Study of 2-D Photonic Band Gaps for NIR applications.

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Abstract: This work consists of the study and characterisation of the photonic band gaps (PGB) for different 2D-crystal structures. It has run with a simulating software called *Optiwave.* We are going to use two methods to study photonic crystals, the Finite-difference time-domain method (FDTD) and the Plane wave expansion method (PWE). This study has been focus on square and hexagonal lattice formed by dielectric cylinders in water, thus one of the important parameters is the ratio radius-to-pitch.

I. INTRODUCTION

A photonic crystal is a periodic optical structure formed by regularly repeating regions of high and low dielectric constant. An incident electromagnetic wave is being affected by the regular lattice in the same way that the periodic potential in a solid-ionic crystal affects electrons motion by defining the energy bands.

According to the statement mentioned above, the photons see the energy bands that they are allowed to propagate and they depend on the wavelength. Wavelengths that are transmitted inside the structure are called modes and on the opposite side, disallowed bands of wavelength are known as photonic band gaps (PBG). The wavelength characteristics of the PBG are dependent of the pitch of the photonic crystal structure. Proximately, the order of magnitude of the pitch must be the half of the wavelength of the electromagnetic wave to be diffracted. Hence, a structure with a PBG in visible spectrum would have a pitch of $\sim 220nm$ for a wavelength $\sim 450nm$ (blue). So as to the fabrication of these structures that run in the visible part of the spectrum is not an irrelevant point.

The tool we have used is a software called *Optiwave.* This simulating software treat photonic crystals as a periodic array of cylinders in a substrate as you can see in Fig.(1).

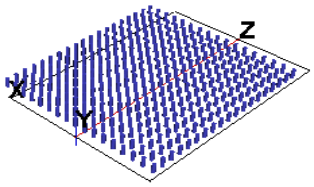

FIG. 1: Screenshot that shows the set of a photonic crystal in *Optiwave*.

In this paper we discuss the calculations of two different structure, the first one is a monoatomic Bravais square lattice. The other one is a monoatomic Bravais hexagonal lattice.

The first task is to study the PBG of several 2D structures and define them. One of the relevant point is the material index of refraction (n), here we do a study from the lowest n value where PBG emerge to $n = 3.6$.

The second task is decide which structures fits better with the lasers we want to work. Being pragmatically it would be useful work in visible range or near-infrared (NIR), where several laser are commercial, or in the infrared (IR) where biological tissues are transparent.

Let me introduce the lasers we contemplated:

Laser	Acronym	$\lambda(um)$
NIR-OC 3rd window	Optic communications	1.55
NIR-OC 1st window	NIR I	0.85
VIS-NIR	NIR II	0.70
He-Ne	He-NE	0.63

TABLE I: The table shows the different lasers we are available to use in the laboratory. Also, the second column shows how we will refer to each laser in charts.

II. OPTIWAVE

This work is based on using *Optiwave*. Even though there are more others goods program on the market, like *EMExplorer* and *Mee*, both are used in the university, we have chosen *Optiwave* due to all the implementation it has.

Optiwave allows us to study the band diagram and the transmission of an electromagnetic wave in a much easier way than going directly to the laboratory.

One of the algorithm of *Optiwave* is based on Finite-difference time-domain (FDTD). It helps study the transmission of electromagnetic waves. This method divides the space into Yee cells, which are small compared to the wavelength. It is characterised because the electric fields are located on the vertex of the box and the magnetic fields are situated on the faces, as you can see an example for a TE wave in Fig.(2).

To solve the problem we consider that the Y-size of the cylinders is infinite and so as Y-direction. It allows us to remove all the partial derivative respect Y from Maxwell's equations. This method solves Maxwell's equations in the time domain, in this approach, both space and time are discretized. The space steps in the X and Z directions are Δx and Δz, recpectively. Both, its order of magnitude is $\sim 0.1\mu m$. And the time step is Δt, and $\Delta t \sim 0.1\ fs$.

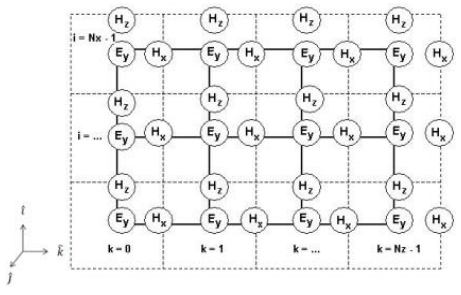

FIG. 2: Location of the TE fields in the computational domain. The indices i and k characterize Δx and Δz. Superscript n labels Δt.

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This method let us express the future components, of both electric and magnetic fields, in terms of the past components, i.e. the Y-Electric component of a TE wave:

$$E_y^n(i,k) = E_y^{n-1}(i,k) + \frac{\Delta t}{\varepsilon \Delta z}\left[H_x^{n-\frac{1}{2}}\left(i,k+\frac{1}{2}\right) - H_x^{n-\frac{1}{2}}(i,k-\frac{1}{2})\right] - \frac{\Delta t}{\varepsilon \Delta z}\left[H_z^{n-\frac{1}{2}}(i+\frac{1}{2},k) - H_z^{n-\frac{1}{2}}(i-\frac{1}{2},k)\right]. \quad (1)$$

In order to solve the band structure, *Optiwave* uses the Plane wave expansion method (PWE). This method solves Maxwell's equations as an eigenvalues problem. We are going to explain it using the electric field. Assuming that the fields are time-harmonic the electric field follows as: $\vec{E}(\vec{r},t) = \vec{E}(\vec{r})e^{i\omega t}$, where ω is the beam frequency. Maxwell's equations can be decoupled as this example shows:

$$\frac{1}{\varepsilon_r}\vec{\nabla}x\vec{\nabla}x\vec{E}(\vec{r}) = \frac{\omega^2}{c^2}\vec{E}(\vec{r}), \quad (2)$$

Notice we already have a eigenvalues problem. According to Bloch theorem, both ε_r and $\vec{E}(\vec{r})$ are periodic along the structure and they can be expanded through Fourier series that let solve the equation (2).

III. FIRST STEPS

In order to be introduced in this simulation field the first steps, apart from *Optiwave* tutorial [1] , have been to look for articles that may can help on our work. Thus, we started simulating the structure that we can find in [2]. The main goal is to achieve the same band structures, and so on, the same PBG, for both TE and TM waves.

This study case is a square lattice with a monoatomic base, composed by Silicon cylinders, $n = 3.45$. These cylinders are laid in air, $n = 1.00$. The other important parameter we need to set is the ratio radius-to-pitch, r/a, where r is the cylinder radio and a the distance between cylinders, both indicated in Fig.(3). In this simulation $r/a = 0.18$, where $a = 1\mu m$.

Fig.(3) shows both direct and reciprocal space of this structure. On the left, the direct space with the primitive cell of a square structure and its primitive vectors. On the right the first Brillouin Zone with its symmetrical points Γ, X and M. Also, r and a are shown.

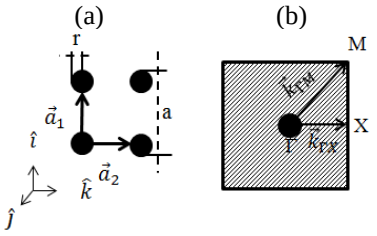

FIG. 3: (a) Layout of direct space. (b) First Brillouin Zone. Both for a monoatomic square structure.

Let me write the primitive vectors for a square structure in the direct space:

$$\vec{a}_1 = a\hat{\imath}$$
$$\vec{a}_2 = a\hat{k}$$
$$\vec{a}_3 = c\hat{\jmath}, \quad (3)$$

notice that the parameter a is the pitch that characterizes the lattice and the parameter c is irrelevant due to is 2-D crystal, but we have to define a base of three vectors in order to calculated the reciprocal vectors:

$$\vec{b}_1 = b\hat{\imath},$$
$$\vec{b}_2 = b\hat{k}$$
$$\vec{b}_3 = d\hat{\jmath}, \quad (4)$$
$$b \equiv \frac{2\pi}{a}, \quad (5)$$

where (3) and (4) are the result of (A.13). Again the third vector only has mathematically meaning.

The Γ point is the center of the first Brillouin Zone, thus X and M points are defined by the vectors:

$$\vec{K}_{\Gamma X} = \frac{b}{2}\hat{\imath}, \quad (6)$$
$$\vec{K}_{\Gamma M} = \frac{b}{2}(\hat{\imath}+\hat{k}). \quad (7)$$

Defining these conditions in *Optiwave* and simulating the PBG structure for a TE wave with PWE method, our results and [2] results:

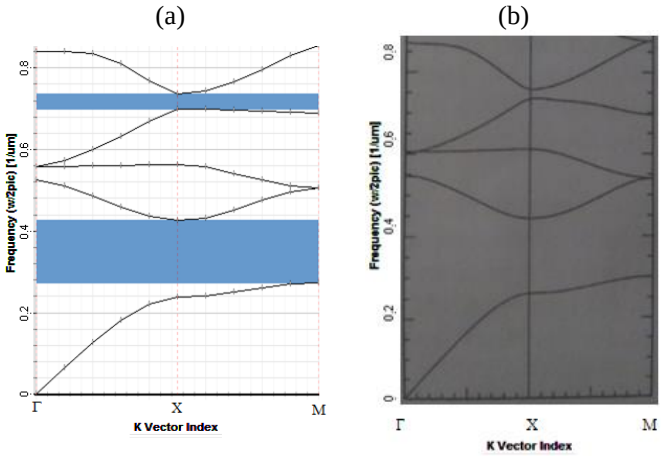

FIG. 4: Band structure along the ΓX and XM directions for a square lattice of silicon cylinders in air and the ratio $r/a = 0.18$. See how two gaps open for TE polarization. (a) Our results running Optiwave. (b) results from the reference [2].

Notice that Fig.(4) gives the results in inverse of wavelength units, to express it in natural wavelength units we have used $\lambda = 2\pi c/\omega$. In this case two band gaps are given, we are going to numerate them in crescendo in energy because it is going to be useful in the future in order to classify PBG.

As we mentioned above:

PBG order	$\frac{\omega_i}{2\pi c}$	$\frac{\omega_f}{2\pi c}$	$\lambda_f(\mu m)$	$\lambda_i(\mu m)$
#0	0.298710	0.442265	3.347729	2.261088
#1	0.733158	0.762272	1.363962	1.311867

TABLE II: The table shows both range of inverse of wavelength and range of wavelength which do not propagate along the photonic crystal for TE polarization. I would like to remark the errors $\delta\left(\frac{\omega}{2\pi c}\right) \sim 10^{-6}\mu m^{-1}$ and applying (A.14) $\delta(\lambda) \sim 2 \cdot 10^{-6}\mu m$.

We remark that the error is so small that we are not going to taking it to account.

In order to contrast these results, we can study the wave transmission along the photonic crystal using FDTD method.

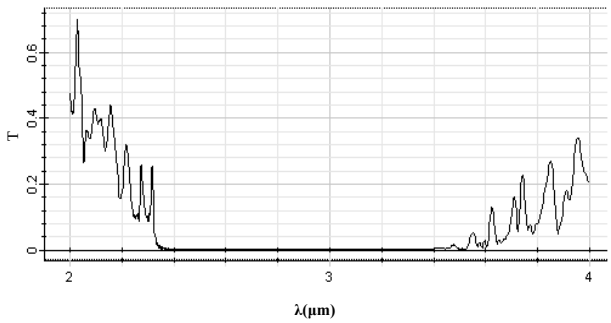

FIG. 5: Transmission spectrum of a Gaussian wave along the photonic crystal. The wavelength range is from $2\mu m$ to $4\mu m$ in order to find the #0 PBG. With both time and space steps we have already explained in II. Optiwave the time simulation is around $\sim 30s$

Notice that Fig.5. proves that exist a PBG between $\sim 2.3\mu m$ and $\sim 3.4\mu m$, approximately. With FDTD method we contrast the PWE results. But from now on all the study is going to be with PWE method due to its higher resolution. Mention that we only have represented the main PBG (#0 order PBG).

Otherwise, for a TM wave no PBG appear:

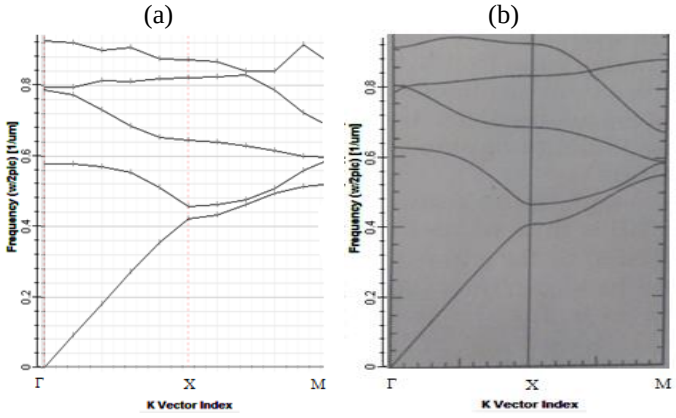

FIG. 6: Band structure along the ΓX and XM directions for a square lattice of silicon cylinders in air and the ratio $r/a = 0.18$. See how no PBG appear for TM polarization. (a) Our results running *Optiwave*. (b) [2] results.

Finally, we obtain the results that we have expected at the beginning of this part. From here, all the study is going to be only with TE waves because of no PBG appear for TM waves. According to quantum mechanics, bang gaps appear because the first band has most of its energy in the dielectric region and the second in the air region, and this energy difference leads to a band gap. So, as bigger is the difference between the permittivity of the cylinders and the substrate, this energy difference will be more remarkable. In TE waves this energy difference is around $\sim 50\%$, while in TM waves $\sim 10\%$, that is why we do not detect PBG for TM waves [3].

IV. SQUARE STRUCTURE

Now we are going to study a Bravais square lattice with a monoatomic base but without fixing the refractive index neither the ratio pitch-to-radius. Furthermore the substrate is going to be water, $n = 1.33$. Thanks to realised that no band gaps appear with TM polarized light all the simulations are going to be with TE waves.

First of all the pitch is set to $1\mu m$. In this particular case the range of ratio r/a is from 0.40 to 0.10 in steps of 0.10. We have no considered work with $r/a = 0.50$ because even though the results may be good, at practice would be a bad way to work.

According to how we numerate the PBG in last part, the first PBG is called #0, and the second #1, and in Fig.(6) they are represented, in units of wavelength, versus the refractive index for various ratio r/a:

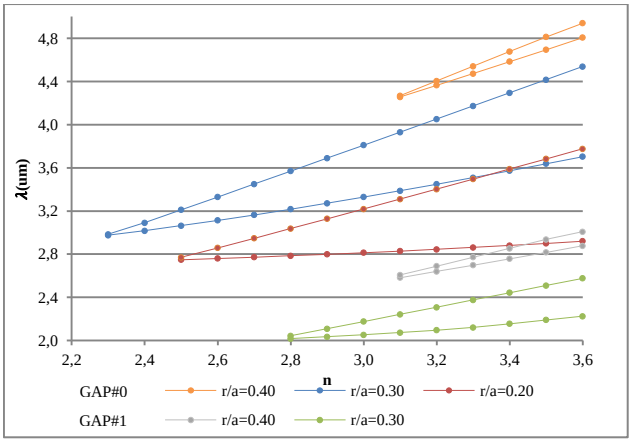

FIG. 7: Position of the #0 and #1 order PBG for TE polarized light. Calculus has been performed for a square lattice of cylinders in water for a pitch of $1\mu m$. The positions of the gaps were extracted from band structure calculations at various values of n. No error bars have been processed due to the fact that they are insignificant.

Notice that in #1 order we only obtain results for both $r/a = 0.40$ and $r/a = 0.30$. And no PBG appear for $r/a = 0.10$.

No more order PBG appear for these conditions. Remark that all these PBG are out of the range that we presented in TableI. They are in the range of mid-infrared, typical of heat sources. Although exist lasers in this range, they are too much expensive and our interest is the visible spectrum and near infrared.

V. HEXAGONAL STRUCTURE

The other interesting structure in 2-D photonic crystal is hexagonal lattice, again we only study TE waves although

PBG can appear for TM waves, but not important as in TE polarization.

Before showing the results it would be good to explain that more PBG appear in the hexagonal structure how we are going to proof. That is why we study two different pitches, the first, as before, is $1\mu m$ and the second is $0.5\mu m$, since we are going to need to reduce the wavelength.

In this case the Fig.(8) presents the hexagonal structure. On the left, the direct space and its primitive vectors, and on the right the first Brillouin Zone, with its symmetrical points Γ, X and M.

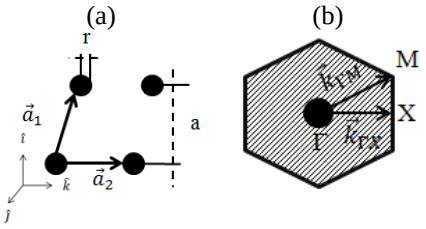

FIG. 8: (a) Layout of direct space. (b) First Brillouin Zone. Both for a monoatomic hexagonal structure.

For an hexagonal structure the primitive vectors are:

$$\begin{aligned}\vec{a}_1 &= a\hat{\imath}\\ \vec{a}_2 &= \frac{a}{2}(\hat{\imath}+\sqrt{3}\hat{k})\\ \vec{a}_3 &= c\hat{\jmath},\end{aligned} \tag{8}$$

again, the third vector only has mathematically meaning.

The vectors in the reciprocal space, using (A.13):

$$\begin{aligned}\vec{b}_1 &= \frac{b}{2}(\sqrt{3}\hat{\imath}-\hat{k})\\ \vec{b}_2 &= b\hat{k}\\ \vec{b}_3 &= d\hat{\jmath},\\ b &\equiv \frac{2\pi}{a}.\end{aligned} \tag{9}$$

How we said, the parameter d has not meaning. Like before, the Γ point is the center of the first Brillouin Zone. And now the X and M points are defined by the vectors:

$$\vec{K}_{\Gamma X} = \frac{b}{2}\hat{\imath}, \tag{10}$$

$$\vec{K}_{\Gamma M} = \frac{b}{3}\left(\frac{3}{2}\hat{\imath}+\sqrt{3}\hat{k}\right) \tag{11}$$

A. Pitch 1µm

The first study case has been to set the pitch to $1\mu m$. In Fig.(8) is represented the #0 and #1 order PBG, in units of wavelength, versus the refractive index for various ratio r/a.

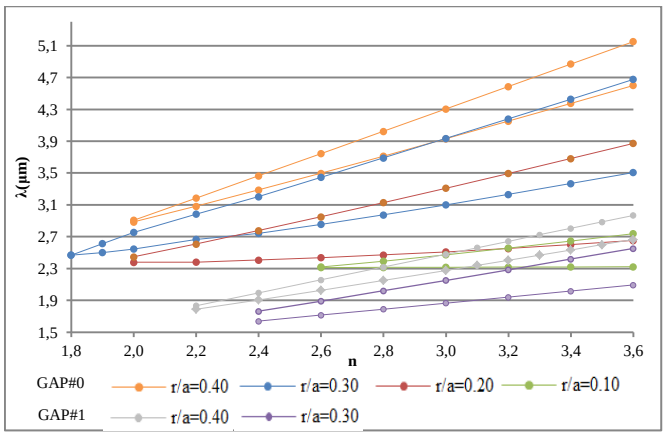

FIG. 8: Position of the #0 and #1 order PBG for TE polarized light. Calculus have been performed for an hexagonal lattice of cylinders in water for a pitch of 1µm.

PBG are located in a high range of wavelength, even going to higher PBG order. We need to reduce the pitch.

B. Pitch 0.5µm

In order to reduce the wavelength of PBG and study a realistic pitch, we thought that a good pitch may be $0.5\mu m$. Also, since we have seen that the biggest PBG appear around $r/a = 0.30$ and $r/a = 0.20$, we are going to study also $r/a = 0.35$ and $r/a = 0.25$. As we have explained and [4] exposes, as biggest is the permittivity difference between cylinders and substrate, the energy difference will be more important and so as PBG. And thanks to the crystal's periodicity we can write the average of the permittivity as:

$$\bar{\varepsilon} = (1-\beta)\varepsilon_s + \beta\varepsilon_d, \tag{12}$$

where, ε_s and ε_d are the permittivity of substrate and cylinders, respectivility. And β the volume fraction of cylinders in the primitivy cell. Maximising (12), [4] shows that $\beta \sim 0.20$.

Fig.(9) shows the first results setting the pitch to $0.5\mu m$. Results are been better due to wavelength reduce the.

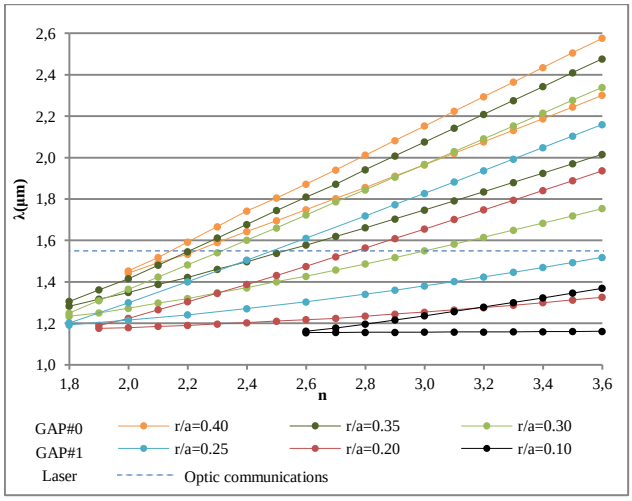

FIG. 9: Position of the #0 order PBG for TE polarized light. Calculus have been performed for an hexagonal lattice of cylinders in water for a pitch of 0.5µm.

No interesting PBG appear in #1 order. Apart from #2 and #3 order PBG, in more higher orders the size of PBG are so small that it would not be pretty efficient to work with them.

In Fig.(10) we can see how #2 and #3 order PBG are in the range of near-infrared and visible spectrum:

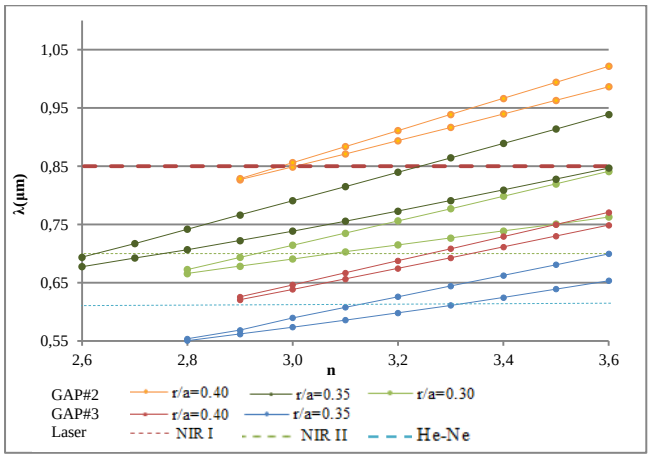

FIG. 10: Position of the #2 and #3 order PBG for TE polarized light. Calculus have been performed for an hexagonal lattice of cylinders in water for a pitch of 0.5 μm.

A summary of what we have obtained:

	Wavelength of lasers			
r/a	$1.55\mu m$	$0.85\mu m$	$0.70\mu m$	$0.63\mu m$
0.40	X	X	X	-
0.35	X	X	X	X
0.30	X	-	X	-
0.25	X	-	-	-
0.20	X	-	-	-

TABLE III: The table shows which structures can work with the wavelength we presented in TableI.

VI. CONCLUSIONS

As far as laser conclusions, concerning for an hexagonal structure with a pitch of $0.5\mu m$, we can say:

- The best results appear for the optic communications laser at $1.55\mu m$. Not only because it fits with five structures, if not the PBG appear for a remarkable range of n.
- The second interesting wavelength would be $0.70\mu m$. Here, three different configurations of r/a can work. Even though, PBG and the range of the index of refraction are not as big as last point.
- For $0.85\mu m$ only two kind of configuration are useful. And finally, for $0.63\mu m$ only can work with one structure, but remark it is in visible spectrum.

Finally, we can conclude that the best structure is an hexagonal lattice with a monoatomic base, with a pitch of $0.5\mu m$ and a ratio equal to $r/a = 0.35$.

I would like to mention that the common material in crystals is Silicon, $n = 3.45$. Silicon has the property that absorb both visible wavelength and near-infrared till $1\mu m$. Hence, for this material the best laser would be optic communications laser. Another choice is to look for a material which does not absorb near-infrared or visible wavelength.

VII. APPLICATION

This final project could be used to study the interaction forces of some damage biological tissues. In order to do that, the tissue is placed onto the top of the photonic crystal and the tissue forces will change the internal structure of the photonic crystal. Thus, the best way to realise how change a photonic crystal is observing its PBG. Although here we have made the study where the substrate is water, it may change depending on tissue and so PBG structures will change. Furthermore, for this application the chosen material would need to be flexible enough in order to be able to change its own internal structure.

VIII. APPENDIX

I would like to mention the equation to pass from the direct space to the reciprocal space:

$$\vec{b}_i = 2\pi \frac{\vec{a}_j \times \vec{a}_k}{\vec{a}_i \cdot (\vec{a}_j \times \vec{a}_k)} \cdot \qquad \text{(A.13)}$$

Finally, for errors calculations:

$$\delta y = \sqrt{\sum_i \left(\frac{\partial y}{\partial x_i}\delta x_i\right)^2} \cdot \qquad \text{(A.14)}$$

Acknowledgments

First of all, I would like to thank you Albert Romano and Mauricio Moreno, both from Electronics department of UB for their patience and also for the knowledge that they have given to me.

Finally, I would also thank to my family and my closest friends who have always supported me.

[1] Optiwave. [Online]. http:// http://optiwave.com/

[2] M.J.A. De Dood, E. Snoeks, A. Moroz and A.Polman Fom. (2002). Optical and Quatum Electronics, **34** 145-159.

[3] Joannopoulos, J.D., R.D. Meade and J.N. Winn. (1995). Photonic Crystals: Molding the Flow of Light, Princeton University Press, Princeton, NJ.

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