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Band gaps in 2D photonic crystals with square symmetry

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The article presents, in detail, a mathematical method useful for calculating dispersion diagrams corresponding to Photonic Crystals with square 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 band gaps and as a result the electromagnetic field, with frequencies inside those gaps, can not propagate through it [1-4].

Therefore, photonic crystals can be defined as periodic media that have the property of forbidden frequency ranges, a radiation with the wavelength in their frequency gaps being unable to propagate inside them. The most usual and interesting type of photonic crystal, to date, is a dielectric material characterized by a cyclic electric permittivity that repents 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 position of photonic crystals band gaps, exists [5], [6]. Unfortunately, when it comes to establishing the dispersion diagrams of this type of periodic 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.

The purpose of the present paper is to start from electromagnetism 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 square symmetry. The case of 1D crystal [7] can easily be particularized from the square one.

2. Atemporal wave equation in square symmetry photonic crystals

In classical physics, the propagation of electromagnetic waves in substance is studied using Maxwell Equations. 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:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \tag{1}$$

$$\nabla \cdot \mathbf{B} = 0, \tag{2}$$

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

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

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 $\mathbf{r}=x\mathbf{e}_x+y\mathbf{e}_y+z\mathbf{e}_z$, where $\mathbf{e}_{x,z,y}$ are versors corresponding to 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 $\mathbf{B}$:

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

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,

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

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. Equations (1)-(4) can have an even simple form if none of the substances under consideration is magnetic,

$$\mu_r = 1, \tag{7}$$

and no density of electric charge or current exists,

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

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 $\mathbf{r}$:

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

Therefore, substituting relations (6)-(9) into Maxwell Equations (1)-(4) and solving the system, two propagation equations: (10) and (11) and two conditions: (12), (13) are obtained:

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

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

$$\nabla\cdot\mathbf{H} = 0, \tag{12}$$

$$\nabla\cdot\left[\varepsilon_r(\mathbf{r})\mathbf{E}\right] = 0, \tag{13}$$

Equations (10) and (11) can be solved using the method of separation of variables. Thus, making the supposition that:

$$(a)\ \mathbf{H}(\mathbf{r},t) = \mathbf{H}(\mathbf{r})H(t), \quad (b)\ \mathbf{E}(\mathbf{r},t) = \mathbf{E}(\mathbf{r})E(t), \tag{14}$$

where $\mathbf{H}(\mathbf{r})$, $H(t)$; $\mathbf{E}(\mathbf{r})$, $E(t)$ are unknown functions, (10) can be rewritten as:

$$-c^2\frac{\nabla\times\left(\frac{1}{\varepsilon_r(\mathbf{r})}\nabla\times\mathbf{H}(\mathbf{r})\right)}{\mathbf{H}(\mathbf{r})} = \frac{\frac{\partial^2 H(t)}{\partial t^2}}{H(t)} = \frac{H''(t_0)}{H(t_0)} \overset{not}{=} -\omega^2 \tag{15}$$

Also, if the constant ω is interpreted as a pulsation, the following notation can be made:

$$\omega = 2\pi f. \tag{16}$$

where f is a quantity interpreted as frequency.

In consequence, (10) transform in two equations, one in $\mathbf{r}$ and the other in t:

$$\nabla\times\left(\frac{1}{\varepsilon_r(\mathbf{r})}\nabla\times\mathbf{H}(\mathbf{r})\right) = \frac{\omega^2}{c^2}\mathbf{H}(\mathbf{r}), \tag{17}$$

$$\frac{\partial^2 H(t)}{\partial t^2} = -\omega^2 H(t). \tag{18}$$

Similar to the equation (17) corresponding to (10), the equation (11) has also an attemporal associate:

$$\frac{1}{\varepsilon_r(\mathbf{r})}\left(\nabla\times\left[\nabla\times\mathbf{E}(\mathbf{r})\right]\right) = \frac{\omega^2}{c^2}\mathbf{E}(\mathbf{r}), \tag{19}$$

The equations (17) and (19) are useful for calculating the dispersion diagrams of various photonic crystals and implicitly for establishing their structures of frequency gaps.

Both of them are 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 case where the medium, taken into consideration, is two-dimensional, a particular situation that splits in two branches (due to the condition which tells that $\mathbf{E}$ and $\mathbf{H}$ are always perpendicular to each other).

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

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

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:

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

where $g(x,y)$ is an unknown 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 imply that $1/\varepsilon_r(x,y)$ is also cyclic with the same period as $\varepsilon_r(x,y)$.

The second possibility is the *transverse magnetic* (**TM**) case, when $\mathbf{H}(\mathbf{r})=H_z\cdot\mathbf{e}_z$. This time, the equation (19) is used. First of all, the quantity $\nabla\times\left[(1/\varepsilon_r(\mathbf{r}))\nabla\times\mathbf{H}(\mathbf{r})\right]$ needs to be evaluated. Thus,

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

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

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

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

3. The Fourier Transform of electric permittivity in square symmetry photonic crystals

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 square symmetry the basic brick of the structure is a square, like in Fig. 1, and in consequence the periodicity of $\varepsilon_r(x,y)$ can be mathematically written as in (24).

The present paragraph gives a method for calculating 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*Fig. 1. Once this transform is found, it can be used for solving equation (24).

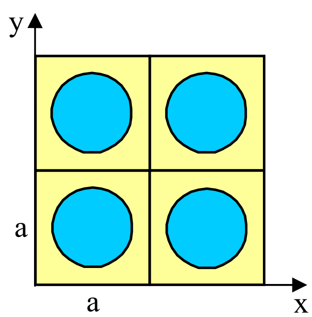


Fig. 1. Photonic crystal with square symmetry.

$$\varepsilon_r(x,y)=\varepsilon_r(x+a,y+a). \tag{24}$$

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

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

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

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

which is satisfied if:

$$e^{ja(k_x+k_y)}=1\Rightarrow(k_x+k_y)=2n\pi \quad \Rightarrow\left|\begin{array}{l} k_x=n_1\dfrac{2\pi}{a} \\ k_y=n_2\dfrac{2\pi}{a}\end{array}\right. n_1,n_2\in Z \tag{27}$$

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

$$\varepsilon_r(x,y)=\frac{1}{a^2}\sum_{n_1=-\infty}^{\infty}\sum_{n_2=-\infty}^{\infty}p\left(n_1\frac{2\pi}{a},n_2\frac{2\pi}{a}\right)e^{j\frac{2\pi}{a}(n_1x+n_2y)}. \tag{28}$$

If we multiplying both members with $e^{-j\frac{2\pi}{a}(m_1x+m_2y)}$ and integrate over one period (see Fig. 1), the expression (28) turns in:

$$\int_{x=0}^{a}\int_{y=0}^{a}\varepsilon_r(x,y)e^{-j\frac{2\pi}{a}(m_1x+m_2y)}dxdy=\frac{1}{a^2}\sum_{n_1=-\infty}^{\infty}\sum_{n_2=-\infty}^{\infty}p\left(n_1\frac{2\pi}{a},n_2\frac{2\pi}{a}\right)\underbrace{\int_{x=0}^{a}\int_{y=0}^{a}e^{j\frac{2\pi}{a}[(n_1-m_1)x+(n_2-m_2)y]}dxdy}_{I}, \tag{29}$$

where I is:

$$I=\frac{a^2}{4\pi^2}\frac{\left(1-e^{j\frac{2\pi}{a}x}\right)\left(1-e^{j\frac{2\pi}{a}y}\right)}{xy}= =\begin{cases}a^2 \text{ for } n_1=m_1,n_2=m_2\\ 0 \text{ for all other cases}\end{cases}. \tag{30}$$

In conclusion:

$$p\left(m_1\frac{2\pi}{a},m_2\frac{2\pi}{a}\right)= =\int_{x=0}^{a}\int_{y=0}^{a}\varepsilon_r(x,y)e^{-j\frac{2\pi}{a}(m_1x+m_2y)}dxdy\approx \approx\frac{1}{N^2}\sum_{q=0}^{N-1}\sum_{r=0}^{N-1}\varepsilon\left(\frac{a}{N}q,\frac{a}{N}r\right)e^{-j\frac{2\pi}{N}(m_1q+m_2r)}. \tag{31}$$

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

4. Method for calculating dispersion diagrams for TE and TM modes

TE modes: As $\varepsilon_r^{-1}(x,y)$ is a function with the same periodicity like $\varepsilon_r(x,y)$, it also can be written in a form similar to (28). Thus,

$$\varepsilon_r^{-1}(x,y)=\frac{1}{a^2}\sum_{n_1=-\infty}^{\infty}\sum_{n_2=-\infty}^{\infty}p_{n_1,n_2}e^{j\frac{2\pi}{a}[n_1x+n_2y]} \qquad (32)$$

Also, $E(x,y)=e^{j(k_xx+k_yy)}g(x,y)$ expands as follows:

$$E(x,y)=\frac{1}{a^2}\sum_{m_1=-\infty}^{\infty}\sum_{m_2=-\infty}^{\infty}h_{m_1,m_2}e^{j\left[(k_xx+k_yy)+\frac{2\pi}{a}(m_1x+m_2y)\right]}, \qquad (33)$$

where p_{n_1,n_2} and h_{m_1,m_2} are the coefficients of the two series. Thus, $\partial^2E(x,y)/\partial x^2+\partial^2E(x,y)/\partial y^2$ can be written as:

$$\frac{\partial^2E(x,y)}{\partial x^2}+\frac{\partial^2E(x,y)}{\partial y^2}=-\frac{1}{a^2}\sum_{m_1=-\infty}^{\infty}\sum_{m_2=-\infty}^{\infty}h_{m_1,m_2}\left[\underbrace{\left(k_x+\frac{2\pi}{a}m_1\right)^2}_{A^2}+\underbrace{\left(k_y+\frac{2\pi}{a}m_2\right)^2}_{B^2}\right]e^{j\left[(k_xx+k_yy)+\frac{2\pi}{a}(m_1x+m_2y)\right]} \qquad (34)$$

and so, (20) transforms into:

$$\sum_{n_1=-\infty}^{\infty}\sum_{n_2=-\infty}^{\infty}\sum_{m_1=-\infty}^{\infty}\sum_{m_2=-\infty}^{\infty}h_{m_1,m_2}p_{n_1,n_2}\left(A^2+B^2\right)e^{j\frac{2\pi}{a}[(m_1+n_1)x+(m_2+n_2)y]}=\frac{\omega^2}{c^2}\sum_{m_1=-\infty}^{\infty}\sum_{m_2=-\infty}^{\infty}h_{m_1,m_2}e^{j\frac{2\pi}{a}(m_1x+m_2y)}. \qquad (35)$$

Multiplying both members of (34) with $\left(1/a^2\right)e^{-j(2\pi/a)[m_1'x+m_2'y]}$ and integrating in respect to x and y over the interval [-*a/2*, *a/2*], the following equality is found:

$$\sum_{n_1=-\infty}^{\infty}\sum_{n_2=-\infty}^{\infty}\sum_{m_1=-\infty}^{\infty}\sum_{m_2=-\infty}^{\infty}h_{m_1,m_2}p_{n_1,n_2}\left(A^2+B^2\right)\underbrace{\frac{\sin[\pi(m_1+n_1-m_1')]}{\pi(m_1+n_1-m_1')}}_{\delta_{m_1+n_1,m_1'}}\underbrace{\frac{\sin[\pi(m_2+n_2-m_2')]}{\pi(m_2+n_2-m_2')}}_{\delta_{m_2+n_2,m_2'}}=\frac{\omega^2}{c^2}\sum_{m_1=-\infty}^{\infty}\sum_{m_2=-\infty}^{\infty}h_{m_1,m_2}\underbrace{\frac{\sin[\pi(m_1-m_1')]}{\pi(m_1-m_1')}}_{\delta_{m_1,m_1'}}\underbrace{\frac{\sin[\pi(m_2-m_2')]}{\pi(m_2-m_2')}}_{\delta_{m_2,m_2'}}. \qquad (36)$$

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

$$\sum_{m_1=-\infty}^{\infty}\sum_{m_2=-\infty}^{\infty}h_{m_1,m_2}p_{m_1'-m_1,m_2'-m_2}\left(A^2+B^2\right)=\frac{\omega^2}{c^2}h_{m_1',m_2'},$$

for **TE** modes (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*) x (*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:

$$p_{n_1,n_2}=\frac{1}{N^2}\sum_{q_1=0}^{4M}\sum_{q_2=0}^{4M}\varepsilon_r^{-1}\left(\frac{a}{N}q_1,\frac{a}{N}q_2\right)e^{-j\frac{2\pi}{N}[n_1q_1+n_2q_2]}, \qquad (38)$$

where the following notations have been made: $N=4M+1$, $n_1=m_1'-m_1$, $n_2=m_2'-m_2$.

In conclusion (39) with $m_1,m_1',m_2,m_2' \in$ [*-M, M*] is a system of the form:

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

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

$$p_{m_1'-m_1,m_2'-m_2}\left(A^2+B^2\right), \qquad (40)$$

which can be calculated for any given $m_1,m_1',m_2,m_2',k_x,k_y$ and **h** is a column matrix possessing (*2M+1*) x (*2M+1*) elements, h_{m_1,m_2}, of unknown values. It can be noticed that (39) is satisfied, independently of **h,** if $\det\left(\mathbf{S}-\omega^2/c^2\right)=0$ which leads to $(2M+1)^2$ 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 remarked, 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 procedure as in the case of **TE** modes, the following expressions can be successively written:

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

$$\begin{aligned}&\frac{\partial}{\partial x}\left(\frac{1}{\varepsilon_r(x,y)}\right)\frac{\partial H(x,y)}{\partial x}+\frac{\partial}{\partial y}\left(\frac{1}{\varepsilon_r(x,y)}\right)\frac{\partial H(x,y)}{\partial y}=\frac{1}{a^2}\sum_{n_1=-\infty}^{\infty}\sum_{n_2=-\infty}^{\infty}p_{n_1,n_2}\left(j\frac{2\pi}{a}n_1\right)e^{j\frac{2\pi}{a}(n_1x+n_2y)}\cdot\sum_{m_1=-\infty}^{\infty}\sum_{m_2=-\infty}^{\infty}h_{m_1,m_2}[jA]e^{j\left[\mathbf{k}\cdot\mathbf{r}+\frac{2\pi}{a}(m_1x+m_2y)\right]}+\\&+\frac{1}{a^2}\sum_{n_1=-\infty}^{\infty}\sum_{n_2=-\infty}^{\infty}p_{n_1,n_2}\left(j\frac{2\pi}{a}n_2\right)e^{j\frac{2\pi}{a}(n_1x+n_2y)}\cdot\sum_{m_1=-\infty}^{\infty}\sum_{m_2=-\infty}^{\infty}h_{m_1,m_2}[jB]e^{j\left[\mathbf{k}\cdot\mathbf{r}+\frac{2\pi}{a}(m_1x+m_2y)\right]}=\\&=-\sum_{n_1=-\infty}^{\infty}\sum_{n_2=-\infty}^{\infty}\sum_{m_1=-\infty}^{\infty}\sum_{m_2=-\infty}^{\infty}h_{m_1,m_2}p_{n_1,n_2}\frac{2\pi}{a}[n_1A+n_2B]e^{j\left[\mathbf{k}\cdot\mathbf{r}+\frac{2\pi}{a}[(m_1+n_1)x+(m_2+n_2)y]\right]}.\end{aligned} \tag{42}$$

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)(23). After simplifying by $e^{j\mathbf{k}\cdot\mathbf{r}}$, multiplying by $\left(1/a^2\right)e^{-j(2\pi/a)[m_1'x+m_2'y]}$ and integrating in respect to x and y over the interval [*-a/2*, *a/2*], the following equality results:

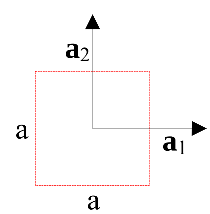
$$\sum_{n_1=-\infty}^{\infty}\sum_{n_2=-\infty}^{\infty}\sum_{m_1=-\infty}^{\infty}\sum_{m_2=-\infty}^{\infty}h_{m_1,m_2}p_{n_1,n_2}\left[\frac{2\pi}{a}n_1A+\frac{2\pi}{a}n_2B+A^2+B^2\right]\cdot\underbrace{\frac{\sin[\pi(m_1+n_1-m_1')]}{\pi(m_1+n_1-m_1')}}_{\delta_{m_1+n_1,m_1'}}\underbrace{\frac{\sin[\pi(m_2+n_2-m_2')]}{\pi(m_2+n_2-m_2')}}_{\delta_{m_2+n_2,m_2'}}=\frac{\omega^2}{c^2}\sum_{m_1=-\infty}^{\infty}\sum_{m_2=-\infty}^{\infty}h_{m_1,m_2}\underbrace{\frac{\sin[\pi(m_1-m_1')]}{\pi(m_1-m_1')}}_{\delta_{m_1,m_1'}}\underbrace{\frac{\sin[\pi(m_2-m_2')]}{\pi(m_2-m_2')}}_{\delta_{m_2,m_2'}} \tag{43}$$

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

$$\sum_{m_1=-\infty}^{\infty}\sum_{m_2=-\infty}^{\infty}h_{m_1,m_2}p_{m_1'-m_1,m_2'-m_2}\cdot\left[\frac{2\pi}{a}(m_1'-m_1)A+\frac{2\pi}{a}(m_2'-m_2)B+A^2+B^2\right]=\frac{\omega^2}{c^2}h_{m_1',m_2'}\quad \text{for } \mathbf{TM} \text{ modes} \tag{44}$$

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

As already explained, by solving (37) and (44) dispersion diagrams, $\omega=\omega(k_x, k_y)$, are obtained. It can be shown that, for photonic crystals with square 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. 3), exists in the spatial frequencies domain (dual space, **D**). Therefore, the periodicity $\varepsilon(\mathbf{r})=\varepsilon(\mathbf{r}+\mathbf{R})$ has a pair in the dual domain, $\omega(\mathbf{k})=\omega(\mathbf{k}+\mathbf{D})$, and in consequence it is enough to compute ω for $\mathbf{k}$ inside just one elementary cell **D**. More than that, if $\varepsilon(\mathbf{r})$ has some symmetry inside the photonic crystal cell, then also $\omega(\mathbf{k})$ has symmetries inside **D** 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. 3), 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.

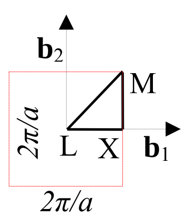


$\mathbf{a}_1=a\mathbf{e}_x;\quad \mathbf{a}_2=a\mathbf{e}_y$

$\mathbf{R}=l_1\mathbf{a}_1+l_2\mathbf{a}_2$

where l_1, l_2 integers

Fig. 2. The vectors that describe normal space, **R**.



$\mathbf{b}_1=(2\pi/a)\mathbf{e}_x;\quad \mathbf{b}_2=(2\pi/a)\mathbf{e}_y$

$\mathbf{D}=n_1\mathbf{b}_1+n_2\mathbf{b}_2$

where n_1, n_2 integers

$L\to(0,0),\ X\to(0,\pi/a)$

$M\to(\pi/a,\pi/a)$

Fig. 3. The vectors that describe the dual space, **D**. *LXML is the path alongh 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 square symmetry, will be calculated. Two configurations are studied. For each situation, the entry parameters are given in the description of the case, beneath the figure or diagram. The signification of these parameters is:

$$\text{(a) } \varepsilon_r(x,y) = \begin{cases} \varepsilon_{ra} \text{ inside the specific geometric element (circle, square)} \\ \varepsilon_{rb} \text{ in the rest of the elementary cell (called backroung)} \end{cases},$$

(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. 4) and d (the length of the square edges, Fig. 9) are given. Another important parameter is N x N = ($2M+1$) x ($2M+1$) (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. 5, Fig. 8, Fig. 10, Fig. 13 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, $a=0.6\ \mu m$, then $\lambda=1.5\ \mu m$ which corresponds to f=66 THz. (2) Both transverse 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 geometry of the dielectric atoms (circular, square shape) are varied.

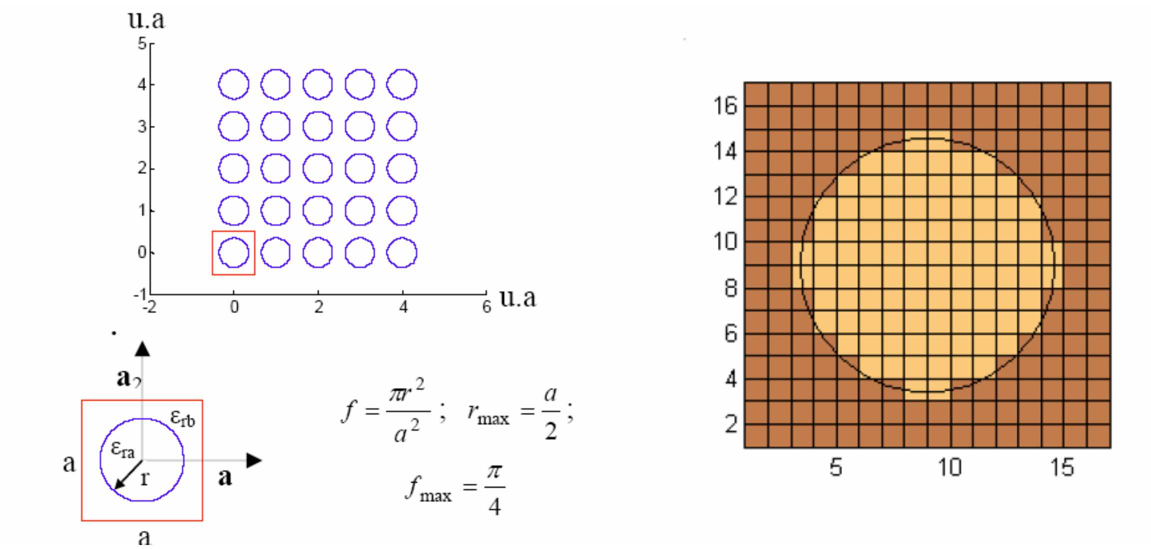


Fig. 4. Square symmetry photonic crystal with circular elements.

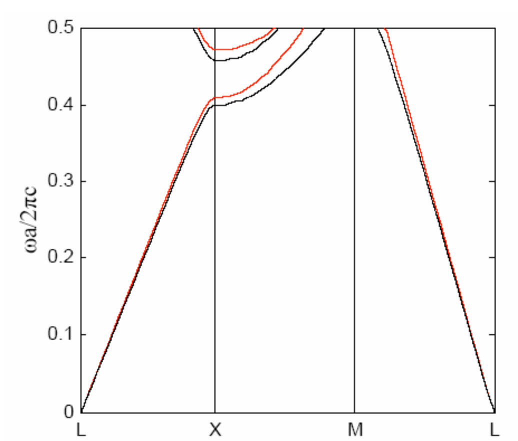


Fig. 5. $r=0.45a$; $\varepsilon_{ra}=1$; $\varepsilon_{rb}=2$; $N\times N=17\times 17$.

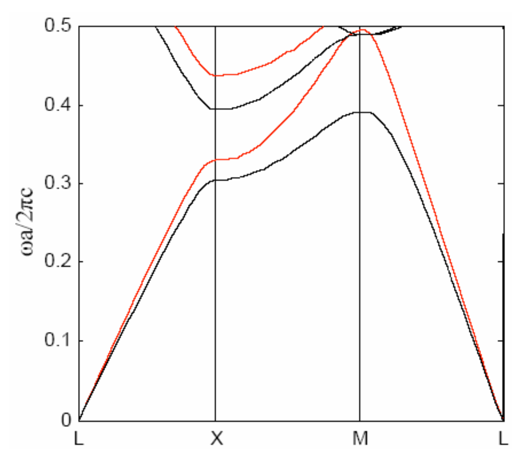


Fig. 6. $r=0.45a$; $\varepsilon_{ra}=1$; $\varepsilon_{rb}=4$; $N\times N=17\times 17$.

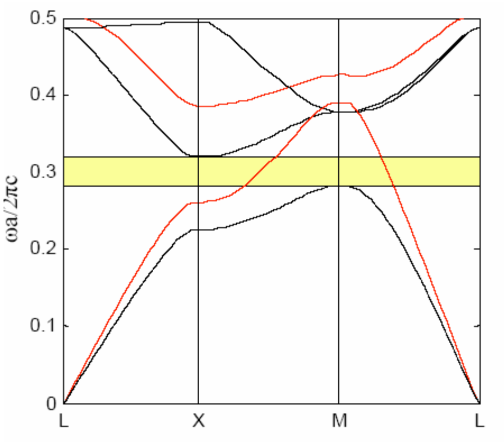


Fig. 7. r=0.45a; ε_{ra}=1; ε_{rb}=8; N×N=17×17.

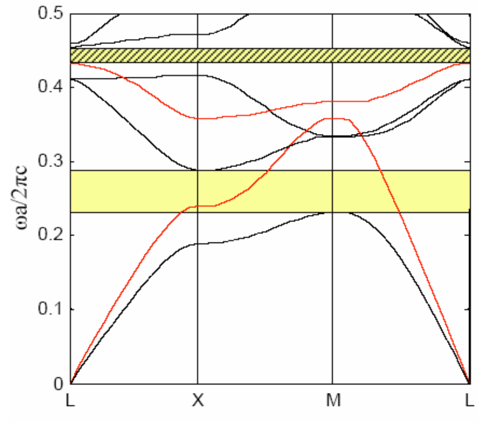


Fig. 8. r=0.47a; ε_{ra}=1; ε_{rb}=13; N×N=33×33

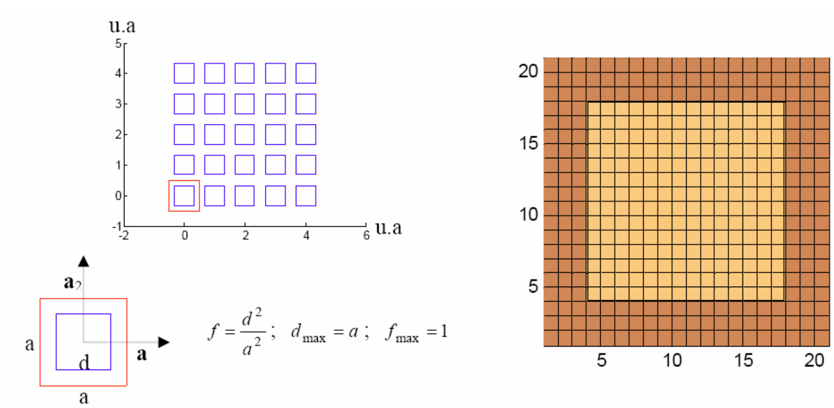


Fig. 9. Square symmetry photonic crystal with square elements.

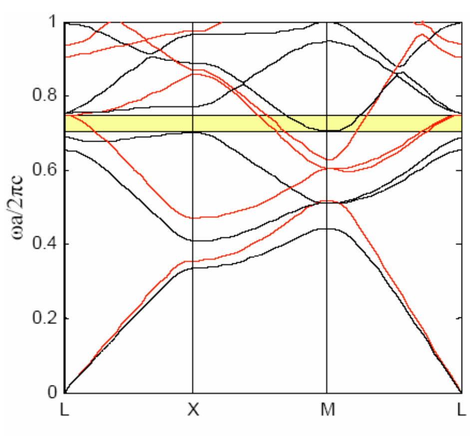


Fig. 10. d=0.85a; ε_{ra}=1; ε_{rb}=5; N×N=26×26.

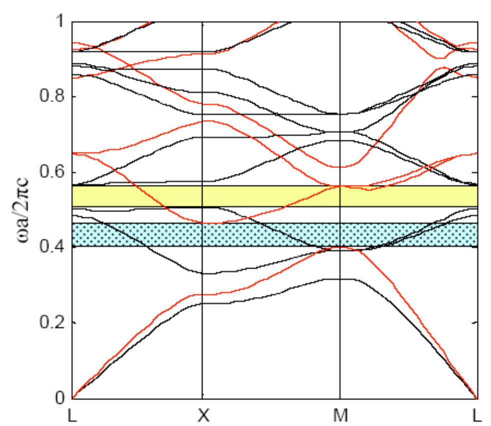


Fig. 11. d=0.85a; ε_{ra}=1; ε_{rb}=13; N×N=26×26.

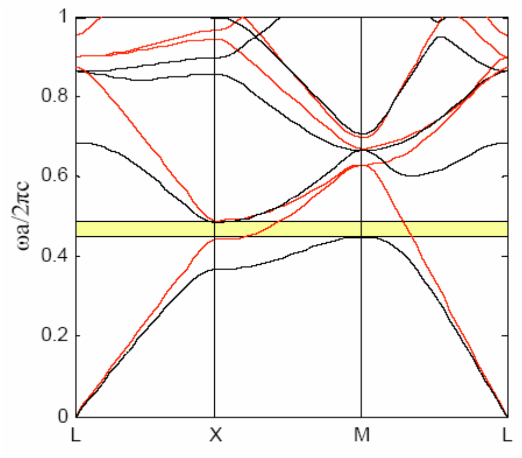


Fig. 12. d=0.35a; ε_{ra}=5; ε_{rb}=1; N×N=26×26.

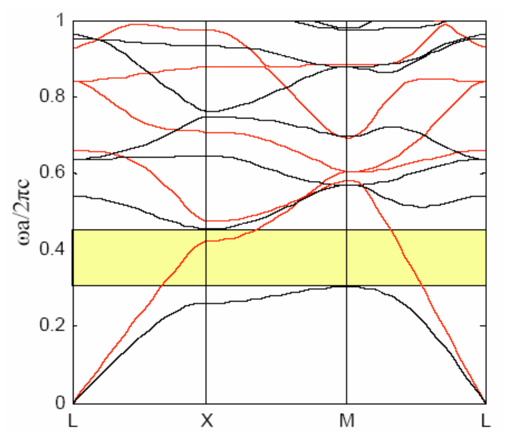


Fig. 13. d=0.35a; ε_{ra}=13; ε_{rb}=1; N×N=26×26

6. 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 square 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 (44) 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, $\mathbf{k}=k_x\mathbf{e_x}+k_y\mathbf{e_y}$, 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 **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 parameter is varied in a certain range of interest.

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