# Experimental and numerical study of the angular dependence of the reflective optical properties of two-dimensional photonic structures with square and hexagonal periodicity

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**ABSTRACT**

In this work we present an experimental and numerical study of the angular dependence of the reflective optical properties of two-dimensional photonic structures with square and hexagonal periodicity, built on a silicon substrate. The work is motivated largely by the need for a new alternative development in telecommunications technology that is purely photonic. The structures that have circular and square inclusions were manufactured with the technique of Focused Ion Beam (FIB). This manufacturing technique was easy to use and has advantages over other techniques; because the structure can be machined in several sessions and we may induce structural defects in the photonic structure. The numerical analysis of the reflective optical properties was through the technique known as Integral Equation Method, that has a great advantage compared to other methods; which only take into account a finite number of sampling points along the contours of the unit cell and inclusion, allowing fewer computational resources. The integral method allows studying both infinite and finite systems. For infinite systems the band structure is obtained and in the case of finite systems, the propagation of electromagnetic waves through the system. When performing the numerical simulations, prohibited bands were obtained by increasing the filling fraction of the square or hexagonal unit cell. Finally, we show the numerical analysis about the wave propagation through photonic structures with similar features to those machined. One of the results was that when considering inclusions in a dielectric plate, considerably improving optical reflectance.

**Keywords:** Photonic structures, Focused Ion Beam, Integral Equation Method.

## Introduction

Photonic crystals (PhC) were proposed simultaneously and independently by Eli Yablonovitch (Yablonovitch, 1987) to control the spontaneous emission and Sajeev John (John, 1987) for the location of the light. Although, periodic structures in the form of stacked plates had been studied before by Lord Rayleigh (Rayleigh, 1888).

PhC is a material that presents a periodic modulation of the refractive index induced by the inclusion of structural defects. The purpose of this type of material is to control the reflection and/or the transmission of light through its structure by the phenomenon of diffraction. These crystals are present in a natural way and are responsible of iridescent color on the opal stone, the coloration of peacock feathers and butterfly wings. Also, they can be manufactured by the man, using modern techniques that allow micro-machined the matter in the regime sub-micrometer and nanometer. The design of such composite structures can be carried out an one, two, or three dimensions. In the 2D PhCs the periodicity is presented in two directions, while the other is invariant. The optical reflective properties of the 2D PhC depend on the type of recurrence, the geometry of the inclusions, the contrast of the refractive index and the filling fraction of photonic structure.

Focussed Ion Beam (FIB) is equipment with some similarity to a SEM. However, while the SEM uses focused electron beams for a picture of the sample, the FIB system uses a gallium focused ion beam, as in the case JEOL JEM9320-FIB equipment of CIMAV. Technical FIB is used particularly in the industry of semiconductor, science of materials, biology, etc., for: modification and repair of devices, obtaining of images, micro and nano machining, micro and nano deposition, among others (Carrillo-Vazquez, 2014).

In this work we used a numerical technique known by Integral Equation Method (Mendoza-Suárez et al., 2006) to calculate the optical reflectance of two-dimensional photonic structures of hexagonal net; one with circular inclusions and the other with square inclusions. Integral Equation Method part of Green theorem applied to Helmholtz equation, for allowing integral equations coupled involving as unknowns to the field and its derivative normal evaluated in the contours that separate regions of the system. To have a finite sampling points, the contours are divided into small regions, $\Delta s$, in this way the coupled equations are approximated by amounts that result in a homogeneous matrix system analysis (infinity) or in a matrix system inhomogeneous (analysis finite) whose solution determines the source function, with which you can get the band gap or optical response of the system, respectively.

## Photonic crystals machining

A silicon monocrystalline substrate of approximately 1 cm² that contains a coating of oxide of zinc (ZnO) of 300 nm, was used for machining them CFs. Each crystal structure consists of 70 holes. In the case of circular holes, the lattice parameter is 1 µm, while for the square holes is 1.5 µm.

To achieve the structure of the Fig. 1(a) was necessary to use ion current of 1000 pA, a dose of 200 µC / µm² to 30 kV in the ion column and a beam exposition time of 15 seconds by hole. For machine structure Fig. 1(b) was necessary to use ion current of 50 pA, a dose of 2.5 µC / µm² to 30 kV in the ion column and beam exposition time of 50 seconds per box.

The Fig. 1(a) shows the surface morphology of PhC with hexagonal lattice and circular inclusion. As you can see the lattice parameter it is approximately 1 µm and the machining hole diameter is ~600 nm. In the same way, the Fig. 1(b) shows the surface morphology of a PhC with hexagonal lattice and square inclusion. In this case the lattice parameter is of approximately 1.4 µm and the length of the box machined is of ~1 µm. This information allows the filling of the unit cell fraction.

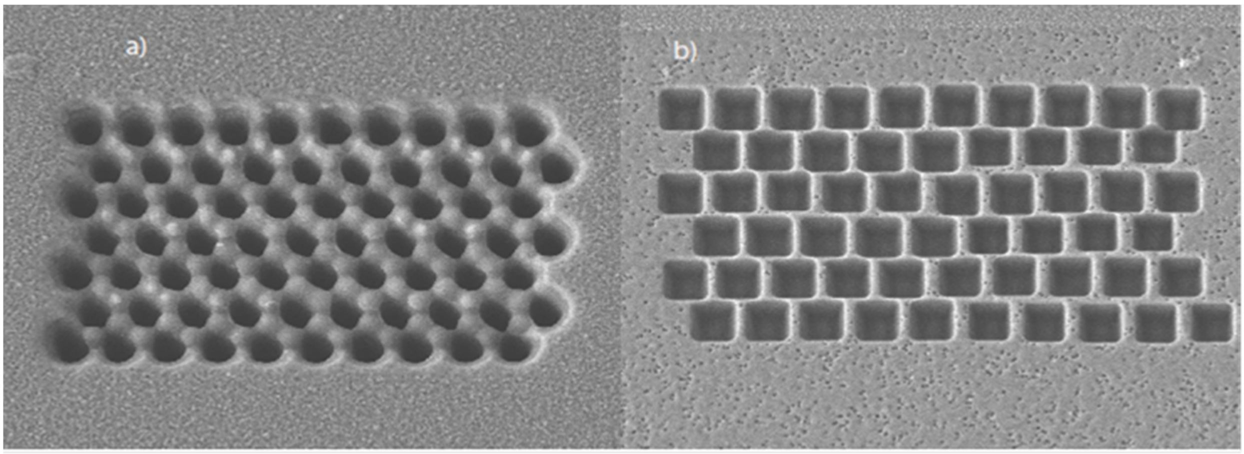


Figure 1. PhC with hexagonal lattice, (a) circular inclusions and (b) square inclusions, machining by FIB technique.

**Integral Equation Method**

Integral method is suitable for calculating the distribution of the electromagnetic field in the region near and distant for 2D PhC of finite lengths.

The general integral equation applicable to the contours involved in 2D PhC is

$$\Psi_{inc}(\boldsymbol{r}) + \frac{1}{4\pi}\int_{\Gamma_j}[G_j(\boldsymbol{r},\boldsymbol{r}')\,\frac{\partial\Psi_j(\boldsymbol{r})}{\partial n'_j} - \Psi_j(\boldsymbol{r})\frac{\partial G_j(\boldsymbol{r},\boldsymbol{r}')}{\partial n'_j})ds'] = \Psi(\boldsymbol{r})\Theta(\boldsymbol{r}) \;, \quad (1)$$

where $\Psi_{inc}(\boldsymbol{r})$ represents the incident field, $G_j(\boldsymbol{r},\boldsymbol{r}')$ is the role of green in the region $R_j$ and $\Theta(\boldsymbol{r})$ is the Heaviside function. Here $\Theta(\boldsymbol{r}) = 1$ if $\boldsymbol{r}$ is within the surface $S'$ and $\Theta(\boldsymbol{r}) = 0$ in the opposite case.

Taking into account the following:

- The contours $C_{1\infty}$, $C_{2\infty}$ and $C_{q\infty}$ are sufficiently away whose disturbance of the fields is null.
- The middle of incidence (region $R_1$) have optical properties given by the electrical permittivity $\varepsilon_1$ and magnetic permeability $\mu_1$.
- The media that contains the inclusions has properties $\varepsilon_2$ and $\mu_2$.
- inclusions have the properties $\varepsilon_3$ and $\mu_3$ if each one of them are of the same material and $\varepsilon_3$, $\mu_3$,..., $\varepsilon_{q-1}$, $\mu_{q-1}$ if they are made of different material.
- The properties of the medium of transmission are given by $\varepsilon_q$ and $\mu_q$, that for our case correspond to $\varepsilon_1$ and $\mu_1$.

Considering the conditions of continuity of the field and its derivative normal along the different contours Γq, the system of equations for 2D PhC finite can be expressed as

$$\sum_{n=1}^{N_a}\left(\delta_{mn(1)} - N_{mn(1)}^{(1)}\right)\Psi_{n(1)} + \frac{f_1}{f_2}\sum_{n=1}^{N_a} L_{mn(1)}^{(1)}\Phi_{n(1)} = \Psi_m^{inc}, \quad (2)$$

$$- \sum_{n=1}^{N_a} N_{mn(1)}^{(2)} \Psi_{n(1)}^{(2)} + \sum_{n=1}^{N_a} L_{mn(1)}^{(2)} \Phi_{n(1)} - \sum_{n=1}^{N_b} N_{mn(2)}^{(2)} \Psi_{n(2)} + \sum_{n=1}^{N_b} L_{mn(2)}^{(2)} \Phi_{n(2)} + \cdots - \sum_{n=1}^{N_q} N_{mn(q)}^{(2)} \Psi_{n(q)} + \sum_{n=1}^{N_q} L_{mn(q)}^{(2)} \Phi_{n(q)} = 0, \quad (3)$$

$$\sum_{n=1}^{N_b} \left(\delta_{mn(2)} - N_{mn(2)}^{(3)}\right) \Psi_{n(2)} + \frac{f_3}{f_2} \sum_{n=1}^{N_b} L_{mn(2)}^{(3)} \Phi_{n(2)} = 0, \quad (4)$$

$$\sum_{n=1}^{N_c} \left(\delta_{mn(3)} - N_{mn(3)}^{(3)}\right) \Psi_{n(3)} + \frac{f_3}{f_2} \sum_{n=1}^{N_b} L_{mn(3)}^{(3)} \Phi_{n(3)} = 0, \quad (5)$$

$$\sum_{n=1}^{N_{q-1}} \left(\delta_{mn(q-1)} - N_{mn(q-1)}^{(3)}\right) \Psi_{n(q-1)} + \frac{f_3}{f_2} \sum_{n=1}^{N_{q-1}} L_{mn(q-1)}^{(3)} \Phi_{n(q-1)} = 0 \quad (6)$$

and

$$\sum_{n=1}^{N_q} \left(\delta_{mn(q)} - N_{mn(q)}^{(4)}\right) \Psi_{n(q)} + \frac{f_4}{f_2} \sum_{n=1}^{N_q} L_{mn(q)}^{(4)} \Phi_{n(q)} = 0. \quad (7)$$

Eqs. (2)-(7) constitute a system not uniform of $2\sum_{p=1}^{q} N_p$ linear equations, which can be solved numerically to determine the functions source (the field and its derivative normal) along contours $\Gamma_j$. With these functions it is possible to obtain the spread field.

To treat problems of 2D PhC is taken into account that there are two types of polarization states complementary. For TE polarization, we will assume that the incident field is given by $\boldsymbol{E}(\boldsymbol{r}) = \hat{k} E_z(x,y)$ and $\boldsymbol{H}(\boldsymbol{r}) = \hat{\imath}\, H_x(x,y) + \hat{\jmath}\, H_y(x,y)$.

If you used the Poynting vector ($\boldsymbol{S} = \boldsymbol{E} \times \boldsymbol{H}^*$) that provides direction and magnitude of the flow of energy per unit of time and integrating on an area, the power incident is written as follows

$$P_{inc} = \frac{1}{2} \frac{\cos\theta_i}{c\,\mu} L_x L_z . \quad (8)$$

In the asymptotic limit (far-field) has to be the power spread is given by

$$P_s = \frac{1}{8\pi k} \frac{L_z}{\mu_0 c} \int_{-\pi/2}^{\pi/2} |\sigma_s(\theta_s)|^2 d\theta_s, \quad (9)$$

here $\sigma_s(\theta_s)$ represents the effective section of a material. For a real material is

$$\sigma_s(\theta_s) = \sum_n \Delta s \Phi_n\, e^{-ik\left(\sin\theta_s x_n + \cos\theta_s y_n\right)} - \sum_n ik\, \Delta s\, \Psi_n \left(\sin\theta_s y_n' - \cos\theta_s x_n'\right) e^{-ik\left(\sin\theta_s x_n + \cos\theta_s y_n\right)}. \quad (10)$$

In the case of TM polarization, the Eqs. (8) and (9) are similar.

## Results

The modeling of the 2D PhC with 70 circular inclusions, as well as the reflectance and transmittance for the TE and TM polarizations are presented in Fig. 3. In the case of

TE polarization, it is estimated that for the 2D PhC with filling fraction of 32.65%, reflectance increases considerably in the regions of angular incidence where there is minimum reflectance for curves of control (plate without inclusions); however in some regions decreases the reflectance. When working with TM polarization we found that there is a filling fraction, specifically 40%, which in the majority of the angles of incidence reflectance improvement. In regard to the transmittance, this decreases for all the filling fractions analyzed.

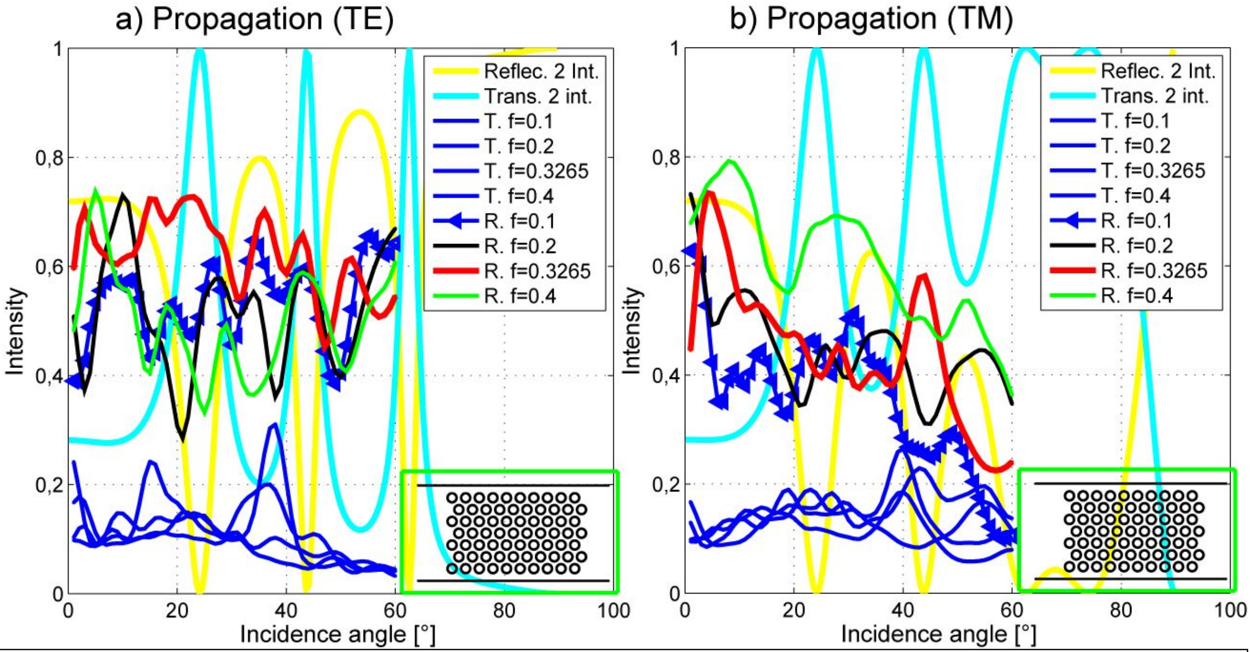


*Figure 3.. Reflectance and Transmittance as a function of incidence angle of a plate with 70 circular inclusions and different filling fraction, to (a)TE polarization and b) TM polarization. Lines of Reflec and Trans correspond to the analytical case and the others in the numeric.*

The other type of inclusions for 2D PhC hexagonal lattice are the square bars of any material, in this case air. The characteristics of the 2D PhC are: lattice parameter of 1.5 μm and filling fraction is 51.32%. In Fig. 4 shows the reflectance and transmittance for different filling fractions to the TE and TM polarizations, using the method of the integral equation. When we working with angles less than 30° has to the PhC is highly reflective for their different filling fractions. It was found a filling fraction (40%) that improves the optical properties reflectivas in most of the angles of incidence. There are two filling fractions (f=40% and f=51%) for which the 2D PhC acquires the property of being highly reflective regardless of the angle of incidence when illuminated with red light (632 nm) and TM polarization.

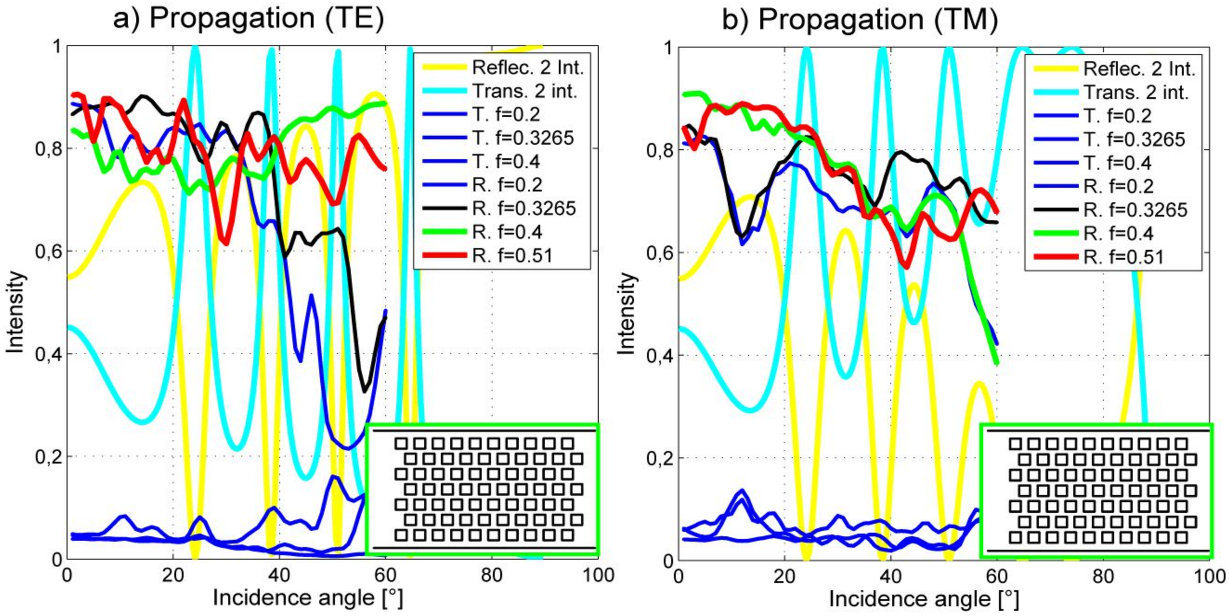


*Figure 4. Reflectance and transmittance as a function of incidence angle of a plate with 70 square inclusions and different filling fraction, to (a) TE polarization and b) TM polarization.*

## Conclusions

When using integral method it was possible to study the propagation of electromagnetic waves through periodic systems truncated. This provided the opportunity to analyze the reflectance and transmittance of two periodic systems of hexagonal lattice, one with 70 circular inclusions and another with 70 square inclusions.

With the results obtained numerically, a comparison was made with the system of a plate without inclusions and the conclusions obtained are:

- To consider the system of a plate with inclusions, optical properties reflectivas have changed considerably since the minimum reflectance that are own of the plate without inclusions do not appear anymore.
- There is a filling fraction the minimum unitary cell where the photonics structure can be considered highly reflective. In the case of square inclusions, the reflective and transmissive properties practically do not change regardless of the polarization of the beam with illuminates the photonic structure.

## References

Carrillo-Vázquez, V. M. (2014). Diseño y caracterización óptica de un material fotónico fabricado mediante haz enfocado de iones.. Tesis de Doctorado, Centro de Investigación en Materiales Avanzados.

John, S. (1987). Strong localization of photons in certain disordered dielectric super-lattices. Phys. Rev. Lett., 58: 2486.2489.

Mendoza-Suárez, A., Villa-Villa, F., y Gaspar-Armenta, J. A. (2006). Numerical method based on the solution of integral equations for the calculation of the band structure and re.ectance of one-and two-dimensional photonic crystals. JOSA B, 23(10): 2249.2256.

Rayleigh, J. W. S. (1888). On the remarkable phenomenon of cristaline re.exion descry-

bed by Prof. Stokes. Phil. Magazine, 26: 256.265.
Yablonovitch, E. (1987). Inhibited spontaneous emission in solid-state physics and electronics. Phys. Rev. Lett., 58: 2059.2062.