Optical properties of two-dimensional square lattices with smooth and randomly rough surfaces that include dispersive left-handed materials

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Abstract. The study of photonic crystals (PCs) is very importance for the development of new optical technologies. An interest in the investigation of PCs is the search of totally optical control of information in a circuit, with the idea of developing new technological applications that have great advantages over conventional electronic devices in the miniaturization of circuits. In the present work, we show a numerical study of the electromagnetic response of two-dimensional square lattices such as finite photonic structures formed by cylinders embedded in air and air holes in a finite plate composed of metamaterial. We applied a numerical technique known as Integral Equation Method (IEM) to calculate the optical response by calculating reflectance and transmittance as a function of the angle of incidence of finite systems proposed. The calculations were performed by varying the filling fractions and introducing a random roughness on the surfaces of the cylindrical inclusions that form our proposed systems, for the transverse magnetic field (TM) polarization. The results obtained show that the random roughness on the surfaces of the cylindrical inclusions affects their reflective and transmissive properties of two-dimensional square lattices. This is an important result to consider in manufacturing of finite two-dimensional square lattices, despite the existence of a well-developed technology for the manufacture of surfaces. These structures can be used, for example, for the development of filters, mirrors and lenses.

1. Introduction

PCs are the subject of much research in recent years because of their potential to develop completely optical integrated circuits. PCs are systems that sometimes involve complicated symmetries and very novel physical properties, such as those corresponding to metamaterials. These artificial materials, also known as Left-Handed Materials (LHMs), have attracted great research interest among researchers in different fields. This enthusiasm can be attributed mainly to its unique electromagnetic characteristics, due to the fact that the light vectors ($\mathbf{E}$, $\mathbf{H}$, $\mathbf{K}$) form a triad of orthogonal vectors with left orientation for a wave propagating through these media [1]. Since these materials have a negative refractive index within a given range of the electromagnetic spectrum, some of the optical phenomena present variations that make them potentially useful for new technological applications, as for example the negative refraction, the invisibility and the transmission of information [2,3]. As a result, the scientific community has begun to study a variety of optical systems that include LHMs as main components.
The study of the propagation of light in PCs is based on numerical methods, some of which were applied first in solid state physics for the study of electronic band structures. In this work, we applied the numerical IEM [4] which presents some advantages in comparison with the Plane Wave Expansion (PWE) [5] method and other methods, since it has the capacity to study different aspects of these systems that have complicated geometries and very novel physical properties, such as those corresponding to the LHMs. As we will see, the proposed formalism has been considered as an alternative to existing methods in the sense that it gives good results unlike others where they often fail.

This paper is organized as follows. In Sec. 2, we present a rigorous numerical method to solve the problems raised. Sec. 3 shows numerical results of the optical response by calculating reflectance and transmittance as a function of the angle of incidence of finite systems such as photonic structures formed by cylinders embedded in air and air holes in a finite plate composed of LHM media, considering a random roughness on the surfaces of the cylindrical inclusions that form our proposed systems. Sec. 4, we show an example of a CF manufactured on a monocrystalline silicon substrate by means of the Focused Ion Beam (FIB) technique. Finally, we present our main conclusions in Sec. 5.

2. Theoretical approach

The present work aims to make a theoretical and numerical study of the electromagnetic response of finite systems such as photonic structures formed by cylinders embedded in air and air holes in a finite plate composed of LHM media, considering a random roughness on the surfaces of the cylindrical inclusions that form our proposed systems. The corresponding finite systems are shown in Fig. 1, where it has been assumed that the incident medium has the optical properties given by the magnetic permeability $\mu_0$ and electrical permittivity $\varepsilon_0$, the medium containing the inclusions has the properties given by $\mu_1$, $\varepsilon_1$, the inclusions considered equal have the properties given by $\mu_2$, $\varepsilon_2$, and the transmission medium has the properties given by $\mu_3$, $\varepsilon_3$.

![Diagram of a two-dimensional square lattice formed by a square unit cell with randomly rough inclusions, containing dielectric means or LHM media. The contours of integration are indicated by dashed curves. $R_0$ and $R_q$ represent the regions enclosing the incident and transmission media, respectively.](image)

The optical properties corresponding to the LHM means are given by the dielectric function [6] $\varepsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2}$, (1) and magnetic permeability $\mu(\omega) = 1 - \frac{F\omega^2}{\omega^2 - \omega_0^2}$, (2)
These functions allow to determine the region where this LHM presents a negative refraction index, which is within the frequency range \( \omega_0 < \omega < \omega_{LM} \) with \( \omega_{LM} = \omega_0 \sqrt{1 - F} \). The parameters used (in reduced units) in these functions are: \( \omega_p = 1.592 \), \( \omega_0 = 0.637 \) and \( F = 0.56 \).

2.1. Integral Equation Method

As we know, if we assume a harmonic time dependence \( e^{-i\omega t} \) for electromagnetic fields, the wave equation is transformed into the Helmholtz equation:

\[
\nabla^2 \Psi_j(r) + k_j^2 \Psi_j(r) = 0.
\]  

(3)

In Eq. (3), \( \Psi_j(r) \) represents the electric field \( E_z \) in the case of TE polarization, and the magnetic field \( H_x \) in the case of the TM polarization, both in the \( j \)-th medium (Fig. 1). It is considered that the electromagnetic field \( \Psi_j(r) \) satisfies the boundary conditions for each polarization. The magnitude of the wave vector is given by \( k_j = n_j(\omega)/(\omega/c) \), where the refractive index \( n_j(\omega) = \pm \sqrt{\mu_j(\omega)e_j(\omega)} \) that involves the material’s properties is given in terms of the electric permittivity \( e_j(\omega) \) and the magnetic permeability \( \mu_j(\omega) \) (Eqs. (1) and (2) from Ref. [6]), both of these functions depending on the frequency \( \omega \) for the case of LHM media. The speed of light is indicated by \( c \). The sign appearing in the refractive index equation must be taken as negative when considering an LHM and positive when the medium is a dielectric material.

Let us now consider the Green’s function \( G_j(r,r') \), which is a solution of the equation:

\[
\nabla^2 G_j(r,r') + k_j^2 G_j(r,r') = -4\pi \delta(r-r'),
\]  

(4)

with \( G_j(r,r') = i\pi H^{(1)}_0(k_j |r-r'|) \) where \( H^{(1)}_0(\zeta) \) is a Hankel function of the first kind and order zero. Firstly applying the two-dimensional Green’s second identity to \( \Psi_j(r) \) and \( G_j(r,r') \) to the vacuum incident region \( j = 0 \) with an incident wave (see Fig. 1), we obtain the total field [6]:

\[
\Psi(r) = \Psi_{inc}(r) + \frac{1}{4\pi} \oint_{\Gamma_1} \left[ \frac{\partial G_0(r,r')}{\partial n'_1} \Psi_0(r') - G_0(r,r') \frac{\partial \Psi_0(r')}{\partial n'_1} \right] ds',
\]  

(5)

where \( \Gamma_1 \) represents the closed contour that delimits the surface \( S_1 \). The source functions \( \Psi_0(r') \) and \( \partial \Psi_0(r')/\partial n'_1 \), which represent the values of the electromagnetic field and its normal derivative evaluated on the contour \( \Gamma_1 \) can be obtained from Eq. (5). For this, an approximation of the observation point is made on the contour delimiting the corresponding region.

Now, applying the two-dimensional Green’s theorem to \( \Psi_j(r,r') \) and \( G_j(r,r') \) for each region corresponding to the \( j \)-th medium (Fig. 1), we get a system of coupled integral equations (see Ref. [6]). The system of integral equations obtained can be solved numerically by means of a discretization on each one of the contours \( \Gamma_j \) (Fig. 1), that under the boundary conditions on the field and its normal derivative along the different contours (see Ref. [6]), we achieve a system of algebraic equations. This system of equations can be expressed as

\[
\sum_{n=1}^{N_j} \left( \delta_{mn(1)} - N_{mn(1)}^{(0)} \right) \Psi_{n(1)}^{(1)} + \int_{\Gamma_1} \sum_{n=1}^{N_j} L_{mn(1)}^{(0)} \Phi_{n(1)}^{(1)} = \Psi_{inc}^{m},
\]  

\[
-\sum_{n=1}^{N_j} N_{mn(1)}^{(1)} \Psi_{n(1)}^{(1)} + \sum_{n=1}^{N_j} L_{mn(1)}^{(1)} \Phi_{n(1)}^{(1)} - \sum_{n=1}^{N_j} N_{mn(2)}^{(1)} \Psi_{n(2)}^{(1)}
\]  

\[
+ \sum_{n=1}^{N_j} L_{mn(2)}^{(1)} \Phi_{n(2)}^{(1)} + \cdots - \sum_{n=1}^{N_j} N_{mn(q)}^{(1)} \Psi_{n(q)}^{(1)} + \sum_{n=1}^{N_j} L_{mn(q)}^{(1)} \Phi_{n(q)}^{(1)} = 0,
\]  

(7)
\[ \sum_{n=1}^{N_z} (\delta_{mn(2)} - N_{mn(2)}) \Psi_{n(2)}^{(1)} + \frac{f_2}{f_1} \sum_{n=1}^{N_z} L_{mn(2)}^{(2)} \Phi_{n(2)}^{(1)} = 0, \] (8)

\[ \sum_{n=1}^{N_z} (\delta_{mn(3)} - N_{mn(3)}) \Psi_{n(3)}^{(1)} + \frac{f_2}{f_1} \sum_{n=1}^{N_z} L_{mn(3)}^{(2)} \Phi_{n(3)}^{(1)} = 0, \] (9)

\[ \vdots \]

\[ \sum_{n=1}^{N_z} (\delta_{mn(q-1)} - N_{mn(q-1)}) \Psi_{n(q-1)}^{(1)} + \frac{f_2}{f_1} \sum_{n=1}^{N_z} L_{mn(q-1)}^{(2)} \Phi_{n(q-1)}^{(1)} = 0, \] (10)

\[ \sum_{n=1}^{N_z} (\delta_{mn(q)} - N_{mn(q)}) \Psi_{n(q)}^{(1)} + \frac{f_2}{f_1} \sum_{n=1}^{N_z} L_{mn(q)}^{(2)} \Phi_{n(q)}^{(1)} = 0. \] (11)

Equations (6)-(11) constitute an inhomogeneous system of \( 2 \sum_{p=1}^{q} N_p \) linear equations that can be solved numerically to determine the fields and their normal derivative along all the contours. To solve the system of equations (6)-(11), we use the FORTRAN programming language with ScaLAPACK libraries employing the LU decomposition method.

Once the \( \Psi_n^{(j)} \) and \( \Phi_n^{(j)} \) sources are obtained, now we can calculate the field at any point and therefore the reflectance and transmittance written as

\[ R(\omega) = \frac{\int_{-\pi/2}^{\pi/2} \hat{h}_r |A(\theta_s, \omega)|^2 d\theta_s}{\int_{-\pi/2}^{\pi/2} \hat{h}_r |A(\theta_s, \omega)|^2 d\theta_s}, \] (12)

and

\[ T(\omega) = \frac{\int_{-\pi/2}^{\pi/2} \hat{h}_t |A(\theta_s, \omega)|^2 d\theta_s}{\int_{-\pi/2}^{\pi/2} \hat{h}_r |A(\theta_s, \omega)|^2 d\theta_s}, \] (13)

where \( h_r \) and \( h_t \) are normalization factors that depend on the incident wave and the length of the \( \Gamma_a \) profile in the direction of \( x \), and \( A(\theta_s, \omega) \) is the far-field amplitude is given by [4]:

\[ A(\theta_s, \omega) = \frac{1}{\Gamma_2} \int_{r'} \left[-i \frac{\omega}{c} (\mathbf{n}_a \cdot \mathbf{r}) \Psi_n^{(1)}(\mathbf{r}') - \frac{\partial \Psi_n^{(1)}(\mathbf{r}')}{\partial n'_u} \right] \times \exp\left(-i \frac{\omega}{c} (\mathbf{r} \cdot \mathbf{r}') \right) ds', \] (14)

being \( \theta_s \) the angle of scattering.

3. **Optical response of finite two-dimensional square lattices composed of cylindrical inclusions with smooth and randomly rough surfaces**

The previously developed method can calculate the electromagnetic field distribution in the far-field regions of the space for a finite two-dimensional square lattice (Fig. 1). Since the size of the system is finite, to avoid edge effects we illuminate it with a tapered Gaussian beam whose intercept with the plane of the interface has a half-width \( g \).

As examples of applications, we consider different systems of finite two-dimensional square lattices such as photonic structures formed by cylinders embedded in air and air holes in a finite plate composed of LHM media, considering a random roughness on the surfaces of the cylindrical inclusions that form our proposed systems. Finite photonic structures are composed of 500 inclusions (125 inclusions in the X-direction and 4 inclusions in direction of the Y-direction). In Figs. 2(a) and (c) show the results obtained from the optical response by calculating the reflectance and transmittance as a function of the incident angle for an incident light beam (Gaussian beam) with wavelength of 1.25 µm (corresponding
to $\omega_r = 0.80$) for finite photonic structures formed by air holes in a finite plate composed of LHM media with filling fractions of $f = 0.04$ and $f = 0.06$, respectively for the TM polarization. To study the effects of roughness in these systems we considered a profile that has random roughness with a correlation length $\delta = 0.05\lambda$ and a standard deviation of heights of $\sigma = 0.02\lambda$ on the surfaces, for the different values of the filling fraction $f$. This profile is defined by a realization of a Gaussian-correlated random process that obeys a negative exponential probability-density function (PDF) [7]. In Figs. 2(b) and (d), we show the results of the equivalent system formed by cylinders embedded in air that include LHM. In this case, the photonic structure is illuminated by a beam with wavelength of 1.17 µm (corresponding to $\omega_r = 0.85$).

When comparing the results of the different systems of finite two-dimensional square lattices with cylindrical inclusions of smooth surface with their corresponding randomly rough surface systems, we can observe that the reflective and transmissive properties are affected for the polarization TM by including a random roughness on the surface of the cylindrical inclusion. This is an important result to consider in manufacturing of finite two-dimensional square lattices, despite the existence of a well-developed technology for the manufacture of surfaces.

4. CF manufactured on a monocrystalline silicon substrate

In Fig. 3, we show a photonic structure corresponding to a PC manufactured on a monocrystalline silicon substrate with the equipment JEOL JEM9320-FIB available at the facilities of the National Nanotechnology Laboratory of the CIMAV.
Figure 3. Diagram of a PC manufactured on a monocrystalline silicon substrate. This is formed by a square unit cell with circular inclusions of 0.8 μm of diameter and lattice parameter of 1 μm. The thickness of the plate is 1 mm [8].

The PC manufactured is composed of 70 circular inclusions of approximately 0.8 μm in diameter and a lattice parameter of 1 μm. To achieve this it was necessary to use an ion beam of 1000 pA, a dose of 200 nC/μm², 30 kV in the ion column, a beam exposure time of 15 seconds per hole and a magnification of 2000X. This photonic structure proves that it is possible to manufacture CFs on a micrometric scale by means of the Focused Ion Beam (FIB) technique. This structure could have an application in the development of completely optical integrated circuits.

5. Conclusions
A numerical method, known as the IEM, was used to calculate the electromagnetic response of finite two-dimensional square lattices such as a finite photonic structure formed by cylinders embedded in air and air holes in a finite plate composed of LHM media, considering a random roughness on the surfaces of the cylindrical inclusions that form our proposed systems. By comparing the results of the optical response by calculating reflectance and transmittance as a function of the angle of incidence, we conclude that the random roughness on the surfaces of the cylindrical inclusions affects the reflective and transmissive properties of the different systems proposed. These theoretical results are very important to take into account in the fabrication of photonic structures, since despite the existence of well-developed technology, rough surfaces are obtained in the scale of the visible wavelength.

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