Modeling of the optical response of two-dimensional hexagonal periodicity photonic structures with cylindrical inclusions with randomly rough surfaces that include dispersive LHM

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Abstract. The interest to develop nanoscale devices is due to their ability to manipulate the optical properties through their structure. With an increasing interest in the recent decades, different types of Photonic Crystals (PC) have also been proposed. A PC is a periodically ordered material in which the refractive index is modulated. It has been shown in recent years that adding new materials to the structure of photonic crystals results in novel properties of these systems, which were originally conceived as composed of purely dielectric materials. One option is to consider this type of systems with dispersive Left-Handed Materials or metamaterials. The optical properties of the PCs depend on the type of periodicity, the geometry of the inclusions, the contrast of the refractive index and the filling fraction of the photonic structure. In this work, a numerical technique known as the Integral Equation Method was used to model the optical response of a two-dimensional photonic structure with a hexagonal lattice of cylindrical inclusions containing smooth and random rough surfaces that include dispersive LHM. It was obtained that the roughness of the inclusions modulates the optical response, in some cases varying the intensity and in others the direction of propagation. This property is very useful and has multiple applications in waveguides, filters, omnidirectional mirrors, beam splitters, etc.

1. Introduction
In 1987, the concept of PC was first used by Eli Yablonovitch [1] and John Sajeev [2] to control the spontaneous emission and location of light, respectively. However, periodic structures in the form of stacked plates had previously been studied by Lord Rayleigh [3] in 1888. A PC is a material that exhibits periodic modulation of the refractive index. For their study, PCs can be classified into one-dimensional (1DPC), two- (2DPC), or three-dimensional (3DPC). In 2DPCs periodicity occurs in two directions, while in the other it is invariant. The purpose of this type of material is to control the reflection and/or transmission of light through its structure by the diffraction phenomenon. These crystals are present naturally and are responsible for the iridescent color in the opal stone and, the coloration of peacock’s feather and butterfly wings. But, they can also be manufactured by man, using modern techniques that allow the material to be machined in the sub-micrometric and nano-metric regime. However, the
fabricated materials are not perfect [4], i.e., they have certain irregularities that can modify the optical properties of the photonic structures. For this reason, the present work is focused on 2DPCs with rough surface in the cylindrical inclusion.

PCs were originally conceived as composed of purely dielectric materials [5, 6], however it has been proved in the past several years that adding news materials to the structure of photonic crystals results in novel properties of these systems. A type of structured material that has recently attracted much interest, from the experimental work of Prendy and colleagues [7, 8], is the Left Handed Material (LHM). Its name is due to the fact that the vectors of the electromagnetic field and the wave (\(E\), \(H\) and \(k\)) form a triad of the left hand for a wave propagating through this medium. This phenomenon was predicted years ago by V. Veselago [9]. The first LHMs were designed as periodic arrays of metallic capacitors and wires with a unitary cell of dimensions much smaller than the wavelength.

When proposing a PC it is necessary to study the optical response of the system. This has been done by numerical simulation calculations using Integral Equation Method (IEM) [10]. The IEM is based on the Second Integral Green’s Theorem applied to the Helmholtz’s equation, in which integral equations are obtained that set as unknowns the field and its normal derivative evaluated in the contours that separate the regions of the system. In order to have a finite sampling of points, the boundaries are divided into small regions, \(\Delta s\), so the coupled equations are approximated by sums that result in an inhomogeneous matrix system, whose solution determines the source functions. With these source functions, the optical response is obtained. In this work, the IEM is used to calculate the optical response of 2DPCs of the hexagonal periodicity with cylindrical inclusions with smooth and randomly rough surfaces, under TE polarization. The results show that the roughness of the surfaces modulates the optical response.

The structure of the paper is as follows: in the next section we give a brief explanation of the IEM applied to a finite 2DPC and validate the method by comparing the optical response obtained from a dielectric plate using the Fresnel’s equations. Section 3 summarizes the results for a finite 2DPC of hexagonal lattice with cylindrical inclusions with smooth and randomly rough surfaces. Finally, in section 4, we state the conclusions of this work.

2. Integral Equation Method applied to 2DPC

In previous works, the IEM has been developed to calculate band structures associated to infinite 2DPC [11, 12]. However, in practice a 2DPC has a finite length. The IEM is suitable to calculate the distribution of the electromagnetic field in the near and far region for a 2DPC of finite length. Figure 1 shows the schematic of a finite 2DPC of hexagonal lattice with cylindrical inclusions with rough surfaces.

![Figure 1](image.png)

**Figure 1.** Scheme of a finite 2DPC. (a) To apply the IEM, the integration contours are indicated by the discontinuous curves. (b) Close view of the system used. The system used consists of \(3 \times 120\) cylinders of dispersive LHM embedded in air.
The general integral equation applicable to the contours involved in this type of systems is expressed by

\[
\Psi_{inc}(r) + \frac{1}{4\pi} \int \left[ G_j(r, r') \Phi_{n_j}(r) - \Psi_j(r) \frac{\partial G_j(r, r')}{\partial n_j} \right] ds' = \Psi(r) \Theta(r),
\]

where \( \Psi_{inc}(r) \) represents the incident field, \( G_j(r, r') \) is the Green’s function in the \( j \)-th region \( R_j \) and \( \Theta(r) = 1 \) if \( r \) is inside the surface \( S' \) and \( \Theta(r) = 0 \) otherwise.

Considering the conditions of continuity of the field and its derivative normal along the different contours \( \Gamma_q \), the system of equations for 2DPhC of finite length can be expressed as

\[
\sum_{n=1}^{N_a} (\delta_{rn(1)} - N_{rn(1)}) \Psi_{n(1)} + f_1 \frac{1}{f_2} \sum_{n=1}^{N_a} f_{rn(1)} \Phi_{n(1)} = \Psi_{inc}^{m},
\]

\[
- \sum_{n=1}^{N_a} N_{rn(1)}^{(2)} \Psi_{n(1)} + \sum_{n=1}^{N_b} f_{rn(1)}^{(2)} \Phi_{n(1)} - \sum_{n=1}^{N_a} N_{rn(1)}^{(1)} \Psi_{n(1)} + \sum_{n=1}^{N_b} f_{rn(1)}^{(1)} \Phi_{n(1)} + \cdots - \sum_{n=1}^{N_q} N_{rn(1)}^{(2)} \Psi_{n(1)} + \sum_{n=1}^{N_q} f_{rn(1)}^{(2)} \Phi_{n(1)} = 0,
\]

\[
\sum_{n=1}^{N_b} (\delta_{rn(2)} - N_{rn(2)}) \Psi_{n(2)} + f_1 \frac{1}{f_2} \sum_{n=1}^{N_b} f_{rn(2)}^{(2)} \Phi_{n(2)} = 0,
\]

\[
\sum_{n=1}^{N_c} (\delta_{rn(3)} - N_{rn(3)}) \Psi_{n(3)} + f_1 \frac{1}{f_2} \sum_{n=1}^{N_c} f_{rn(3)}^{(3)} \Phi_{n(3)} = 0,
\]

\[
\cdots,
\]

\[
\sum_{n=1}^{N_q-1} (\delta_{rn(q-1)} - N_{rn(q-1)}) \Psi_{n(q-1)} + f_1 \frac{1}{f_2} \sum_{n=1}^{N_q-1} f_{rn(q-1)}^{(q-1)} \Phi_{n(q-1)} = 0,
\]

and

\[
\sum_{n=1}^{N_q} (\delta_{rn(q)} - N_{rn(q)}) \Psi_{n(q)} + f_1 \frac{1}{f_2} \sum_{n=1}^{N_q} f_{rn(q)}^{(q)} \Phi_{n(q)} = 0.
\]

Thus, Eqs. (2) - (7) constitute an inhomogeneous system of \( 2 \sum_{p=1}^{q} N_p \) linear equations, which can be solved numerically to determine the source functions (the field and its normal derivative) along \( \Gamma_q \) contours. With these functions it is possible to obtain the scattered field.

The far-field amplitude is given by

\[
A(\theta, \omega) = \int_{\Gamma_q} \left[ -i \frac{\omega}{c} \left( \hat{n}_q \cdot \hat{r} \right) \Psi_q(\mathbf{r'}) - \frac{\partial \Psi_q(\mathbf{r'})}{\partial \hat{n}_q} \right] \times \exp \left( -i \frac{\omega}{c} \mathbf{r'} \cdot \hat{r} \right) ds',
\]

with \( \hat{r} = (-\cos \theta, \sin \theta) \). Then the differential reflectance coefficient can be obtained by

\[
\frac{\partial R}{\partial \theta} = h |A(\theta, \omega)|^2,
\]

where \( h \) is a normalization factor that depends on the incident wave. In the case of an incident Gaussian wave, this factor is

\[
h = \left( 2(2\pi)^{3/2} g k \cos \theta_0 \right)^{3/2},
\]

being \( g \) the 1/e half-width of the modulus projected on the plane \( x = 0 \), and \( k \) represent the wave number. The reflectance as a function of the frequency is obtained by one’s integrating over all the scattering angles in the incident region. That is,
In a similar way, it is possible to apply an analogous procedure to determine the far-field amplitude in the transmission zone to calculate the transmittance.

To validate the application of the IEM to finite systems, the reflective optical properties were obtained as a function of the incidence angle of a dielectric plate without inclusions and compared with those obtained by the Fresnel equations for multiple reflections, as show in figure 2. The curves obtained with the IEM overlap the curves obtained with Fresnel equations; with this the validity of the integral equation method is verified.

Figure 2. Reflectance (R) and transmittance (T) as a function of the incidence angle of a glass plate (n = 1.52) embedded in air, under TE polarization. The dimensions of the plate are 3×100 µm and it was illuminated with a Gaussian beam with a wavelength of 850 nm and a half-beam of 12 µm. The solid curves correspond to optical response using IEM and the dashed lines represent the optical properties obtained with the Fresnel equations.

3. Optical response of a finite 2DPC
The results of the optical response obtained by modeling 2DPhCs composed of array of dielectric cylindrical inclusions with smooth and rough surfaces have already been studied [13]. As an extension of the work, we present the modeling of the optical response of two-dimensional photonic structures that include dispersive LHM. Optical properties of dispersive LHM are given by the dielectric function \[ \varepsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2}, \] and the magnetic permeability \[ \mu(\omega) = 1 - \frac{F\omega_0^2}{\omega^2 - \omega_0^2}, \] where the plasma frequency is \( \omega_p = 10c/D \), the resonance frequency is \( \omega_0 = 4c/D \) and the LHM filling fraction is \( F = 0.56 \). The speed of light in vacuum is \( c \), and lattice parameter is \( D \) [14]. The region where the LHM presents a negative refraction index is in the frequency range comprised of \( \omega_p < \omega < \omega_{\text{LH}} \), here \( \omega_{\text{LH}} = \omega_0 / \sqrt{(1 - F)} \). In our analysis, was considered \( D = 1 \mu m \). With this, the plasma and resonance frequencies (in reduced units) are: \( \omega_p = 1.592 \) and \( \omega_0 = 0.637 \), respectively.

The optical response obtained by the modeling of 2DPhC with 360 dispersive LHM cylindrical inclusions with smooth and rough surfaces embedded in air with the Integral Method is presented in figure 3. In this case, the roughness was modeled with a Gaussian profile in which the parameters are the correlation length \( l_c = 0.05\lambda \) and the standard deviation of heights \( \sigma = 0.01\lambda \) for a filling fraction \( f = 0.10 \). The parameters for \( f = 0.20 \) were \( l_c = 0.08\lambda \) and \( \sigma = 0.02\lambda \).

In some cases, the optical response is not modulated due to the roughness of the surface of the inclusions, as shown in figure 3(a). However, by increasing the filling fraction and the roughness parameters, a modulation of the optical response is obtained due to the roughness. This is shown in figures 3(c) and 3(d).
Figure 3. Reflectance (R) and transmittance (T) as a function of the incidence angle of a system of 360 cylinders of dispersive LHM with smooth and randomly rough surfaces, under TE polarization, for a filling fraction $f = 0.10$ and a reduced frequency of (a) $\omega_r = 0.82$ ($\lambda = 1.21\mu m$) and (b) $\omega_r = 0.85$ ($\lambda = 1.17\mu m$); and for $f = 0.20$ with (c) $\omega_r = 0.82$ and (d) $\omega_r = 0.85$.

Once it is possible to predict the behavior of the optical response of the two-dimensional photonic structures is possible, and if the fabrication of them is feasible, the experimental verification is carried out. In Mexico, plate-shaped two-dimensional photonic structures have already been fabricated on silicon substrates using the focused ion beam technique, in Laboratorio Nacional de Nanotecnologia at CIMAV. Focused Ion Beam (FIB) allows a micro-machining without the need to use masks or irregularities in the material. To manufacture the 2DPhCs using the FIB technique, it is only necessary to indicate to the equipment the pattern where it should be erode and establish the erosion parameters. The main drawback of this method is the redeposition of the eroded material, which makes the walls of the holes are not parallel. Another technique for manufacturing 2DPhCs is metal-assisted chemical etching (MACE). The main advantages of MACE are: it is an easy and inexpensive method to manufacture nanostructures on silicon and it allows the control of the orientation of silicon nanostructures with respect to the substrate. As immediate future work, photonic structures will be obtained through soft lithography by MACE technique. In figure 4 two micrographs of 2DPhC reported previously with similar techniques, are shown.

Figure 4. Micrographs of (a) dielectric plate with air holes, self-image; and (b) dielectric rods embedded in air, image taken of [15].
4. Conclusions

Using the integral method, it was possible to study the propagation of electromagnetic waves through truncated periodic systems and has been shown to have great advantage in comparison with other methods. It takes into account a finite number of sampling points along the contours of the inclusions, which allows the modelling of the optical response using less computational resources. This provided the opportunity to analyze the reflectance and transmittance of periodic hexagonal lattice systems with cylindrical inclusions containing smooth and randomly rough surfaces, under TE polarization. It is observed that for some systems formed by an array of inclusions with little roughness, the reflective optical properties are modified. By taking into account the roughness of the systems, you can have better control of the power, which is important when developing technological applications.

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