the partial differential equations relevant to different physical quantities cause user to be able to get deep realization of complicated systems. A typical work out of the method involves (1) dividing the domain of the problem into a collection of subdomains, (2) finding special equations that describe physical structure of the problem, (3) representing each subdomain by a set of element equations to the original problem, (4) Recombining systematically all sets of element equations into a global system of equations for the final calculation. (5) Considering all boundary condition refers to the problem, (6) solving the system of equations. The global system of equations can be calculated from the initial values of the original problem to obtain a numerical answer¹².

4.2 Simulation Configuration

In simulating two-dimensional PhC waveguide, first, we design a square as the crystal surface and a close packed triangle arrangement of circles as air holes, then, by creating defect and eliminating a number of holes, we set the slope of the removing holes path for the electromagnetic wave to be 60 degrees. We complete the simulation by setting the slab to be made of GaInAsP. In order to avoid light reflection towards the inside of the crystal we use the dispersion boundary condition emit the electromagnetic wave in Z direction in the designed path as it is shown

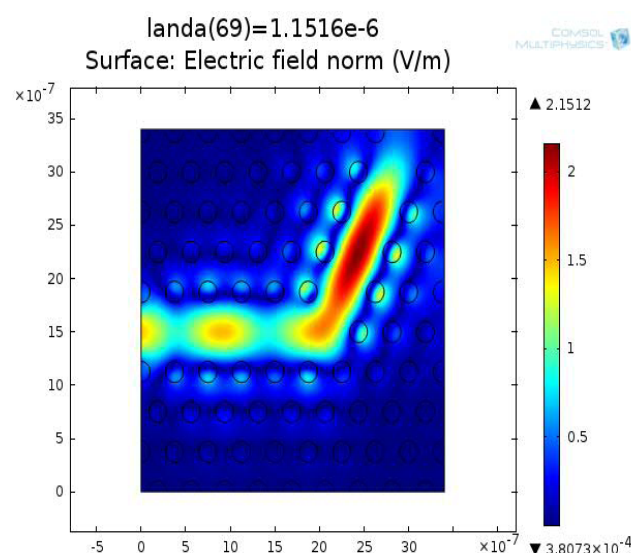


Figure 4. Transmission of electromagnetic wave in $1.2\mu\text{m}$ wavelength in 2D waveguide.

in Figure 4. By introducing the widespread parameters we consider the visible light wavelength and solve it by using its correlation with frequency points in the considered time interval and plot the transmission diagram. The diagram changes with variations in refractive index. Therefore, we calculate the n_{eff} by using refractive index and available effective dielectric constant, and finally we obtain the crystal transmission with respect to n_{eff} .

We consider the PhC waveguide, which we have simulated its two-dimensional structure, as slab of the PhC and sandwich it between two layers of semiconductors made of InP and investigate the wave transmission again.

In this simulation, PhC slab is drawn as a square of dielectric GaInAsP with refractive index of 3.35 and with the dimension of $34\mu\text{m}$. This slab is drilled air holes with radius $0.01\mu\text{m}$ and is designed as PhC waveguide. We consider the filling factor and lattice constant of this crystal to be 0.3 and 375 nm respectively and emit incident light in wavelength interval of $[1.2, 1.7]$ perpendicular to waveguide. We set the L_{decay} to be $360\mu\text{m}$ and filling factor to be 0.03 for penetration depth of $Z_0 = 0.86\mu\text{m}$ ^{10,11,13}. Then, using the problem data, we introduce the efficient refraction index and efficient dielectric constant, according to our simulation, to be 3.7 and 0.361 respectively. We increase efficiency of PhC to some extent by setting the refractive index as the efficient refractive index of three-dimensional crystal core. In order to reach the optimum structure for PhC waveguide (i.e. the highest level of transmission) we need to optimize other contributing

factors in the problem, therefore, we calculate the effective refractive index for two layers of InP semiconductors using the equations stated in the present study.

In three-dimensional simulation, the GaInAsP dielectric is simulated with the same characteristics as the two-dimensional slab and with the height of 434 nm which is sandwiched between two layers of InP semiconductors with the height of 200 and 600 nm and the refractive index of 3.17 as shown in Figure 5. The air cavities in the dielectric are drilled in cylindrical shapes with core ends similar to the expected shape of the drillings done according to figure of experimental sample of

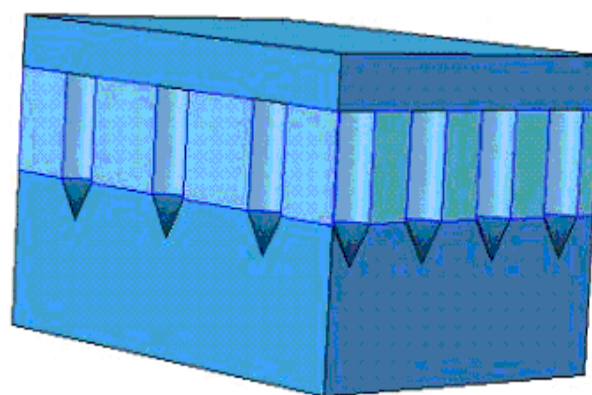


Figure 5. 3D model of PhC waveguide.

drilled holes⁹. The effective radius of these holes is calculated to be 76 nm and the penetration level of the drills in substrate is considered to be $0.86\mu\text{m}$.

As it is expected, given the z_{eq} , filling factor for the structure should be calculated; then refractive index and efficient dielectric coefficient should be calculated. Here, by approximating $z_{\text{eff}} = z_0$ we compute the coefficient dielectric constant for the wavelength of $1.3\mu\text{m}$ to be 0.164 and efficient refractive index for two layers of semiconductors to be 3.21. Finally, we introduce the structure for PhC waveguide and by considering effective refractive index we compare the transmission for both two-dimensional and three-dimensional structure compared.

4.3 Simulation Result

As stated in the private section, at first we simulated a two-dimensional structure or PhC slab and computed the effective refractive index, then, we set this slab between two layers of semiconductors and considering the effects

of loss, we also calculated the effective refractive index for the semiconductors. Finally by applying these coefficients in three-dimensional simulation we suggested an opti-

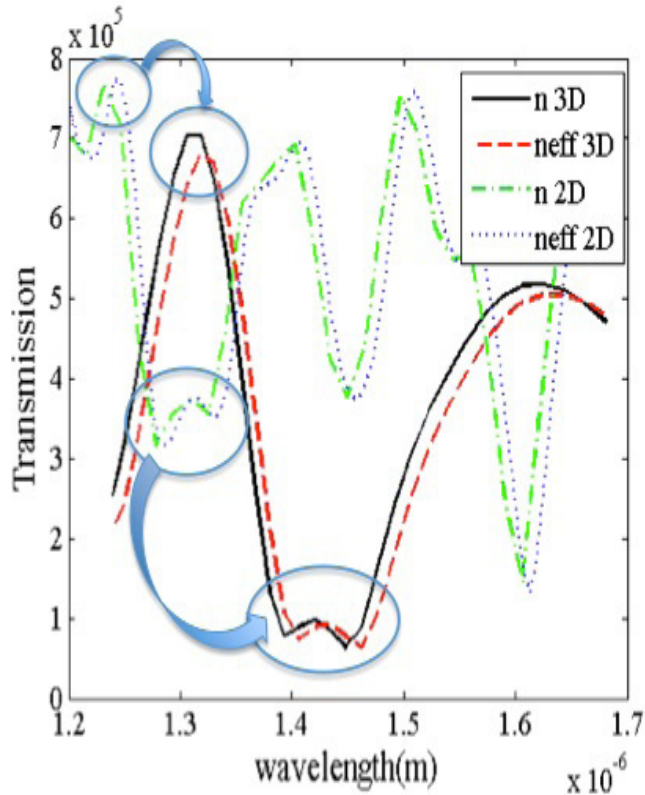


Figure 6. Transmission comparison of PhC waveguide between 2D and 3D structure.

imum structure. We compared the transmission for these two structures and presented the results of this comparison in Figure 6.

As observed in Transmission comparison of PhC waveguide between 2D and 3D structure figure, and it was predictable from the theory, the movement field transmission spectrum versus with wavelength is the same for two and three dimensional structures and match well in the considered intervals. The transmission level is decreased noticeably in three-dimensional structure in comparison to two-dimensional waveguide structure. Also, a red shift has occurred in three-dimensional structure which decrease due to the resultant loss of the out of plane losses in three-dimensional structure, the displacement towards larger wavelength is due to the transmission difference in two-dimensional structure with a background efficient refraction index and three-dimensional structure with

interlayer refractive index contrast. In each of the structures the transmission decrease for efficient refractive index is well observed, which this transmission decrease is the sign of the noticeable change in decrease of out of plane loss and improvement of the quality and performance of PhC tools.

5. Conclusion

With respect to the shape and type of the drillings of the holes are very effective in transmission, loss and the PhC quality used in tools such as LEDs and in as much as ideal cavities in the crystal cannot be created, we have considered the approximate shapes close to what can be created in reality using various drilling techniques and have calculated the throughput rate which is the refractive index in this simulation, cylindrical cavities with cone end the same as the empirical drilling have been considered. Also, we have considered the transmission path angle to be 60 degrees, which is the optimum state for the transmission of the electromagnetic wave transmission in close-packed PhC. We often ignore one dimension and the problem simulated in two dimensions due to the required computer sources limitation and three-dimensional simulation is time consuming. Although this decrease causes the destruction of some data, as it is shown in this study, we can obtain useful information but due to the high cost of the production of the crystals and the tendency of the consumers to have high quality electronic devices and reasonable cost, despite the problems stated in three dimensional simulation some studies are also needed to be done so that by considering the majority of the parameters affecting quality, we can introduce the most optimum structure and in the end decrease the final cost of the product significantly. One of the most effective parameters in quality or PhCs loss is their drilling type which is discussed in detail in this paper and its closest type to experimental type is considered by doing these kinds of simulations effective refractive index with various shapes of holes can be calculated which this can be very useful and efficient for increasing quality of calculation that are based on PhC like LEDs. Also, by comparing the refractive index between different shapes of holes it can be a goal for increasing the drilling techniques and reaching the highest efficiency in tools, which are based on PhC and are considered to be among the most practical tools in industry and human life.

6. References

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