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A Systematic Approach to Photonic Crystal Based Metamaterial Design

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ABSTRACT— **Photonic crystal design procedure for negative refraction has so far been based on trial and error. In this paper, for the first time, a novel and systematic design procedure based on physical and mathematical properties of photonic crystals is proposed to design crystal equi-frequency contours (EFCs) to produce negative refraction. The EFC design is performed by the help of rectangular stair-case (RSC) photonic crystals. The RSC crystal is then converted to more common structures like pillar crystals by matching Fourier coefficients of periodic electric permittivity. Methods to design common crystals which have approximately equal Fourier components to the RSC crystal are also discussed. The proposed procedure can be used to design metamaterials without the difficulties of large trial and error. The devised procedure can also be applied in designing other structures involving photonic crystals.**

KEYWORDS: Negative Refraction; Photonic Crystals; Metamaterials.

I. INTRODUCTION

Optical metamaterials are materials which exhibit negative index of refraction. Metamaterials can have unprecedented electromagnetic properties and therefore can produce unique functionality which naturally occurring materials are not able to produce.

The idea of materials with negative optical refraction and their properties was considered long time ago. The possibility of negative refraction and optical properties of metamaterials were first studied by L.I. Mandel'stam [1], D.V. Sivukhin [2], and V.G. Veselago [3]. Years later John Pendry made some predictions about the potential applications of optical metamaterials the most important of which is superlens with resolution beyond the diffraction limit [4].

No naturally existing metamaterial has yet been discovered. Therefore, in order to obtain negative refraction, we should design and fabricate artificial materials in a way that they show $n_{\mathrm{eff}}<0$. For this purpose, deep understanding of optical mechanisms leading to negative refraction is required. This goal was first achieved in microwave regime thanks to the contributions made by Smith *et al.* [5-7]. The key idea used in these structures has also been adopted with smaller dimensions in order to extend the negative refraction to optical frequencies by employing advanced nanofabrication techniques [8-10].

There are several approaches to obtain negative refraction such as photonic crystals [11-18] and transmission lines [19-20]. In photonic crystals, certain conditions for equi-frequency contours (EFCs) guarantee negative refraction [12]. Design of optical metamaterials based on photonic crystals has so far been based on trial and error. In this paper, we report a systematic design process to achieve negative refraction in photonic crystals. The novel design process described in this paper uses rectangular stair-case (RSC) photonic crystals because analytical relations exist between crystal parameters and their propagation frequency. The RSC is then transformed by the help of mathematical tools to conventional crystals that are easier to fabricate.

The paper is organized as follows: in Section 2, theory of light refraction in photonic crystals is explained. In Section 3, our systematic design process is described. Methods to convert the designed crystal into more common crystals which are easier to fabricate are discussed in Section 4, and Section 5 concludes the paper.

II. THEORY

Photonic crystals can be designed to exhibit negative refraction, i.e. in photonic crystals, light can propagate in such a way as if the medium has negative refractive index. Therefore, in order to investigate negative refraction in photonic crystals, we should be able to predict light trajectory inside crystal when there is an incident light from a different medium with a known angle. For ordinary homogeneous and isotropic media, the problem has been solved long time ago by Snell's rule. But photonic crystals have periodic modulation of electric permittivity and therefore don't follow Snell's rule.

Bloch-Floquet theory is the key theory for light propagation inside photonic crystals, but it only determines the allowed propagation frequencies and not the light trajectory. Therefore it is not adequate for our purpose. Several theories were presented by different groups in order to predict light path in photonic crystals but all of them proved to be insufficient [21-27]. Notomi eventually proposed a theory which clarified the subject and was also in good agreement with experiments [12].

As is reported in [12], the light trajectory in photonic crystals is determined by the use of equi-frequency contours (EFCs). EFC is the locus of all of the wave vectors in reciprocal lattice which have a certain frequency of propagation as their eigen-value.

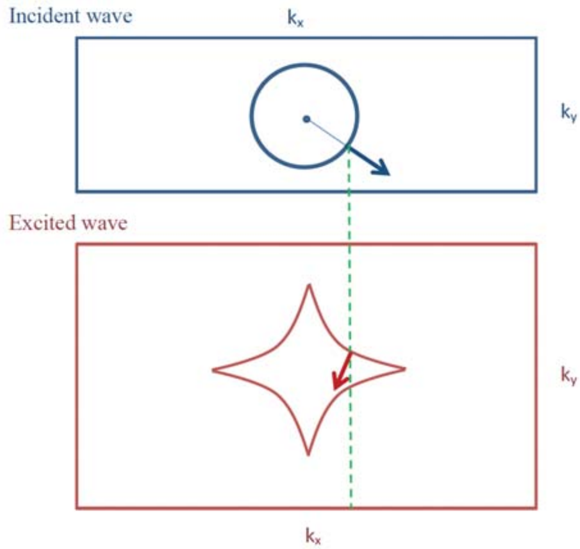

Fig. 1: Equi-frequency contours of an isotropic and homogeneous medium (top) and schematic EFC of a 2D photonic crystal (bottom). The *k* vector in the crystal is determined by the continuity of the tangential components across the boundary. The light propagation direction inside the photonic crystal is oriented to the gradient of the EFC.

In order to predict the propagation angle of the excited wave in photonic crystal, we draw the EFC of the medium from which light is incident, on top of the EFC of photonic crystal. Figure 1 shows EFC of an isotropic and homogeneous medium (top) and schematic EFC of a 2D photonic crystal (bottom). The EFC of the first medium is circular because for a homogeneous and isotropic medium we have:

$$\omega = ck/n = c\sqrt{k_x^2 + k_y^2}\Big/n \qquad (1)$$

where ω and c are frequency and speed of light, respectively; k is wavenumber and n is the refractive index of medium. This equation shows that for a homogeneous and isotropic medium, the points in k_x-k_y space that correspond to a certain frequency form a circle.

As we see in the figure, a vertical line is drawn from the k_x point of the incident wave to determine the value of k_x in photonic crystal. This is because the tangential components of the electric field are the same in the two media in order to meet electromagnetic boundary conditions. The intersection of the vertical line with the EFC of photonic crystal, determines the Bloch wave number of the excited wave in photonic crystal.

Note that, the propagation direction of the excited wave in photonic crystal is in the direction of the group velocity vector which is the gradient of angular frequency with respect to wave vector v=grad$_\kappa\omega$. As we know, the gradient of angular frequency with respect to wave vector is perpendicular to EFC, because EFC is a contour formed by wave vectors which belong to a certain frequency. Therefore, light propagation direction in photonic crystals is perpendicular to EFC at the Bloch wavenumber.

The perpendicular line to the EFC can be drawn inward or outward. The true direction is obviously the direction of the gradient. Therefore, if the EFCs are growing by increasing frequency, the perpendicular line should be outward, and if the contours are getting smaller by increasing frequency, the line should be drawn inward.

A. *Negative Refraction Necessities*

As is now clear from Fig. 1, if the EFC of the photonic crystal has inward gradient, the incident light will propagate in a way as if the crystal is showing negative refractive index. Therefore, in order to have a photonic crystal with negative refraction, we should design a crystal whose EFCs at the range of interest show inward gradient. Moreover, circular EFCs make photonic crystals mimic homogeneous behavior at the wavelength range of interest.

III. DESIGN

The design procedure of photonic crystals for negative refraction has so far been based on trial and error. This means that crystal parameters are randomly selected and large numbers of simulations are done in order to reach the desired shape of EFCs for negative refraction in a crystal. In this section we report a systematic design procedure.

The key idea towards EFC design is to use a specific kind of crystal that somehow eases the design procedure. It is known from transfer matrix method (TMM) that stair-case profiles can lead to closed form relations between frequency and crystal parameters [28]. Therefore, we consider a two- dimensional rectangular stair case (RSC) crystal whose permittivity function is defined as [28]:

$$\varepsilon(x) = A(x) + B(y) \tag{2}$$

in which A and B are stair-case profiles:

$$A(x) = \varepsilon_a + \left[u(x+t/2) - u(x-t/2)\right](\varepsilon_b - \varepsilon_a)$$

$$|x| \le X/2 \qquad A(x) = A(x+mX) \tag{3-a}$$

and

$$B(y) = \varepsilon_c + \left[u(y+s/2) - u(y-s/2)\right](\varepsilon_d - \varepsilon_c)$$

$$|y| \le Y/2 \qquad B(y) = B(y+nY) \tag{3-b}$$

u is the unit step function and X and Y are the periods of the functions along x and y directions. m and n are integers and t and s are positive constants for which we have: $t<X$ and $s<Y$. Schematic of such a crystal is shown in Fig. 2.

Two dimensional wave equation for TE waves is expressed by:

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)E(x,y) + \frac{\omega^2}{c^2}\varepsilon(x,y)E(x,y) = 0 \tag{4}$$

where $E(x,y)$ is the electric field amplitude and ω and c are frequency and speed of light, respectively.

Using the permittivity function of Eq. (2) and assuming $E(x,y) = \Lambda(x)\Psi(y)$ we reach [28]:

$$\frac{\partial^2}{\partial x^2}\Lambda(x) + \frac{\omega^2}{c^2}\left[A(x) + \beta\right]\Lambda(x) = 0 \tag{5-a}$$

$$\frac{\partial^2}{\partial y^2}\Psi(y)+\frac{\omega^2}{c^2}\left[B(y)-\beta\right]\Psi(y)=0 \qquad \text{(5-b)}$$

where β is a separation constant. $A(x)+\beta$ and $B(y)-\beta$ are periodic functions by periods of X and Y. Therefore, equations 5-a and 5-b have Bloch solutions of the form $\Lambda_\kappa(x)=\lambda_\kappa(x)\exp(-j\kappa x)$ and $\Psi_\eta(y)=\psi_\eta(y)\exp(-j\eta y)$, where κ and η are Bloch wave numbers. Doing lengthy arithmetic we obtain [28]:

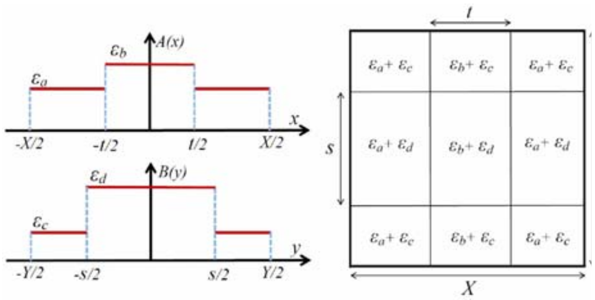

Fig. 2: Unit cell of the rectangular stair-case profile used in the design

$$\cos(\kappa X)=\frac{q_{11}}{2}\exp\left\{-j\omega\frac{X}{c}\left[A\left(-\frac{X}{2}\right)+\beta\right]^{1/2}\right\}+$$
$$\frac{q_{22}}{2}\exp\left\{-j\omega\frac{X}{c}\left[A\left(-\frac{X}{2}\right)+\beta\right]^{1/2}\right\} \qquad \text{(6-a)}$$

$$\cos(\eta Y)=\frac{p_{11}}{2}\exp\left\{-j\omega\frac{Y}{c}\left[B\left(-\frac{Y}{2}\right)-\beta\right]^{1/2}\right\}+$$
$$\frac{p_{22}}{2}\exp\left\{+j\omega\frac{Y}{c}\left[B\left(-\frac{Y}{2}\right)-\beta\right]^{1/2}\right\} \qquad \text{(6-b)}$$

q_{ii} and p_{ii} are the diagonal elements of transfer matrix in x and y directions which are related to the electrical permittivity function. Inserting the relations for diagonal elements of transfer matrix into Eq. (6-a) and Eq. (6-b) we have:

$$\cos(\kappa X)=\cos\left(\frac{\omega}{c}\sqrt{\varepsilon_b+\beta}t\right)\cos\left[\frac{\omega}{c}\sqrt{\varepsilon_a+\beta}(X-t)\right]-$$
$$\frac{\varepsilon_a+\varepsilon_b+2\beta}{2\sqrt{\varepsilon_a+\beta}\sqrt{\varepsilon_b+\beta}}\sin\left(\frac{\omega}{c}\sqrt{\varepsilon_b+\beta}t\right)\sin\left[\frac{\omega}{c}\sqrt{\varepsilon_a+\beta}(X-t)\right]$$

(7-a)

$$\cos(\eta Y)=\cos\left(\frac{\omega}{c}\sqrt{\varepsilon_d+\beta}s\right)\cos\left[\frac{\omega}{c}\sqrt{\varepsilon_c+\beta}(Y-s)\right]-$$
$$\frac{\varepsilon_c+\varepsilon_d+2\beta}{2\sqrt{\varepsilon_c+\beta}\sqrt{\varepsilon_d+\beta}}\sin\left(\frac{\omega}{c}\sqrt{\varepsilon_d+\beta}s\right)\sin\left[\frac{\omega}{c}\sqrt{\varepsilon_c+\beta}(Y-s)\right]$$

(7-b)

Crystal design can be done by calculation of degrees of freedom in these equations: ε_a, ε_b, ε_c, ε_d, t, s, X and Y. We can set X and Y to unity for the sake of normalization. Therefore, we have 6 degrees of freedom which can be used in design procedure. Thus, we can write a set of 6 simultaneous nonlinear equations to solve for the six unknown variables:

1:

$$\cos(\kappa_1 X)=\cos\left(\frac{\omega}{c}\sqrt{\varepsilon_b+\beta}t\right)\cos\left[\frac{\omega}{c}\sqrt{\varepsilon_a+\beta}(X-t)\right]-$$
$$\frac{\varepsilon_a+\varepsilon_b+2\beta}{2\sqrt{\varepsilon_a+\beta}\sqrt{\varepsilon_b+\beta}}\sin\left(\frac{\omega}{c}\sqrt{\varepsilon_b+\beta}t\right)\sin\left[\frac{\omega}{c}\sqrt{\varepsilon_a+\beta}(X-t)\right]$$

2:

$$\cos(\eta_1 Y)=\cos\left(\frac{\omega}{c}\sqrt{\varepsilon_d+\beta}s\right)\cos\left[\frac{\omega}{c}\sqrt{\varepsilon_c+\beta}(Y-s)\right]-$$
$$\frac{\varepsilon_c+\varepsilon_d+2\beta}{2\sqrt{\varepsilon_c+\beta}\sqrt{\varepsilon_d+\beta}}\sin\left(\frac{\omega}{c}\sqrt{\varepsilon_d+\beta}s\right)\sin\left[\frac{\omega}{c}\sqrt{\varepsilon_c+\beta}(Y-s)\right]$$

3:

$$\cos(\kappa_2 X)=\cos\left(\frac{\omega}{c}\sqrt{\varepsilon_b+\beta}t\right)\cos\left[\frac{\omega}{c}\sqrt{\varepsilon_a+\beta}(X-t)\right]-$$
$$\frac{\varepsilon_a+\varepsilon_b+2\beta}{2\sqrt{\varepsilon_a+\beta}\sqrt{\varepsilon_b+\beta}}\sin\left(\frac{\omega}{c}\sqrt{\varepsilon_b+\beta}t\right)\sin\left[\frac{\omega}{c}\sqrt{\varepsilon_a+\beta}(X-t)\right]$$

4:

$$\cos(\eta_2 Y)=\cos\left(\frac{\omega}{c}\sqrt{\varepsilon_d+\beta}s\right)\cos\left[\frac{\omega}{c}\sqrt{\varepsilon_c+\beta}(Y-s)\right]-$$
$$\frac{\varepsilon_c+\varepsilon_d+2\beta}{2\sqrt{\varepsilon_c+\beta}\sqrt{\varepsilon_d+\beta}}\sin\left(\frac{\omega}{c}\sqrt{\varepsilon_d+\beta}s\right)\sin\left[\frac{\omega}{c}\sqrt{\varepsilon_c+\beta}(Y-s)\right]$$

5:

$$\cos(\kappa_3 X)=\cos\left(\frac{\omega}{c}\sqrt{\varepsilon_b+\beta}t\right)\cos\left[\frac{\omega}{c}\sqrt{\varepsilon_a+\beta}(X-t)\right]-$$
$$\frac{\varepsilon_a+\varepsilon_b+2\beta}{2\sqrt{\varepsilon_a+\beta}\sqrt{\varepsilon_b+\beta}}\sin\left(\frac{\omega}{c}\sqrt{\varepsilon_b+\beta}t\right)\sin\left[\frac{\omega}{c}\sqrt{\varepsilon_a+\beta}(X-t)\right]$$

6:

$$\cos(\eta_3 Y)=\cos\left(\frac{\omega}{c}\sqrt{\varepsilon_d+\beta s}\right)\cos\left[\frac{\omega}{c}\sqrt{\varepsilon_c+\beta}(Y-s)\right]-\frac{\varepsilon_c+\varepsilon_d+2\beta}{2\sqrt{\varepsilon_c+\beta}\sqrt{\varepsilon_d+\beta}}\sin\left(\frac{\omega}{c}\sqrt{\varepsilon_d+\beta s}\right)\sin\left[\frac{\omega}{c}\sqrt{\varepsilon_c+\beta}(Y-s)\right] \quad (8)$$

(κ_i,η_i) , i=1,2,3 are points in reciprocal lattice that we want to include them in the EFC. By proper selection of these points, we can shape the EFC for our desired purpose. The set of equations in (8) can then be solved using Trust-Region-Dogleg method [29].

When the EFC points are chosen, we should note that all the symmetries existing in the crystal unit cell are transferred to the reciprocal lattice. Therefore, EFCs have all the symmetries existing in crystal unit cell [30]. As seen in Fig. 2, due to symmetries of unit cell, RSC profile can be built by only a quarter of the cell. Thus, for designing a circular EFC, it is adequate to design a 90° arc.

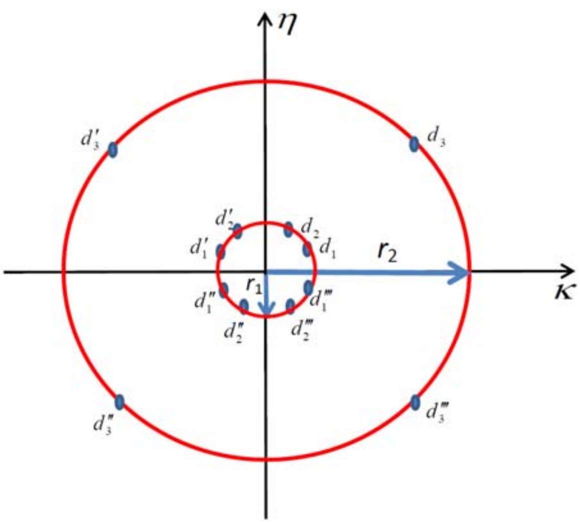

Fig. 3: Points used in equi-frequency contour design

In order to design a crystal with negative refraction, we choose the points $d_1(\kappa_1,\eta_1)$ and $d_2(\kappa_2,\eta_2)$ located on a circle with radius r_1 with angles 30° and 60°, as shown in Fig. 3:

$$\kappa_1=r_1\cos(\pi/6)=\sqrt{3}r_1/2$$
$$\eta_1=r_1\sin(\pi)=r_1/2$$
$$\kappa_2=r_1\cos(\pi/3)=r_1/2$$
$$\eta_2=r_1\sin(\pi/3)=\sqrt{3}r_1/2 \quad \text{(9-a)}$$

Due to symmetries, there are three replicas of d_1 at 150° and 210° and 330° defined by d_1', d_1'' and d_1'''. Similarly $d_2(\kappa_2,\eta_2)$ has its replicas at 120° and 240° and 300° to form d_2', d_2'' and d_2'''. These eight points make a circle with radius of r_1. We arbitrarily choose r_1=0.1 and the corresponding normalized frequency to be ω_1=0.5. In the next step, we locate $d_3(\kappa_3,\eta_3)$ in a way to force EFCs with greater frequencies to have smaller sizes. As shown in the figure, we locate $d_3(\kappa_3,\eta_3)$ on a circle with radius r_2 with the angle 45°:

$$\kappa_3=r_2\cos(\pi/4)=0.7r_2$$

$$\eta_3=r_2\sin(\pi/4)=0.7r_2 \quad \text{(9-b)}$$

We also arbitrarily choose r_2=0.2 and its corresponding normalized frequency at ω_2=0.49 in order to make the EFCs have inward gradient, which is the basic requirement to have negative refraction.

By inserting the values listed in Eq. (9-a) and (9-b) in the set of equations in Eq. (8) and solving for the unknowns by 1% accuracy we obtain:

$$\begin{array}{lll} \varepsilon_a=0.70 & \varepsilon_b=6.99 & t=0.64 \\ \varepsilon_c=0.73 & \varepsilon_d=6.81 & s=0.57 \end{array} \quad (10)$$

These parameters are expected to yield nearly circular EFC with inward gradient and therefore exhibit negative refraction.

IV. Verification of Results

In order to verify the design, we should be able to draw equi-frequency contours (EFCs) of the crystal. This can be done by the help of plane wave expansion method (PWEM) [31]. Defining $\eta(r)=\dfrac{1}{\varepsilon(r)}$ and writing electric field as a Bloch wave like $E(r)=\Phi_\kappa(r)e^{-j\kappa.r}$ in Eq. (4) we reach:

$$\eta(r)\left[\nabla - j\kappa\right]^2 \Phi_\kappa(r) + \frac{\omega^2}{c^2}\Phi_\kappa(r) = 0 \tag{11}$$

Knowing that $\eta(r)$ and $\varphi(r)$ are periodic functions we can write their Fourier series expansions as:

$$\eta(r) = \sum_{mn} \eta_{mn} \exp(-G_{mn}.r) \tag{12}$$

$$\Phi_\kappa(r) = \sum_{mn} \Phi_{mn}(\kappa) \exp(-G_{mn}.r) \tag{13}$$

where η_{mn} and φ_{mn} are Fourier coefficients and G_{mn} is reciprocal lattice vector. Inserting Eq. (12) and Eq. (13) in Eq. (11) and doing some lengthy arithmetic we have [31]:

$$\left\{S_{mnpq}\right\}\left\{\Phi_{pq}\right\} = \frac{\omega^2(\kappa)}{c^2}\left\{\Phi_{mn}\right\} \tag{14}$$

where

$$\{S_{mnpq}\} = \left\{\eta_{m-p,n-q}\left|G_{pq}+\kappa\right|^2\right\} \tag{15}$$

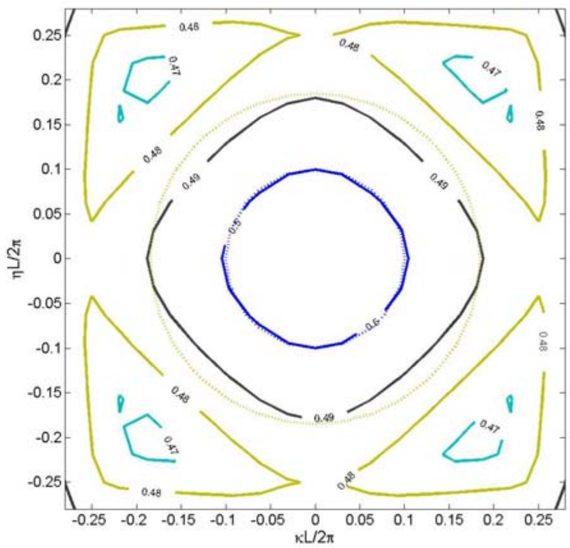

Fig. 4 EFCs of the RSC crystal with parameters listed in Eq. (10)

This is an eigenvalue-eigenvector equation. We can draw EFC of the RSC crystal by using PWEM and by sweeping Bloch wavenumber in the entire surface of the first Brillouin zone. We then find the locus for all the points in the Brillouin zone which have a certain frequency. The locus is obviously the EFC.

The EFCs of the rectangular stair-case (RSC) crystal depicted in Fig. 2 with the parameters listed in (10) are drawn in Fig. 4. The number of plane waves used in the method is N= [-50, 50] and each side of the first Brillouin zone is divided to 100 points. In this figure, contours of normalized frequency ($\omega/2\pi c$) are drawn in the reciprocal lattice. As we see in the figure, EFCs approximately satisfy our design requirement, that is a circular EFC for ω_1=0.5 with radius r_1=0.1, and another EFC for ω_2=0.49 with r_2=0.2. Dotted circles with redii 0.1 and 0.2 are also drawn in the figure for visual aid.

V. Converting to Standard Crystal

The rectangular stair-case (RSC) crystal that is designed in the previous section can be converted to common structures like pillar structures that are more straight-forward to fabricate. As a photonic crystal is a periodic structure, we can write Fourier series expansion for the electrical permittivity function. In a rectangular crystal we have

$$\varepsilon(x+mX, y+nY) = \varepsilon(x,y) \tag{16}$$

where X and Y are dimensions of crystal unit cell and m and n are integer numbers. Thus we have

$$\varepsilon(x,y) = \sum_m \sum_n \varepsilon_{mn} \exp\left[j2\pi\left(m\frac{x}{X}+n\frac{y}{Y}\right)\right] \tag{17}$$

$$\varepsilon_{mn} = \frac{1}{XY}\iint_{unit-cell} \varepsilon(x,y) * \exp\left[-j2\pi\left(m\frac{x}{X}+n\frac{y}{Y}\right)\right] dxdy \tag{18}$$

It has been already demonstrated that if the first three non-zero ε_{m0} or ε_{0n} coefficients of two crystals are approximately equal, the two crystals exhibit similar behaviors in terms of EFC shapes [28]. Therefore, if we can properly select parameters of an standard crystal so that its first Fourier coefficients are nearly equal to those of the RSC crystal that we designed in section 3, then we expect to have an EFC diagram similar to Fig. 4. By applying Eq. (18) to a crystal unit cell shown in Fig. 5 we have:

$$\varepsilon_{mn} = \begin{cases} \varepsilon_b + (\varepsilon_a - \varepsilon_b)\pi r_a^2 / XY & \text{for } m = 0 \\ \dfrac{2\pi r_a^2}{XY}\left(\dfrac{1}{\varepsilon_a} - \dfrac{1}{\varepsilon_b}\right)\dfrac{J_1\left(\sqrt{m^2+n^2}\,r_a\right)}{\sqrt{m^2+n^2}\,r_a} & \text{for } n = 0 \end{cases} \quad (19)$$

where $J_1(x)$ is the Bessel's function of the first kind and order 1. On the other hand, Fourier coefficients of the RSC crystal shown in Fig. 2 are:

$$\varepsilon_{mn} = \begin{cases} \dfrac{\varepsilon_b - \varepsilon_a}{\pi m}\sin\left(\dfrac{\pi m t}{X}\right) & \text{for } m \neq 0, n = 0 \\ \dfrac{\varepsilon_d - \varepsilon_c}{\pi n}\sin\left(\dfrac{\pi n s}{Y}\right) & \text{for } m = 0, n \neq 0 \\ \dfrac{(\varepsilon_b - \varepsilon_a)t}{X} + \varepsilon_a + \dfrac{(\varepsilon_d - \varepsilon_c)s}{Y} + \varepsilon_c & \text{for } m = 0, n = 0 \\ 0 & \text{elsewhere} \end{cases} \quad (20)$$

Using Eq. (20), Fourier coefficients of RSC crystal with parameters in Eq. (10) are listed in Table 1.

According to Eq. (19) and by choosing parameters of the crystal depicted in Fig. 5 as X=Y=1, r=0.47, ε_a=12.45 and ε_b=1, Fourier coefficients of the crystal are shown in Table 2. Calculation method of the pillar crystal parameters is discussed in detail in the next section.

Table 1 Fourier Coefficients of the designed RSC crystal.

m \ *n*	*n*=-2	*n*=-1	*n*=0	*n*=1	*n*=2
m=-2	0	0	-0.77	0	0
m=-1	0	0	1.81	0	0
m=0	-0.41	1.89	8.92	1.89	-0.41
m=1	0	0	1.81	0	0
m=2	0	0	-0.77	0	0

Table 2 Fourier Coefficients of the standard crystal.

m \ *n*	*n*=-2	*n*=-1	*n*=0	*n*=1	*n*=2
m=-2	0.51	-0.30	-0.79	-0.30	0.51
m=-1	-0.30	-0.49	1.91	-0.49	-0.30
m=0	-0.79	1.91	8.84	1.91	-0.79
m=1	-0.30	-0.49	1.91	-0.49	-0.30
m=2	0.51	-0.30	-0.79	-0.30	0.51

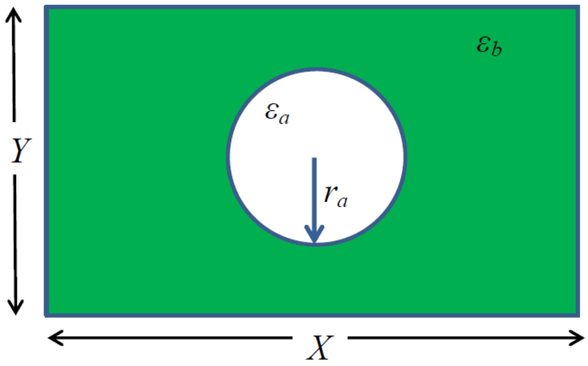

Fig. 5: Schematic of unit cell of a common crystal which is easy to fabricate

As we see, there is a good conformity between the non-zero coefficients of the two crystals along the η_{m0} column. Therefore, we expect the EFC shapes of the two to be similar. The EFC diagram of the crystal depicted in Fig. 5 with X=Y=1, r=0.47, ε_a=12.45 and ε_b=1 is plotted in Fig. 6. As is clear in the figure, the EFC shapes are quite similar to those of the RSC crystal.

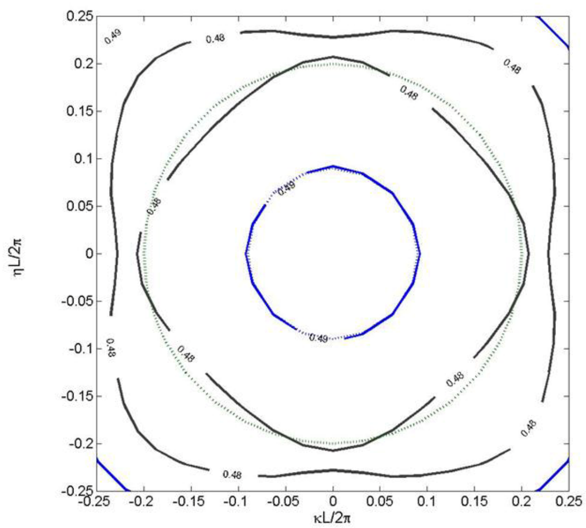

Fig. 6 EFCs of the crystal depicted in Fig. (5) with X=Y=1, r=0.47, ε_a=12.45 and ε_b=1

Dotted circles with radii r=0.09and r=0.2 are also drawn for visual aid. As shown in Fig. 4, we designed an EFC with inward gradient at r=0.1 and at ω=0.5. Knowing that $n = \dfrac{|\mathbf{k}_{normalized}|}{\omega_{normalized}}$, it is clear that this EFC can show effective refractive index of n=-0.2. Corresponding to this EFC, an EFC exists in Fig. 6 but by ω=0.49 and r=0.09. The calculation of refractive index for this EFC results in n=-0.18. As we see, the quantitative similarity between the two figures is satisfactory. Therefore, by this method we could design a photonic crystal showing negative refraction which is quite easy to fabricate. This completes the process to design metamaterials based on photonic crystals. The designed crystal shows negative refraction around $\omega/2\pi c$=0.49. Based on scaling rules, by reducing unit cell dimensions to L=0.76μm, we have negative refraction in the optical communication wavelength λ=1.55μm.

B. *Choosing crystal parameters*

As stated earlier, we can choose parameters of the crystal depicted in Fig. 5 in such a way that its Fourier coefficients become approximately equal to those of the RSC crystal. This can be done by one of the following two methods:

1: The Fourier coefficients of the two crystals are determined by Eq. (19) and Eq. (20). We choose the same magnitude for X and Y in the two crystals. Then we form a set of equations by equating three corresponding coefficients of the two crystals. The set of equations can then be solved using Trust-Region Dogleg Method [29] to find the three unknown r_a, ε_a and ε_b. For example by equating ε_{00}, ε_{10} and ε_{20} of the two crystals we have:

$$\begin{cases} \varepsilon_b + (\varepsilon_a - \varepsilon_b)\pi r_a^2 / XY = \varepsilon_{a-st} + \varepsilon_{c-st} + \\ \dfrac{(\varepsilon_{b-st} - \varepsilon_{a-st})t}{X} + \dfrac{(\varepsilon_{d-st} - \varepsilon_{c-st})s}{Y} \\ \dfrac{2\pi r_a^2}{XY}\left(\dfrac{1}{\varepsilon_a} - \dfrac{1}{\varepsilon_b}\right)\dfrac{J_1(r_a)}{r_a} = \\ \dfrac{\varepsilon_{b-st} - \varepsilon_{a-st}}{\pi}\sin\left(\dfrac{\pi t}{X}\right) \end{cases}$$

$$\frac{2\pi r_a^2}{XY}\left(\frac{1}{\varepsilon_a} - \frac{1}{\varepsilon_b}\right)\frac{J_1(2r_a)}{2r_a} = \frac{\varepsilon_{b-st} - \varepsilon_{a-st}}{2\pi}\sin\left(\frac{2\pi t}{X}\right) \tag{21}$$

2: There are closed-form relations for finding r_a, ε_a, and ε_b, provided that in the RSC crystal we have: $\varepsilon_a=\varepsilon_c$ and $\varepsilon_b=\varepsilon_d$. in this case we have [28]:

$$t - \frac{X}{\pi}\cos^{-1}\left\{\frac{\mathrm{Re}\left(\dfrac{2\pi r_a^2}{XY}\left(\dfrac{1}{\varepsilon_a} - \dfrac{1}{\varepsilon_b}\right)\dfrac{J_1(2r_a)}{2r_a}\right)}{\mathrm{Re}\left(\dfrac{2\pi r_a^2}{XY}\left(\dfrac{1}{\varepsilon_a} - \dfrac{1}{\varepsilon_b}\right)\dfrac{J_1(r_a)}{r_a}\right)}\right\} = 0$$

$$\varepsilon_{a-st} + \frac{\pi t\,\mathrm{Re}\left(\dfrac{2\pi r_a^2}{XY}\left(\dfrac{1}{\varepsilon_a} - \dfrac{1}{\varepsilon_b}\right)\dfrac{J_1(r_a)}{r_a}\right)}{X\sin\left(\dfrac{\pi t}{X}\right)} = \frac{\varepsilon_b + (\varepsilon_a - \varepsilon_b)\pi r_a^2}{2XY}$$

$$\frac{\pi\,\mathrm{Re}\left(\dfrac{2\pi r_a^2}{XY}\left(\dfrac{1}{\varepsilon_a} - \dfrac{1}{\varepsilon_b}\right)\dfrac{J_1(r_a)}{r_a}\right)}{\sin\left(\dfrac{\pi t}{X}\right)} = \varepsilon_{b-st} - \varepsilon_{a-st} \tag{22}$$

These equations can also be solved using Trust-Region-Dogleg method. If the conditions of $\varepsilon_a=\varepsilon_c$ and $\varepsilon_b=\varepsilon_d$ are not met in the RSC crystal, the equations can be solved using average values of $(\varepsilon_a+\varepsilon_c)/2$ and $(\varepsilon_b+\varepsilon_d)/2$. The calculated parameters can then be fine-tuned for best results.

VI. Conclusion

In this paper, for the first time, a novel and systematic design procedure was proposed to design crystal EFCs to produce negative refraction. The EFC design is performed by the help of a special two dimensional RSC photonic crystal. The closed form relations between light frequency and crystal parameters in RSC crystal were helpful for systematic design. Circular EFCs and their inward gradient were realized by choosing appropriate points in crystal EFC. EFCs of the crystal were drawn by the help of PWEM in order to verify the design. We were able to convert RSC crystal to more common structures like pillar crystals, by matching Fourier coefficients of periodic electric permittivity. Two methods to design common crystals which have approximately equal

Fourier components to the RSC crystal were also presented. The designed crystal can show negative refraction at λ=1.55μm by reducing unit cell dimensions to L=0.76 μm. The proposed procedure can be used to design metamaterials and also other photonic crystal based structures. The devised procedure can also be helpful in designing other structures involving photonic crystals.

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