

Band gaps in 2d photonic crystals with hexagonal symmetry

B. LAZĂR, P. STERIAN*

Academic Center for Optical Engineering and Photonics, Faculty of Applied Sciences, University "Politehnica" Bucharest, Romania

The article presents, in detail, a mathematical method useful for calculating dispersion diagrams corresponding to Photonic Crystals with hexagonal symmetry. In the end, a few numerical results are given to confirm the validity of the method.

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1. Introduction

Mathematical calculations and practical experiments show that a composite, formed by a repetitive succession of media with different dielectric permittivities, named also Photonic Crystal, possesses frequency gaps and as a result the electromagnetic fields, with speeds of oscillation inside those gaps, cannot propagate through it [1], [2], [3], [4].

Therefore, photonic crystals can be defined as periodical media that have the property of forbidden frequency ranges, a radiation with the wavelength in their frequency gaps being unable to propagate inside these repetitive composites. The most usual and interesting type of photonic crystal, to date, is a dielectric material characterized by a cyclic electric permittivity that repeats in space with a period comparable, as linear dimensions, with the wavelength of the radiation interacting with the dielectric.

No simple formula, able to predict the size and positions of photonic crystals band gaps, exists [5], [6]. Unfortunately, when it comes to establishing the dispersion diagrams of this type of alternating structures, various articles present the results specifying that they have been obtained using a certain numerical method (for instance PWM – Plane Wave Method) implemented with a software conceived by the author, which if available is not well documented and written in a language you are not familiar with. For this reason, programs that calculate the structures of forbidden bands are hard to integrate in your own software, designed to study various properties of photonic crystals, and in conclusion, many people have to write their own piece of code able to calculate the dispersion diagrams, in other words, to solve Maxwell Equations for a periodic dielectric medium in the frequency space.

The purpose of the present paper is to start from these equations and finally get a mathematical set of expressions that can be easily implemented in software, especially Matlab, with the goal of obtaining dispersion diagrams for

any 2D dielectric photonic crystal having hexagonal symmetry. The cases of 1D crystals [7] and 2D structures with square symmetry can easily be particularized from the hexagonal one.

2. The wave equation in the frequency domain

In classical physics, the propagation of electromagnetic waves in substance is studied using Maxwell Equations. The photonic crystals, being a repetitive succession of media, each of them extending in a volume many orders of magnitude greater than the dimensions of atoms, are perfectly suitable to be treated with these equations whose general form is:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad (1)$$

$$\nabla \cdot \mathbf{B} = 0 \quad (2)$$

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{j}(\mathbf{r}, t) \quad (3)$$

$$\nabla \cdot \mathbf{D} = \rho(\mathbf{r}, t) \quad (4)$$

where: $\mathbf{E}=\mathbf{E}(\mathbf{r},t)$ is the intensity of the electric field, $\mathbf{B}=\mathbf{B}(\mathbf{r},t)$ the magnetic induction, $\mathbf{H}=\mathbf{H}(\mathbf{r},t)$ the intensity of magnetic field, $\mathbf{D}=\mathbf{D}(\mathbf{r},t)$ the electric induction, $\mathbf{j}(\mathbf{r},t)$ the current density and $\rho(\mathbf{r},t)$ the electric charge density.

In Cartesian coordinates, the position vector \mathbf{r} has the expression $\mathbf{r}=xe_x+ye_y+ze_z$, where $\mathbf{e}_{x,y,z}$ are versors corresponding to the x, y, z spatial directions.

The quantities \mathbf{D} and \mathbf{H} are, in general, for an arbitrary medium, complicated function of the following four variables: $t, \mathbf{r}, \mathbf{E}$ and \mathbf{B} :

$$\mathbf{D} = \mathbf{D}(t, \mathbf{r}; \mathbf{E}, \mathbf{B}), \quad \mathbf{H} = \mathbf{H}(t, \mathbf{r}; \mathbf{E}, \mathbf{B}). \quad (5)$$

However, for an entire group of substances, relations (5) turn into simple linear dependencies if the intensities of \mathbf{E} and \mathbf{B} are relatively small. Thus,

$$\mathbf{D} = \varepsilon \mathbf{E} = \varepsilon_0 \varepsilon_r \mathbf{E}, \quad \mathbf{H} = \frac{\mathbf{B}}{\mu} = \frac{\mathbf{B}}{\mu_0 \mu_r}, \quad (6)$$

where: ε is the electric permittivity of the medium, μ - magnetic permeability, ε_0 , μ_0 - electric permittivity and magnetic permeability of vacuum respectively and ε_r , μ_r - electric permittivity and magnetic permeability of the medium in respect to vacuum. The equations (1) ÷ (14) can have an even simple form if none of the substances under consideration is magnetic,

$$\mu_r = 1, \quad (7)$$

and no density of electric charge or current exists,

$$\mathbf{j}(\mathbf{r}, t) = 0, \quad \rho(\mathbf{r}, t) = 0. \quad (8)$$

Conditions (7) and (8) are met for the majority of dielectrics, at small intensities of electric and magnetic fields. Unfortunately, all simplifications end here because photonic crystals have position dependent electric permittivity in the form of a repetitive function of \mathbf{r} :

$$\varepsilon_r(\mathbf{r}) = \varepsilon_r(\mathbf{r} + \mathbf{A}), \quad \text{where } \mathbf{A} \text{ is the period.} \quad (9)$$

Therefore, substituting relations (6) ÷ (9) into Maxwell Equations (1) ÷ (4) and solving the system, two equivalent propagation equations: (10) and (11) and two conditions: {(12), (14)} or {(13), (15)} can be written:

$$\nabla \times \left(\frac{1}{\varepsilon_r(\mathbf{r})} \nabla \times \mathbf{H} \right) = -\frac{1}{c^2} \frac{\partial^2 \mathbf{H}}{\partial t^2}, \quad (10)$$

$$\frac{1}{\varepsilon_r(\mathbf{r})} [\nabla \times (\nabla \times \mathbf{E})] = -\frac{1}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2}, \quad (11)$$

$$\nabla \cdot \mathbf{H} = 0, \quad (12)$$

$$\nabla \cdot \mathbf{H} = 0, \quad (13)$$

$$\nabla \cdot [\varepsilon_r(\mathbf{r}) \mathbf{E}] = 0, \quad (14)$$

$$\nabla \cdot [\varepsilon_r(\mathbf{r}) \mathbf{E}] = 0, \quad (15)$$

In the case of photonic crystals, of great interest is solving the two equations in the frequency domain. For that purpose \mathbf{H} and \mathbf{E} are considered being harmonic:

$$(a) \mathbf{H}(\mathbf{r}, t) = \mathbf{H}(\mathbf{r}) e^{j\omega t}, \quad (b) \mathbf{E}(\mathbf{r}, t) = \mathbf{E}(\mathbf{r}) e^{j\omega t}, \quad (16)$$

where ω is the pulsation of the field:

$$\omega = 2\pi f \quad (17)$$

By replacing (16) (a) in (10) or (16) (b) in (11) the following atemporal expressions are obtained:

$$\nabla \times \left(\frac{1}{\varepsilon_r(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) \right) = \frac{\omega^2}{c^2} \mathbf{H}(\mathbf{r}), \quad (18)$$

$$\frac{1}{\varepsilon_r(\mathbf{r})} (\nabla \times [\nabla \times \mathbf{E}(\mathbf{r})]) = \frac{\omega^2}{c^2} \mathbf{E}(\mathbf{r}). \quad (19)$$

The equations (18) and (19) are useful for calculating the dispersion diagrams of various photonic crystals and implicitly for establishing their structures of frequency gaps. The equality (19), for instance, is general and can be solved for the full 3D case or simplifications in one or two dimensions. As stated in the beginning, this article deals only with the circumstance where the medium, taken into consideration, is two-dimensional, a case that splits in two branches.

The first is the transversal electric possibility when $\mathbf{E} = E_z \cdot \mathbf{e}_z$ that once replaced in (19) transforms it in (20) (the \mathbf{e}_z versor and z index will be considered implicit).

$$-\frac{1}{\varepsilon_r(x, y)} \left(\frac{\partial^2 E(x, y)}{\partial x^2} + \frac{\partial^2 E(x, y)}{\partial y^2} \right) = \frac{\omega^2}{c^2} E(x, y) \quad \text{for TE modes.} \quad (20)$$

The relation (20) belongs to a category of equations that can be solved using the Bloch-Floquet theorem which (for the current situation) states that: if $1/\varepsilon_r(x, y)$ is a periodic function then:

$$E(x, y) = e^{j(k_x x + k_y y)} g(x, y), \quad (21)$$

where $g(x, y)$ is a repetitive function having the same period as $1/\varepsilon_r(x, y)$.

In the particular situation of photonic crystals, $\varepsilon_r(x, y)$ is by definition periodic which also imply that $1/\varepsilon_r(x, y)$ is also cyclic with the same period as $\varepsilon_r(x, y)$.

The second case is the transversal magnetic one, when $\mathbf{H}(\mathbf{r}) = H_z(x, y, z) \cdot \mathbf{e}_z$. This time, the equation (18) is used. First of all, the quantity $\nabla \times \left[\left(\frac{1}{\varepsilon_r(\mathbf{r})} \right) \nabla \times \mathbf{H}(\mathbf{r}) \right]$ needs to be evaluated. Thus,

$$\nabla \times \left(\frac{1}{\varepsilon_r(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) \right) = -\frac{\partial}{\partial y} \left(\frac{1}{\varepsilon_r(x, y)} \frac{\partial H_z}{\partial y} \right) \cdot \mathbf{e}_z - \frac{\partial}{\partial x} \left(\frac{1}{\varepsilon_r(x, y)} \frac{\partial H_z}{\partial x} \right) \cdot \mathbf{e}_z \quad (22)$$

Therefore, the following equation in \mathbf{H} is obtained (where the z index and \mathbf{e}_z versor are considered implicit):

$$-\left[\frac{\partial}{\partial x} \left(\frac{1}{\varepsilon_r(x, y)} \frac{\partial H(x, y)}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{1}{\varepsilon_r(x, y)} \frac{\partial H(x, y)}{\partial y} \right) + \frac{1}{\varepsilon_r(x, y)} \left(\frac{\partial^2 H(x, y)}{\partial x^2} + \frac{\partial^2 H(x, y)}{\partial y^2} \right) \right] = \frac{\omega^2}{c^2} H(x, y) \quad (23)$$

which can be used for calculating dispersion diagrams for TM modes.

3. The Fourier Transform for periodic electric permittivity

The equation (20), with ε_r repetitive, can be solved by applying the Fourier Transform to both sides of the equality. In the case of photonic crystals with hexagonal symmetry the basic brick of the structure is rhombic, like in Fig. 1, and in consequence the periodicity of $\varepsilon_r(x,y)$ can be mathematically written as in expression (24). The present paragraph calculates the Fourier Transform of ε_r , $1/\varepsilon_r$ or in general, of any repetitive 2D function having a periodicity as that in Fig. 1. Once this transform is found, it can be used for solving equation (20).

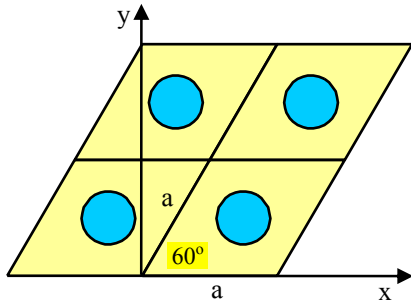


Fig. 1. Photonic crystal with hexagonal symmetry.

$$\varepsilon(x, y) = \varepsilon\left(x + a\left(1 + \cos\frac{\pi}{3}\right), y + a\sin\frac{\pi}{3}\right). \quad (24)$$

By definition, a square integrable function with n variables can be written as an integral sum in the following form [8]:

$$\int_{y=0}^{\frac{a\sqrt{3}a+y}{\sqrt{3}}} \int_{x=-\frac{y}{\sqrt{3}}}^{\frac{a\sqrt{3}a+y}{\sqrt{3}}} \varepsilon(x, y) e^{-j\frac{2\pi}{a}\left(m_1x + \frac{2m_2-m_1}{\sqrt{3}}y\right)} dx dy = \underbrace{\frac{2}{a^2\sqrt{3}} \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} p\left(n_1 \frac{2\pi}{a}, \frac{2n_2-n_1}{\sqrt{3}} \frac{2\pi}{a}\right) \int_{y=0}^{\frac{a\sqrt{3}a+y}{\sqrt{3}}} \int_{x=-\frac{y}{\sqrt{3}}}^{\frac{a\sqrt{3}a+y}{\sqrt{3}}} e^{j\frac{2\pi}{a}\left[(n_1-m_1)x + \frac{2(n_2-m_2)-(n_1-m_1)}{\sqrt{3}}y\right]} dx dy}_I \quad (29)$$

where I is:

$$I = \frac{a^2\sqrt{3}}{8\pi^2} \frac{\left(1 - e^{j\frac{2\pi}{a}x}\right)\left(1 - e^{j\frac{2\pi}{a}y}\right)}{xy} = \begin{cases} \frac{a^2\sqrt{3}}{2} \text{ pt. } n_1 = m_1, n_2 = m_2 \\ 0 \text{ for the remaining cases} \end{cases} \quad (30)$$

In conclusion:

$$f(x_1, x_2 \dots x_n) = \frac{1}{(2\pi)^n} \int_{k_{x1}=-\infty}^{\infty} \int_{k_{x2}=-\infty}^{\infty} \dots \int_{k_{xn}=-\infty}^{\infty} p(k_{x1}, k_{x2} \dots k_{xn}) e^{j(k_{x1}x_1 + k_{x2}x_2 + \dots + k_{xn}x_n)} dk_{x1} dk_{x2} \dots dk_{xn} \quad (25)$$

where p is the Fourier Transform of f . Consequently, using (25), where f is replaced by ε , both members of the equality (24) can be expanded as follows:

$$\frac{1}{(2\pi)^2} \int_{k_x=-\infty}^{\infty} \int_{k_y=-\infty}^{\infty} p(k_x, k_y) e^{j(k_x x + k_y y)} dk_x dk_y = \frac{1}{(2\pi)^2} \int_{k_x=-\infty}^{\infty} \int_{k_y=-\infty}^{\infty} p(k_x, k_y) e^{j\left[k_x\left(x + \frac{3a}{2}\right) + k_y\left(y + \frac{a\sqrt{3}}{2}\right)\right]} dk_x dk_y, \forall x, y \quad (26)$$

which is satisfied if:

$$e^{j\frac{a\sqrt{3}}{2}(k_x\sqrt{3} + k_y)} = 1 \Rightarrow \frac{a\sqrt{3}}{2}(k_x\sqrt{3} + k_y) = 2n\pi \Rightarrow \begin{cases} k_x = n_1 \frac{2\pi}{a} \\ k_y = \frac{2n_2 - n_1}{\sqrt{3}} \frac{2\pi}{a} \end{cases} \quad (27)$$

n_1, n_2 integers.

As a result, $\varepsilon_r(x,y)$ is constrained to have the decomposition:

$$\varepsilon(x, y) = \frac{2}{a^2\sqrt{3}} \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} p\left(n_1 \frac{2\pi}{a}, \frac{2n_2-n_1}{\sqrt{3}} \frac{2\pi}{a}\right) e^{j\frac{2\pi}{a}\left(n_1x + \frac{2n_2-n_1}{\sqrt{3}}y\right)} \quad (28)$$

By multiplying both members with $e^{-j\frac{2\pi}{a}\left(m_1x + \frac{2m_2-m_1}{\sqrt{3}}y\right)}$ and integrating over one period (see Fig. 1), the expression (28) turns in:

$$p\left(m_1 \frac{2\pi}{a}, \frac{2m_2-m_1}{\sqrt{3}} \frac{2\pi}{a}\right) = \int_{y=0}^{\frac{a\sqrt{3}}{2}} \int_{x=0}^{\frac{a\sqrt{3}}{2}} \varepsilon(x, y) e^{-j\frac{2\pi}{a}\left(m_1x + \frac{2m_2-m_1}{\sqrt{3}}y\right)} dx dy \approx \frac{1}{N^2} \sum_{q=0}^{N-1} \sum_{r=0}^{N-1} \varepsilon\left(\frac{a}{N}q, \frac{a\sqrt{3}}{2N}r\right) e^{-j\frac{2\pi}{N}\left(m_1q + \frac{2m_2-m_1}{2}r\right)} \quad (31)$$

Using (31), equations (20) and (23) can be solved (see the next paragraph).

4. The matrices that give the dispersion diagrams for TE, TM modes

TE modes: Using

(28)(28), $\epsilon_r^{-1}(x,y)$ from (20) can be put in the form:

$$\epsilon_r^{-1}(x,y) = \frac{2}{a^2\sqrt{3}} \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} p_{n_1,n_2} e^{j\frac{2\pi}{a}\left[n_1x + \frac{(2n_2-n_1)}{\sqrt{3}}y\right]} \quad (32)$$

Also, $E(x,y) = e^{j(k_x x + k_y y)} g(x,y)$ is expanded as follows:

$$\frac{\partial^2 E(x,y)}{\partial x^2} + \frac{\partial^2 E(x,y)}{\partial y^2} = -\frac{2}{a^2\sqrt{3}} \sum_{m_1=-\infty}^{\infty} \sum_{m_2=-\infty}^{\infty} h_{m_1,m_2} \left[\left(k_x + \frac{2\pi}{a}m_1\right)^2 + \left(k_y + \frac{2\pi}{a}\frac{(2m_2-m_1)}{\sqrt{3}}\right)^2 \right] e^{j\left[(k_x+k_y)x + \frac{2\pi}{a}\left(m_1x + \frac{(2m_2-m_1)}{\sqrt{3}}y\right)\right]} \quad (34)$$

and so, (20) transforms into:

$$\begin{aligned} & \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \sum_{m_1=-\infty}^{\infty} \sum_{m_2=-\infty}^{\infty} h_{m_1,m_2} p_{n_1,n_2} \left[\left(k_x + \frac{2\pi}{a}m_1\right)^2 + \left(k_y + \frac{2\pi}{a}\frac{(2m_2-m_1)}{\sqrt{3}}\right)^2 \right] e^{j\frac{2\pi}{a}\left[(m_1+n_1)x + \frac{2m_2-m_1+2n_2-n_1}{\sqrt{3}}y\right]} = \\ & = \frac{\omega^2}{c^2} \sum_{m_1=-\infty}^{\infty} \sum_{m_2=-\infty}^{\infty} h_{m_1,m_2} e^{j\frac{2\pi}{a}\left(m_1x + \frac{2m_2-m_1}{\sqrt{3}}y\right)} \end{aligned} \quad (35)$$

Multiplying both members of (35): with $\left(1/a^2 \sin(\pi/3)\right) e^{-j(2\pi/a)[m_1'x + (2m_2'-m_1')y/\sqrt{3}]}$ and integrating with respect to y over the interval $[-a\sqrt{3}/4, a\sqrt{3}/4]$ and x

$$E(x,y) = \frac{2}{a^2\sqrt{3}} \sum_{m_1=-\infty}^{\infty} \sum_{m_2=-\infty}^{\infty} h_{m_1,m_2} e^{j\left[(k_x+k_y)x + \frac{2\pi}{a}\left(m_1x + \frac{(2m_2-m_1)}{\sqrt{3}}y\right)\right]} \quad (33)$$

where p_{n_1,n_2} and h_{m_1,m_2} are the coefficients of the two series.

Thus, $\partial^2 E(x,y)/\partial x^2 + \partial^2 E(x,y)/\partial y^2$ can be written as:

over $[y/\sqrt{3} - a/2, y/\sqrt{3} + a/2]$, the following equality is found:

$$\begin{aligned} & \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \sum_{m_1=-\infty}^{\infty} \sum_{m_2=-\infty}^{\infty} h_{m_1,m_2} p_{n_1,n_2} \left[\left(k_x + \frac{2\pi}{a}m_1\right)^2 + \left(k_y + \frac{2\pi}{a}\frac{(2m_2-m_1)}{\sqrt{3}}\right)^2 \right] \frac{\sin[\pi(m_1+n_1-m_1')]\sin[\pi(m_2+n_2-m_2')]}{\underbrace{\pi(m_1+n_1-m_1')}_{\delta_{m_1+n_1,m_1'}} \underbrace{\pi(m_2+n_2-m_2')}_{\delta_{m_2+n_2,m_2'}}} = \\ & = \frac{\omega^2}{c^2} \sum_{m_1=-\infty}^{\infty} \sum_{m_2=-\infty}^{\infty} h_{m_1,m_2} \frac{\sin[\pi(m_1-m_1')]\sin[\pi(m_2-m_2')]}{\underbrace{\pi(m_1-m_1')}_{\delta_{m_1,m_1'}} \underbrace{\pi(m_2-m_2')}_{\delta_{m_2,m_2'}}} \end{aligned} \quad (36)$$

For an arbitrary (m_1',m_2') pair, the majority of terms, situated left and right in respect to the equality sign, will disappear and (36) simplifies to:

$$\begin{aligned} & \sum_{m_1=-\infty}^{\infty} \sum_{m_2=-\infty}^{\infty} h_{m_1,m_2} p_{m_1'-m_1,m_2'-m_2} \left[\left(k_x + \frac{2\pi}{a}m_1\right)^2 + \left(k_y + \frac{2\pi}{a}\frac{(2m_2-m_1)}{\sqrt{3}}\right)^2 \right] =, \\ & = \frac{\omega^2}{c^2} h_{m_1',m_2'} \end{aligned} \quad \text{for TE modes} \quad (37)$$

which represents a system of equations that, if solved, gives a set of eigen frequencies, ω_k .

In practice, the m indexes will be taken: $m_1, m_1', m_2, m_2' \in [-M, M]$ where M is a positive integer. For each of the $(2M+1) \times (2M+1)$ values of (m_1', m_2') an equation like (37) exists where the coefficients $p_{m_1'-m_1, m_2'-m_2}$ have indexes that vary in the interval $[-2M, 2M]$ and can be calculated (see (31)) with the formula:

$$\begin{aligned} p_{n_1,n_2} & = \\ & = \frac{1}{(4M+1)^2} \sum_{q_1=0}^{4M} \sum_{q_2=0}^{4M} \epsilon_r^{-1} \left(\frac{a}{4M+1} q_1, \frac{a\sqrt{3}}{2(4M+1)} q_2 \right) e^{-j\frac{2\pi}{4M+1}\left[n_1q_1 + \frac{(2n_2-n_1)}{2}q_2\right]} \end{aligned} \quad (38)$$

where the following notations have been made: $n_1 = m_1' - m_1, n_2 = m_2' - m_2$.

In conclusion (37) with $m_1, m_1', m_2, m_2' \in [-M, M]$ is a system in the form:

$$\mathbf{S} \cdot \mathbf{h} = \frac{\omega^2}{c^2} \mathbf{h} \text{ or } \left(\mathbf{S} - \frac{\omega^2}{c^2} \right) \cdot \mathbf{h} = 0, \quad (39)$$

where \mathbf{S} is a square matrix having $(2M+1)^4$ elements of the type:

$$p_{m_1'-m_1, m_2'-m_2} \left[\left(k_x + \frac{2\pi}{a}m_1\right)^2 + \left(k_y + \frac{2\pi}{a}\frac{(2m_2-m_1)}{\sqrt{3}}\right)^2 \right] \quad (40)$$

that can be calculated for any given $m_1, m_1', m_2, m_2', k_x, k_y$. \mathbf{h} is a column matrix possessing $(2M+1) \times (2M+1)$ elements, h_{m_1,m_2} , of unknown values. It can be noticed

that (39) is satisfied, independently of \mathbf{h} , if $\det(\mathbf{S} - \omega^2/c^2) = 0$ which gives $(2M+1)^2$ possible ω_k .

Therefore, for any given (k_x, k_y) , $(2M+1)^2$ values for ω are found and, in this way, the dispersion diagram $\omega = \omega(k_x, k_y)$ is obtained. As can be noticed, a single pair of given (k_x, k_y) require solving a system of $(2M+1)^2$ equations where for good precisions M have to be increased till no difference is observed between $\omega = \omega(k_x,$

$k_y)$ calculated with $(2M+1)^2$ and with $(2(M+1)+1)^2$ equations.

TM modes: The expression (37) is valid only for the TE modes. For finding its equivalent corresponding to the TM situation, the equation (23) have to be utilized as starting point. Using the same deductions as in the case of TE modes, the following expressions can be successively written:

$$\frac{1}{\varepsilon_r(x,y)} \left(\frac{\partial^2 H(x,y)}{\partial x^2} + \frac{\partial^2 H(x,y)}{\partial y^2} \right) = -\frac{2}{a^2 \sqrt{3}} \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \sum_{m_1=-\infty}^{\infty} \sum_{m_2=-\infty}^{\infty} h_{m_1, m_2} p_{n_1, n_2} \left[\left(k_x + \frac{2\pi}{a} m_1 \right)^2 + \left(k_y + \frac{2\pi}{a} \frac{(2m_2 - m_1)}{\sqrt{3}} \right)^2 \right] e^{j \left[\mathbf{k} \cdot \mathbf{r} + \frac{2\pi}{a} \left[(m_1 + n_1)x + \frac{2m_2 - m_1 + 2n_2 - n_1}{\sqrt{3}} y \right] \right]} \tag{41}$$

$$\begin{aligned} \frac{\partial}{\partial x} \left(\frac{1}{\varepsilon_r(x,y)} \right) \frac{\partial H(x,y)}{\partial x} + \frac{\partial}{\partial y} \left(\frac{1}{\varepsilon_r(x,y)} \right) \frac{\partial H(x,y)}{\partial y} &= \\ &= \frac{2}{a^2 \sqrt{3}} \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} p_{n_1, n_2} \left(j \frac{2\pi}{a} n_1 \right) e^{j \frac{2\pi}{a} \left(n_1 x + \frac{2n_2 - n_1}{\sqrt{3}} y \right)} \cdot \sum_{m_1=-\infty}^{\infty} \sum_{m_2=-\infty}^{\infty} h_{m_1, m_2} \left[j \left(k_x + \frac{2\pi}{a} m_1 \right) \right] e^{j \left[\mathbf{k} \cdot \mathbf{r} + \frac{2\pi}{a} \left(m_1 x + \frac{2m_2 - m_1}{\sqrt{3}} y \right) \right]} + \\ &+ \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} p_{n_1, n_2} \left(j \frac{2\pi}{a} \frac{(2n_2 - n_1)}{\sqrt{3}} \right) e^{j \frac{2\pi}{a} \left(n_1 x + \frac{2n_2 - n_1}{\sqrt{3}} y \right)} \cdot \sum_{m_1=-\infty}^{\infty} \sum_{m_2=-\infty}^{\infty} h_{m_1, m_2} \left[j \left(k_y + \frac{2\pi}{a} \frac{(2m_2 - m_1)}{\sqrt{3}} \right) \right] e^{j \left[\mathbf{k} \cdot \mathbf{r} + \frac{2\pi}{a} \left(m_1 x + \frac{2m_2 - m_1}{\sqrt{3}} y \right) \right]} = \\ &= - \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \sum_{m_1=-\infty}^{\infty} \sum_{m_2=-\infty}^{\infty} h_{m_1, m_2} p_{n_1, n_2} \frac{2\pi}{a} \left[n_1 \left(k_x + \frac{2\pi}{a} m_1 \right) + \frac{(2n_2 - n_1)}{\sqrt{3}} \left(k_y + \frac{2\pi}{a} \frac{(2m_2 - m_1)}{\sqrt{3}} \right) \right] e^{j \left[\mathbf{k} \cdot \mathbf{r} + \frac{2\pi}{a} \left[(m_1 + n_1)x + \frac{2m_2 - m_1 + 2n_2 - n_1}{\sqrt{3}} y \right] \right]} \end{aligned} \tag{42}$$

The decompositions obtained from (41) and (42) together with (32) and (33) (where $E(x,y)$ is replaced by $H(x,y)$) are introduced in (23). After simplifying by $e^{j\mathbf{k} \cdot \mathbf{r}}$, multiplying by $(1/a^2 \sin(\pi/3)) e^{-j(2\pi/a)[m_1'x + (2m_2' - m_1')y/\sqrt{3}]}$

and integrating in respect to y over the interval $[-a\sqrt{3}/4, a\sqrt{3}/4]$ and to x over $[y/\sqrt{3} - a/2, y/\sqrt{3} + a/2]$, the following equality results:

$$\begin{aligned} &\sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \sum_{m_1=-\infty}^{\infty} \sum_{m_2=-\infty}^{\infty} h_{m_1, m_2} p_{n_1, n_2} \left[\frac{2\pi}{a} n_1 \left(k_x + \frac{2\pi}{a} m_1 \right) + \frac{2\pi}{a} \frac{(2n_2 - n_1)}{\sqrt{3}} \left(k_y + \frac{2\pi}{a} \frac{(2m_2 - m_1)}{\sqrt{3}} \right) + \left(k_x + \frac{2\pi}{a} m_1 \right)^2 + \left(k_y + \frac{2\pi}{a} \frac{(2m_2 - m_1)}{\sqrt{3}} \right)^2 \right] \cdot \tag{43} \\ &\frac{\sin[\pi(m_1 + n_1 - m_1')] \sin[\pi(m_2 + n_2 - m_2')]}{\pi(m_1 + n_1 - m_1') \pi(m_2 + n_2 - m_2')} = \frac{\omega^2}{c^2} \sum_{m_1=-\infty}^{\infty} \sum_{m_2=-\infty}^{\infty} h_{m_1, m_2} \frac{\sin[\pi(m_1 - m_1')] \sin[\pi(m_2 - m_2')]}{\pi(m_1 - m_1') \pi(m_2 - m_2')} \end{aligned}$$

For an arbitrary pair (m_1', m_2') , the majority of terms from the left and right of the equal sign disappear, (43) turning in:

$$\sum_{m_1=-\infty}^{\infty} \sum_{m_2=-\infty}^{\infty} h_{m_1, m_2} p_{m_1 - m_1', m_2 - m_2'} \cdot \left[\frac{2\pi}{a} (m_1' - m_1) \left(k_x + \frac{2\pi}{a} m_1 \right) + \frac{2\pi}{a} \frac{2(m_2' - m_2) - (m_1' - m_1)}{\sqrt{3}} \left(k_y + \frac{2\pi}{a} \frac{(2m_2 - m_1)}{\sqrt{3}} \right) + \left(k_x + \frac{2\pi}{a} m_1 \right)^2 + \left(k_y + \frac{2\pi}{a} \frac{(2m_2 - m_1)}{\sqrt{3}} \right)^2 \right] = \frac{\omega^2}{c^2} h_{m_1', m_2'} \tag{44}$$

for **TM** modes where the same explanations as given for equation (37), corresponding to the TE situation, remain valid.

As already explained, by solving (37) and (44) the dispersion diagrams, $\omega = \omega(k_x, k_y)$, are obtained. It can be shown that, for a photonic crystal with hexagonal symmetry (whose basic cell is described by the vectors \mathbf{a}_1 and \mathbf{a}_2 as in Fig. 2), a reciprocal cell, defined by $\mathbf{b}_1, \mathbf{b}_2$ (see Fig. 2), exists in the spatial frequencies domain (dual space). Therefore, the periodicity $\varepsilon(\mathbf{r}) = \varepsilon(\mathbf{r} + \mathbf{A})$ has a pair in

the dual domain, $\omega(\mathbf{k}) = \omega(\mathbf{k} + \mathbf{B})$, and in consequence it is enough to compute ω for \mathbf{k} inside just one elementary cell \mathbf{B} . More than that, if $\varepsilon(\mathbf{r})$ has some symmetry inside the photonic crystal cell, then also $\omega(\mathbf{k})$ has symmetries inside \mathbf{B} and this property further reduces the range of \mathbf{k} for which ω have to be evaluated. In the particular cases of the crystals given as examples, in the following paragraph, it is sufficient to calculate the dispersion diagrams just for values of \mathbf{k} lying inside the triangular domain LXM (see Fig. 2), called irreducible Brillouin zone. More, numerical

calculations show that the worst scenario, with the smallest band gaps, happens for wavenumbers \mathbf{k} along the contour LXML, and for this reason, diagrams $\omega=\omega(\mathbf{k})$ will

not be represented for the entire surface of the triangle LXM but just for the contour LXML.

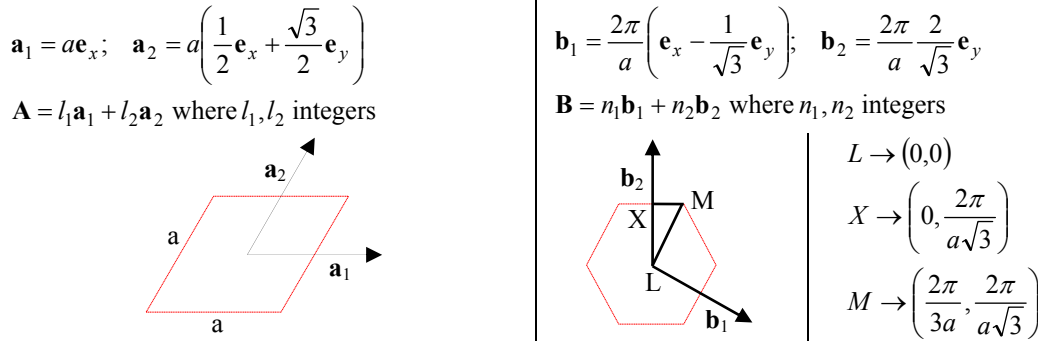


Fig. 2. The vectors that describe: normal space (left) and the dual space (right). LXML is the path along which the dispersion diagrams will be graphed.

5. Dispersion diagrams and band gaps. Numerical results.

Using (37) and (44) the dispersion diagrams for the TE and TM modes, corresponding to a few particular geometries of photonic crystals with hexagonal symmetry, will be calculated. A total of three configurations are studied. For each situation, the entry parameters are given in the description of the case, beneath the figure or diagram. The significations of these parameters are:

(a)

$$\epsilon_r(x, y) = \begin{cases} \epsilon_{ra} & \text{inside the specific geometric element (circle, triangle, hexagon)} \\ \epsilon_{rb} & \text{in the rest of the elementary cell (called background)} \end{cases}$$

- (b) f = the filling factor defined as the fraction between the surface of the geometric element and that of the entire cell.
- (c) f_{max} = maximum filling factor attainable. Also, for each case, some specific parameters as r (the radius of the circular element in Fig. 3) and d (the length of the triangle or hexagon edges, Fig. 6, Fig. 9) are given. Another important parameter is $N \times N = (2M+1) \times (2M+1)$ (see the

explanations for the equation (37)) that represents the number of discretisation elements in which the basic cell of the crystal is divided.

Regarding the diagrams in Fig. 4, Fig. 5, Fig. 7, Fig. 8, Fig. 10, Fig. 11 a few explanations have to be given: (1) A scaled frequency, $\omega a/2\pi c$, was represented on the y axis in order the dispersion diagrams could be read at any frequency and any elementary cell size. Thus, supposing that $\omega a/2\pi c=0.4$ (see one of the diagrams) which is equivalent to $fa/c=0.4$ ($\omega=2\pi f$) or $a/\lambda=0.4$, and knowing the crystal cell edge length, $a=0.6 \mu\text{m}$, then $\lambda=1.5 \mu\text{m}$ which corresponds to $f=66 \text{ THz}$. (2) Both transversal electric and magnetic diagrams have been represented on the same figure for each crystal. The curves with dotted line correspond to TM modes and the ones with solid line to TE modes. Also, for clarity, the TM and TE gaps have been marked using color bands and in the case of total forbidden frequency zones (for both modes) the gap was hatched with oblique lines. As can be seen from diagrams, various band structures are obtained when ϵ_{ra} , ϵ_{rb} and the geometrical figure shape, inside the crystal cell, are varied.

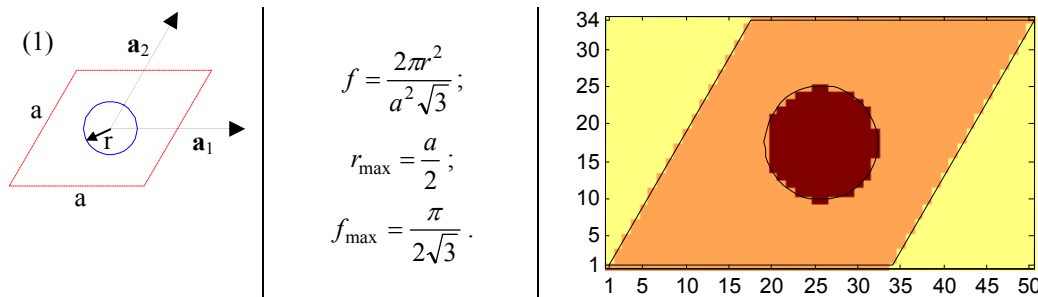


Fig. 3. Periodic element defined by: $r=0.2a$; $N \times N=33 \times 33$ (two cases of $(\epsilon_{ra}, \epsilon_{rb})$ are considered).

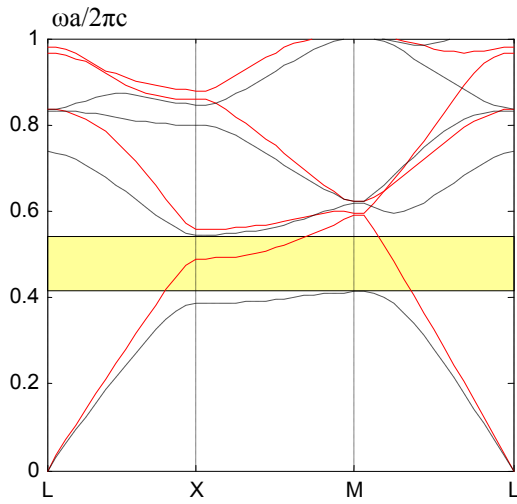


Fig. 4. $r=0.2a$; $\epsilon_{ra}=5$; $\epsilon_{rb}=1$; $N \times N=33 \times 33$.

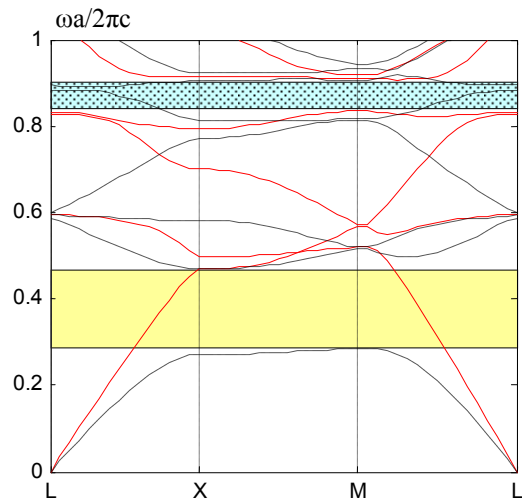


Fig. 5. $r=0.2a$; $\epsilon_{ra}=12$; $\epsilon_{rb}=1$; $N \times N=33 \times 33$.

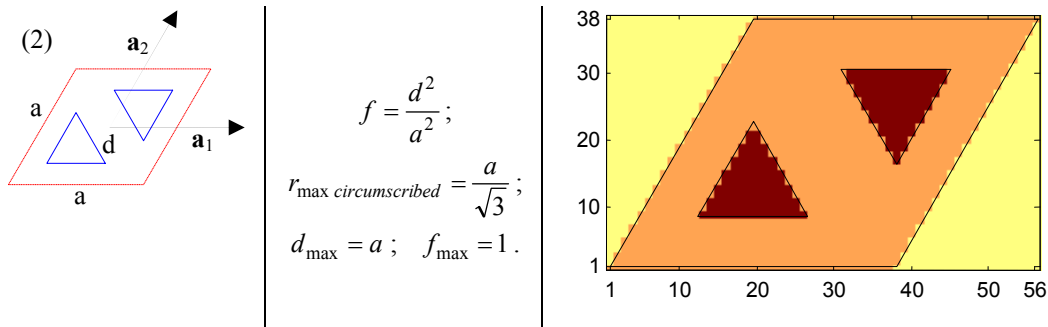


Fig. 6. Periodic element defined by: $r_{cc}=0.42a$; $N \times N=37 \times 37$ (two cases of $(\epsilon_{ra}, \epsilon_{rb})$ are considered).

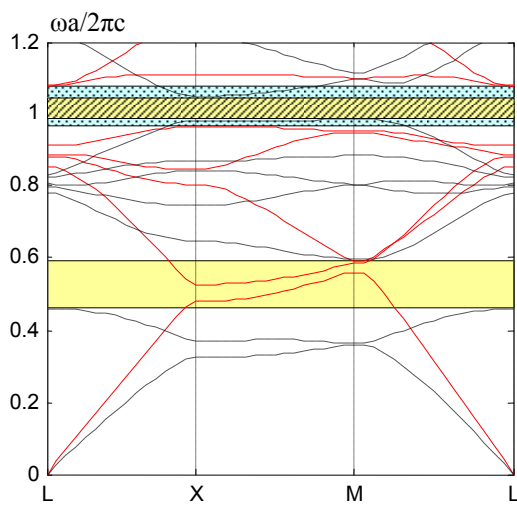


Fig. 7. $r_{cc}=0.22a$; $\epsilon_{ra}=12$; $\epsilon_{rb}=1$; $N \times N=37 \times 37$.

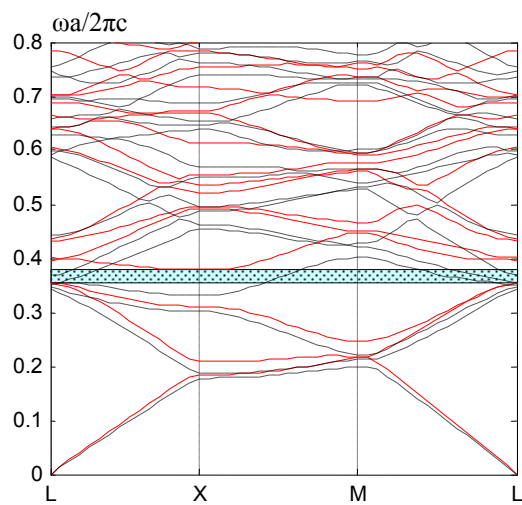


Fig. 8. $r_{cc}=0.22a$; $\epsilon_{ra}=1$; $\epsilon_{rb}=12$; $N \times N=37 \times 37$.

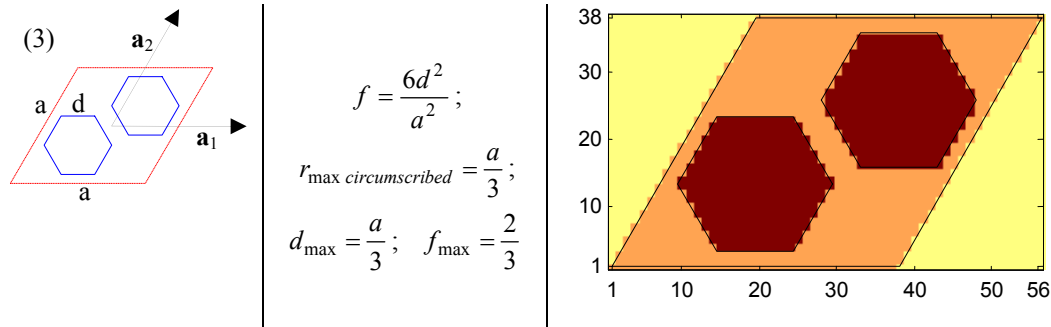


Fig. 9. Periodic element defined by: $r_{cc}=0.27a$; $N \times N=37 \times 37$ (two cases of $(\epsilon_{ra}, \epsilon_{rb})$ are considered).

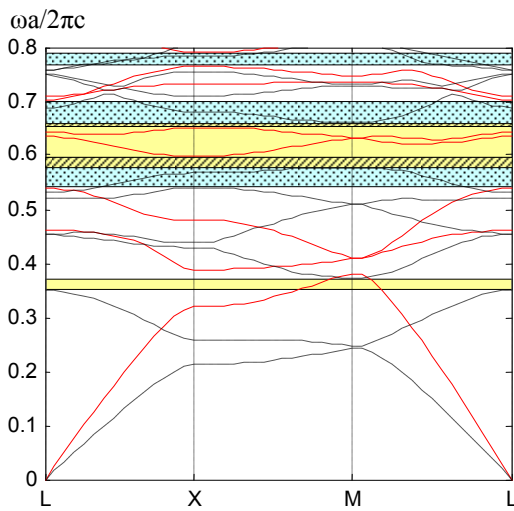


Fig. 10. $r_{cc}=0.27a$; $\epsilon_{ra}=12$; $\epsilon_{rb}=1$; $N \times N=37 \times 37$.

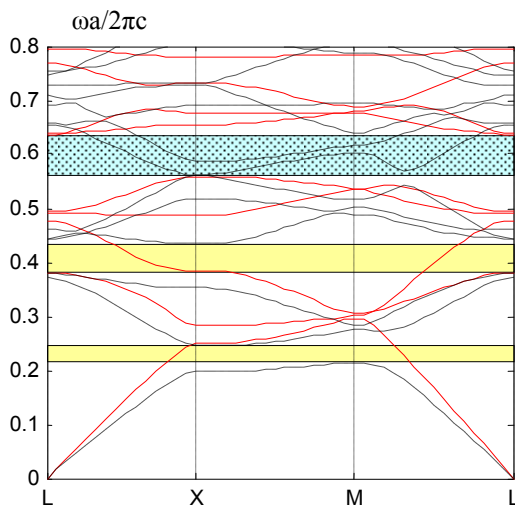


Fig. 11. $r_{cc}=0.27a$; $\epsilon_{ra}=1$; $\epsilon_{rb}=12$; $N \times N=37 \times 37$.

5. Conclusions

Systems (37) and (44) can be used for obtaining dispersion diagrams and implicitly band gaps for a variety of dielectric two-dimensional photonic crystals with hexagonal symmetry. Both systems are in a form that can be easily implemented in software, especially in Matlab

where, due to the richness of the already existing subroutines, just a few program loops need to be written for computing the coefficients in (37) and (44) with which a square matrix is generated and finally the eigenvalues of it are extracted using a general function already available in Matlab. Each set of ω eigenvalues corresponds to a wavenumber, $\mathbf{k}=\mathbf{k}_x\mathbf{e}_x+\mathbf{k}_y\mathbf{e}_y$, that can be chosen to vary along an arbitrary path or in a given domain. In practice, due to symmetry reasons, it is enough to take \mathbf{k} along LXML path (see Fig. 2).

As regarding the numerical examples, they are given just for demonstrative purposes, in order to show the correctness of the formula written in the current paper. For a thorough investigation, on how the size of certain band gaps are affected by the contrast between ϵ_{ra} , ϵ_{rb} and other parameters of the crystal cell, many diagrams have to be computed while a single entry value is varied in a certain range of interest.

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*Corresponding author: sterian@physics.pub.ro