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A different approach in the calculation of two-dimensional local density of states has been presented for a two-dimensional finite rectangular-lattice photonic crystal with a separable profile of permittivity. Approximate staircase structures are already shown to be useful for their ability to reproduce actual properties of practical square lattice photonic crystals. Using the effective resonance approach in a Fabry–Perot resonator and transfer matrix method an analytical expression for calculating a two-dimensional local density of states can be derived for both polarisations in the structure. It is shown that for this geometry one can resolve the modes as a product of two separate functions each being a function of x- and y-coordinates. The results have been investigated for the two-dimensional local density of states in the ordered finite structure and in the disordered structure. The main advantage of this method in calculating the local density of states is its extremely efficient numerical evaluations. As an application we introduce a cavity-like defect in the vicinity of a waveguide-like defect and examine the variation of local density of states in the plane of the structure at band gap frequency.

1. Introduction

The concept of photonic crystal (PC) that was introduced by seminal works of Yablonovitch [1] and John [2] is concerned with the ability to modify the photonic density of states (DOS) in periodic permittivity structures. Two new optical principles, i.e. the localisation of light in bulk materials and the complete inhibition of spontaneous emission over a broad range, were then introduced in the field of photonics. In these new concepts, the emission and absorption properties of radiating sources (atoms and molecules) which are placed within the structure can be prohibited or enhanced through the changing of the DOS with respect to its free space and depends on the degree of tuning to or detuning from the relevant atomic

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transition frequencies. This modification can also be explained by the formation of a photonic band gap (PBG) in these structures that prevents them from propagating electromagnetic fields without evanescent decay inside the gap regions [3].

As a general point of view, the PCs can be investigated using two methods: (1) calculation of band structures accompanied by evaluation of reflection and transmission spectra [4], and (2) by calculation of DOS in the structure [1,2]. The second approach is more suitable especially when the main goal is to study the radiation dynamic of a radiating source placed within the structure [5–7]. This salient property of PCs opens up a new way to attain integrated photonics. For example, applications of these structures are to improve efficiency in semiconductor devices such as lasers and solar cells [4] and in fabrication of new devices such as low-threshold micro lasers, optical memories and ultra-fast optical switches as well as all-optical transistors [8]. Therefore, it seems that the calculation of DOS in these structures is a crucial task to give us a real insight into the optical properties of photonic crystals.

Moreover, the spatial variations of the optical parameters in these structures are to be in scales of the optical wavelength; so, the spatial dependence of DOS function should be considered when investigating the radiation dynamics. But, the DOS only considers an average quantity over a unit cell. This deficiency can be removed by considering somehow the eigen-mode profile of PCs in the DOS function [9,10]. Therefore, the fundamental quantity that predicts the radiation dynamics is spatially resolved or local density of states (LDOS). This quantity describes the local availability of modes to which a source can couple and emit a photon [11]. However, the calculation of these two quantities is rigorously hard because of the existence of singularities that happen in a band where the group velocity tends to zero [12]. Furthermore, for infinite structures, the LDOS becomes zero inside a complete band gap with corresponding radiating source transition frequency, but it is not exactly zero for a finite structure because of the incompleteness of structure periodicity [10,13]. From a computational point of view, calculation of LDOS for an infinite structure is easier than a finite one because of using the capability of the Bloch method in infinite structures, although the results are not realistic.

Several methods have been developed to calculate the LDOS in specific PC structures. To date, the LDOS have been calculated for an infinite two-dimensional (2D) array of cylinders [10,14], and an array of spheres [15] as well as cylinders ordered in a woodpile 3D geometry [16] using the Bloch method. In one-dimensional (1D) finite structure, the LDOS has been calculated using multiple scattering theory [17] and the transfer matrix method [18]. Another approach in calculating the LDOS and so the spontaneous emission rates in finite-sized PCs is using the finite difference time domain (FDTD) method [19,20]. Among the methods, the method of Green’s tensor is an applicable approach in calculating the DOS and LDOS in 2D and 3D finite-sized PC structures [21,22]. Moreover, it has been shown that applying a Rayleigh-multipole method in calculating the Green’s tensor of a finite 2D cluster of cylinders results in a more accurate and efficient method for computation of the 2D and 3D LDOS [11,12, 23–25]. The LDOS has also been calculated for collections of spherical scatterers using the multiple-scattering theory [26].
Among these results, there are some useful papers in examining numerical stability and efficiency of different algorithms in analysing 1D and 2D periodic structures [27–29] such as gratings. Also, the validity of the staircase approximation used to describe arbitrary-shaped gratings and the modal methods has been studied numerically [30].

Moreover, localised defect modes (LDM) in band gap region which is emerged by introducing defect or disorder in the periodic of dielectric structure, are important in designing new optical devices like low threshold lasers [31], optical memories and high-quality factor resonators [32,33]. Optimal design of such new devices depends on the emission characteristic of atoms and molecules that place within the structure. The first proposed application was the ability to inhibit the spontaneous emission by suppressing the density of state. For using this ability in designing the new photonic devices one must introduce new modes inside the bad gap region, named localised defect modes.

In this article, we introduce a different approach in calculating local density of states for both perfect and defect 2D finite-sized structures in which the permittivity function can be resolved to two staircase permittivity profiles along $x$- and $y$-axes, referred to here as the separable profile of permittivity (SPP). It has been previously shown that the band structure of a general rectangular–lattice photonic crystal can be easily reproduced from a properly fitted staircase structure [34], which provides an efficient way to design of optical devices base on rectangular-lattice photonic crystals. So, the investigation of optical response of this structure can be useful in figuring out their general properties. We have recently studied the problem of DOS of an infinite-sized staircase structure where no defects were considered [35]. Perfect 2D periodicity enabled us to employ the Bloch wave formalism in calculating the DOS. It is the purpose of this paper to include both orthogonal polarisations in calculation of Local DOS corresponding to finite-sized photonic crystals. We demonstrate excellent numerical stability and convergence together with superior efficiency in derivation of DOS and LDOS.

In calculating the LDOS, we are inspired by the works of Bendickson et al. [36] and Rudzinski et al. [37], in finding an analytical expression for electromagnetic mode density and the density of states in finite 1D PC, respectively. Finding an analytical expression leads to calculation of the DOS and LDOS efficiently at a very shorter CPU time. Moreover, we can investigate localised defect mode by introducing desired disorder in the SPP structure and calculating its local density of states. With introducing proper defect in the structure, we can engineer new optical devises for specific application. In this approach, it is not hard to introduce defect in the structure. We must only alter the appropriate parameters of SPP unit cell and consider them in matrix transformation operator for calculating the LDOS. In the following section we investigate the LDOS and LDM in SPP structure.

This article begins with defining the SPP structure in Section 2. Then, after proving the ability of resolving the 2D wave equation into two separate 1D differential equation for E- and H-polarisation in Section 3, we introduce the method for calculating of the LDOS in Section 4. The method is used in Section 5 to calculate the LDOS in a SPP structure without and with defect as a cavity resonator and as a waveguide.
2. Defining the structure

The unit cell of a SPP structure is a square or rectangular-lattice photonic crystal that is illustrated in Figure 1. With this definition for the structure we can write the permittivity function as a sum of two one variable functions in x and y directions, i.e. \( \varepsilon(x,y) = X(x) + Y(y) \). So, it is possible to resolve the permittivity function as two staircase permittivity profiles along x and y axes.

The independent parameters in this unit cell are \( L_x, L_y, d_{i,x}, d_{i-1,x}, d_{i,y}, d_{i-1,y}, \varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4 \), which one can change for the desired structure. The desired structure consists of \( n_x \) and \( n_y \) clusters of this unit cell in x and y directions, respectively.

3. Wave equations

For 2D structure when, the direction of wave vector is parallel to the structure plane, i.e. normal incident, there is always a possibility to decouple the general wave equation to TM- and TE-modes. So, one can investigate the two polarisations independently as two kinds of eigen-functions. The E-polarisation that means the electric field is perpendicular to the structure plane and the H-polarisation for which the magnetic field is perpendicular to the structure.

It will be shown that having a SPP 2D PC and under normal incidence, one can resolve the modes as a product of two separate terms each being a function of x- and y-coordinates. This resolution can be done easily in a very simple fashion for E-polarisation equation, but it is not straightforward to substantiate the resolution for H-polarisation and it will be done in a little more complicated manner than E-polarisation. In the following subsection, it will be shown that not only

Figure 1. The unit cell of the 2D structure and corresponding staircase functions have been shown.
the E-polarisation equation can be resolved but also one can decompose the H-polarisation equation and reduce them into two separate differential equations, so one 2D structure has been divided into two separate 1D structures, one being a 1D PC with periodic permittivity in the horizontal direction and the other in the vertical direction.

3.1. E-polarisation in SPP structure
In a 2D non-magnetic photonic crystal the wave equation for the electric field vector can be considered as follows

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r}) = \frac{\omega^2}{c^2} \varepsilon_\varepsilon(\mathbf{r}) \mathbf{E}(\mathbf{r}), \quad \varepsilon(\mathbf{r}) = \varepsilon_0 \varepsilon_\varepsilon(x, y)$$

(1)

where $\varepsilon(\mathbf{r})$ is the permittivity of the medium and $\varepsilon_\varepsilon(x, y)$, $\omega$ are the relative permittivity function of the PC and eigen-angular frequency, respectively. ‘$c$’ is the speed of light in vacuum. Also, we use $\varepsilon_0 \mu_0 = c^{-2}$ for defining the vacuum permittivity $\varepsilon_0$. $\mathbf{E}(\mathbf{r})$ is the electric wave vector. For E-polarisation, $\mathbf{E}(\mathbf{r}) = \mathbf{E}(x, y, z) = E_z(\mathbf{r}) \hat{z}$ the divergence of the field always is zero. Moreover, in the case of normal propagation when the incident wave is propagating in the plane of PC, we can conclude that the electric field is only a function of $x$ and $y$ spatial coordinate system.

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) E_z(x, y) = -\frac{\omega^2}{c^2} \varepsilon_\varepsilon(x, y) E_z(x, y).$$

(2)

In a SPP structure, we assume the permittivity to be a sum of two terms, each being single functions of $x$- and $y$-coordinates, then the electric field can be written down as product of two separately function of $x$- and $y$-coordinates $E_z(x, y) = \chi(x) \psi(y)$ using the method of separation of variables. With this expression for the electric field it can be concluded that

$$\frac{\partial^2}{\partial x^2} \chi(x) + \frac{\omega^2}{c^2} [X(x) + \beta] \chi(x) = 0$$

$$\frac{\partial^2}{\partial y^2} \psi(y) + \frac{\omega^2}{c^2} [Y(y) - \beta] \psi(y) = 0$$

(3)

where $\beta$ is the separation constant of the partial derivative. Equation (1) reduces into two separate differential equations, so one 2D structure has been divided into two separate 1D structures.

3.2. H-polarisation in SPP structure
The wave equation for magnetic field in a 2D non-magnetic PC can be consider as follows

$$\nabla \times \left[ \frac{1}{\varepsilon_\varepsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) \right] = \frac{\omega^2}{c^2} \mathbf{H}(\mathbf{r}), \quad \varepsilon(\mathbf{r}) = \varepsilon_0 \varepsilon_\varepsilon(x, y)$$

(4)
where $\varepsilon(\mathbf{r})$ is the permittivity of the medium and $\varepsilon_\text{i}(x,y)$ and $\omega$ are the relative permittivity function of the PC and eigen-angular frequency, respectively. $c$ is the speed of light in vacuum. Only the normal component of the magnetic field $\mathbf{H}(\mathbf{r}) = H_z(\mathbf{r})\hat{z}$ would be non zero. By simplifying the Equation (4), we can derive the equation for magnetic field component

$$\nabla \times [\eta \nabla \times \mathbf{H}(\mathbf{r})] = \nabla \eta \times [\nabla \mathbf{H}(\mathbf{r})] + \eta \nabla [\nabla \cdot \mathbf{H}(\mathbf{r})] - \eta \nabla^2 \mathbf{H}(\mathbf{r})$$

(5)

where $\eta$ is reverse of material permittivity $\eta = \frac{1}{\varepsilon(\mathbf{r})}$.

The permeability of a non-magnetic material is supposed to be that of free space. So, we can write

$$\nabla \cdot \mathbf{H}(\mathbf{r}) = 0.$$  

(6)

Thus, from Equations (4), (5), and (6) we obtain

$$\nabla \eta \times [\nabla \times \mathbf{H}(\mathbf{r})] - \eta \nabla^2 \mathbf{H}(\mathbf{r}) = \frac{\omega^2}{c^2} \mathbf{H}(\mathbf{r}).$$

(7)

In a Cartesian coordinate system the former equation can be simplified as follows

$$\frac{\partial}{\partial x} \eta \frac{\partial}{\partial x} H_z(\mathbf{r}) + \frac{\partial}{\partial y} \eta \frac{\partial}{\partial y} H_z(\mathbf{r}) + \eta \frac{\partial^2}{\partial x^2} H_z(\mathbf{r}) + \eta \frac{\partial^2}{\partial y^2} H_z(\mathbf{r}) + \eta \frac{\partial^2}{\partial z^2} H_z(\mathbf{r}) = -\frac{\omega^2}{c^2} H_z(\mathbf{r}).$$

(8)

Using Fourier transform, it would be possible to write the solution to Equation (8) in the following form

$$H_z(x, y, z) = A(x, y) \exp(-i\gamma z)$$  

(9)

where, the $\gamma$ coefficient corresponds to the angle of the wave vector respect to $z$-axis and $A(x, y)$ is a scalar function. Inserting Equation (9) into Equation (8) we can write

$$\frac{\partial}{\partial x} \eta \frac{\partial}{\partial x} A(x, y) + \frac{\partial}{\partial y} \eta \frac{\partial}{\partial y} A(x, y) + \eta \frac{\partial^2}{\partial x^2} A(x, y) + \eta \frac{\partial^2}{\partial y^2} A(x, y) = \left(\gamma^2 \eta - \frac{\omega^2}{c^2}\right) A(x, y).$$

(10)

If it is assumed that the permittivity is a sum of two terms, each being single functions of $x$- and $y$-coordinates, as in the case of SPP structure, then $\eta = [X(x) + Y(y)]^{-1}$ and thus the above equation becomes

$$\frac{-\frac{\partial}{\partial x} X}{(X + Y)^2} \frac{\partial}{\partial x} A + \frac{-\frac{\partial}{\partial x} Y}{(X + Y)^2} \frac{\partial}{\partial y} A + \frac{1}{X + Y} \frac{\partial^2}{\partial x^2} A + \frac{1}{X + Y} \frac{\partial^2}{\partial y^2} A = \left(\gamma^2 \frac{1}{X + Y} - \frac{\omega^2}{c^2}\right) A.$$  

(11)

Using the method of separation of variables, the field can be written as product of two separately function of $x$- and $y$-coordinates as $A(x, y) = \chi(x) \psi(y)$; hence, the
final form of the set of H-polarisation wave equation in the structure for in-plane propagation can be obtained as follows

\[
\begin{align*}
\frac{\partial^2}{\partial x^2} \chi(x) - \left[ \frac{1}{X(x) + Y(y)} \frac{\partial}{\partial x} X(x) \right] \frac{\partial}{\partial x} \chi(x) + \left[ \frac{\omega^2}{c^2} X(x) - \beta_1 \right] \chi(x) &= 0 \quad (12a) \\
\frac{\partial^2}{\partial y^2} \psi(y) - \left[ \frac{1}{X(x) + Y(y)} \frac{\partial}{\partial y} Y(y) \right] \frac{\partial}{\partial y} \psi(y) + \left[ \frac{\omega^2}{c^2} Y(y) + \beta_1 \right] \psi(y) &= 0 \quad (12b)
\end{align*}
\]

where \( \beta_1 \) is the separation constant of the partial derivative.

As a result, the 2D problem is reduced to two pseudo 1D problems. Notice that while according to Equation (12), \( \frac{\partial}{\partial x} X(x) \) and \( \frac{\partial}{\partial y} Y(y) \) are not really 1D, but we would rather conclude \( \frac{\partial}{\partial x} X(x) = \frac{\partial}{\partial x} X(x, y) \), and similarly \( \frac{\partial}{\partial y} Y(y) = \frac{\partial}{\partial y} Y(y, x) \). However, one can still solve Equation (12a) and Equation (12b) as simple ordinary differential equations, treating, respectively, \( y \) and \( x \) arguments as constants.

At this point, we make use of the method of changing variables to transform each of the above equations into forms similar to that of E-polarisation equations in the previous section. Initially consider the uncoupled system of equations

\[
\begin{align*}
\frac{\partial^2}{\partial x^2} \chi(x) + a(x, y) \frac{\partial}{\partial x} \chi(x) + b(x) \chi(x) &= 0 \quad (13a) \\
\frac{\partial^2}{\partial y^2} \psi(y) + c(x, y) \frac{\partial}{\partial y} \psi(y) + d(y) \psi(y) &= 0 \quad (13b)
\end{align*}
\]

where the following definitions have been adopted

\[
a(x, y) = -\frac{1}{X(x) + Y(y)} \frac{\partial}{\partial x} X(x), \quad c(x, y) = -\frac{1}{X(x) + Y(y)} \frac{\partial}{\partial y} Y(y) \\
b(x) = \frac{\omega^2}{c^2} X(x) - \beta_1, \quad d(y) = \frac{\omega^2}{c^2} Y(y) + \beta_1. \quad (14)
\]

For solving (13a) we can use the following new variable

\[
\chi(x) = V(x) \exp \left( -\frac{1}{2} \int a(x, y) dx \right). \quad (15)
\]

Then, one can solve the differential equation

\[
\frac{\partial^2}{\partial x^2} V(x) + \left[ -\frac{1}{2} \frac{\partial}{\partial x} a(x, y) - \frac{1}{4} a(x, y)^2 + b(x) \right] V(x) = 0. \quad (16)
\]

With the same method we can infer the Equation (13b) as follows

\[
\frac{\partial^2}{\partial y^2} V(y) + \left[ -\frac{1}{2} \frac{\partial}{\partial y} c(x, y) - \frac{1}{4} c(x, y)^2 + d(y) \right] V(y) = 0 \quad (17)
\]

\[
\psi(y) = V(y) \exp \left( -\frac{1}{2} \int c(x, y) dy \right). \quad (18)
\]
As a result, the solution of normal component of magnetic field can be derived as product of $\chi(x)$ and $\psi(y)$. These two functions are derived from (16) and (17), and we finally obtain

$$H_z(x, y) = \chi(x)\psi(y; x). \quad (19)$$

### 4. Modelling the local density of states in a SPP structure

In the calculation of local density of states (LDOS), we use the method of effective resonance approach. In this approach each layers of 1D PC can be considered as a Fabry–Perot resonator and the rest of the structure acts as two separate multi-Bragg reflectors constituting the forward and backward mirrors of the resonator. These coefficients act as the boundary condition for finding the eigen-fields inside the FP resonator. Then, with imposing the boundary condition on the exciting fields one can find the effective field amplitude inside the resonator. This effective amplitude shows the probability of existence specific modes inside the resonator and its real value can be a criterion for the number of mode inside the resonator. If this amplitude is a maximum quantity for a specific frequency and wave vector, the exciting field $E_x(d, k)$ is a resonator mode located in position $d$ inside the structure. Moreover, this satisfies the resonance condition in the resonator and will be a longitudinal eigen-mode with the resonance frequency of the resonator. So, these eigen values $\rho_e(d, k)$ are proportional to mode density, related to distribution of modes in wave vector domain within a factor which can be find through the well known mode density of empty space.

If one assumes that operator $Q$ operates on the exciting electric field $E^ex$ that acts on the resonator, it will yield an effective electric field $E^eff$ that is a possible mode for the resonator.

$$E^eff = QE^ex = QE_0 \exp(i k \cdot d) \quad (20)$$

where $k$ is the wave vector on the layers and $d$ is the position vector. $E_0$ is the amplitude of the exciting field.

In 1D with respect to $x$ or $y$ direction, the operator $Q$ acts on scalar field. So we can write the operation relation in each direction as follows

$$E^eff_x = Q_x E_0 \exp(i k d_x)$$

$$E^eff_y = Q_y E_0 \exp(i k d_y). \quad (22)$$

In 2D in the $x$-$y$ plane the operator $Q$ acts on a vector field. If we consider the TE- or TM-polarised light for the structure explained in the previous section then, we will be able to write the electric and magnetic field as a product of to term one being as a function of $x$ coordinate and the other as a function of $y$ coordinate.

$$E^eff = Q_{xy} E_0, \exp(i k \cdot d) = Q_{xy}(E_0, \exp(i k_x d_x) E_0, \exp(i k_y d_y)) \hat{z}. \quad (23)$$
So, we should look for an expression for the 2D operator $Q_{xy}$. In order to do this, we can consider the product of Equation (21) and Equation (22), leading to

$$E_x^{\text{eff}} E_y^{\text{eff}} = Q_x E_0^x \exp(ikdx) \exp(ikd_y) = Q_x Q_y E_0^{xy} \exp(\mathbf{k} \cdot \mathbf{d}). \quad (24)$$

In the last expression, we have made use of the field as a product of two scalar functions.

By comparing Equations (23) and (24), we can conclude that the operator form in 2D structure must be the product of the two 1D operators in $x$ and $y$ direction, only if it is possible to write its eigen-field as a product of eigen-fields of each direction, i.e.

$$Q_{xy} = Q_x Q_y. \quad (25)$$

As it turned out in the previous section, for SPP structure the solution of TE-polarised and TM-polarised fields, can be individually derived as product of two independent 1D functions and the 2D structure has been divided into two separate 1D structures, one being a 1D PC with periodic permittivity in the horizontal direction and the other in the vertical direction. So, it is possible to calculate the local density of state in a simple manner using (25). In TM-polarised and TE-polarised light cases, the electric and magnetic fields, respectively, are normal to the plane of PC; therefore, we only need to find the projection of $\mathbf{k}$ vector in $x$ and $y$ direction for finding the effective waves. This effective field can be obtained from summation of plane waves, moving back and forth between the mirrors of the resonator. Since the field eigen-values are real quantities it is necessary to take the real part of the effective waves inside the resonator. So that

$$E_{x, \varepsilon}^{\text{eff}}(d_{ix}, k) = \text{Re} \left\{ E_0 \sum_n (r_{\text{right}, \varepsilon}(d_{ix}) r_{\text{left}, \varepsilon}(d_{ix}) \exp(-2ik_{ix}d_{ix}))^n \right\} \quad (26)$$

$$E_{y, \varepsilon}^{\text{eff}}(d_{iy}, k) = \text{Re} \left\{ E_0 \sum_n (r_{\text{up}, \varepsilon}(d_{iy}) r_{\text{down}, \varepsilon}(d_{iy}) \exp(-2ik_{iy}d_{iy}))^n \right\}. \quad (27)$$

The parameters in the two above equations are introduced here.

$r_{\text{left}}(d_{ix})$, $r_{\text{right}}(d_{ix})$, $r_{\text{up}}(d_{iy})$ and $r_{\text{down}}(d_{iy})$ are the reflection coefficient of the left, right, up and down mirrors of FP resonator placed in $x$ and $y$ directions, respectively. These reflection coefficients are a function of space that is specified by the position of the FP-layer in the structure. The position of each layer is indicated by the $i$-index in $d_{ix}$ and $d_{iy}$ which are the thicknesses of the $i$th layers in the $x$ and $y$ directions, respectively. Furthermore, $k_{ix}$ and $k_{iy}$ are the projection of wave vector for $i$th layer in $x$ and $y$ direction, respectively. ‘Re’ denotes real part of the complex functions. The parameter $\varepsilon$ indicates one of E- or H-polarisations. The geometry for calculating the LDOS has been shown in the (Figure 2). After performing the summations in Equations (26) and (27) and taking the amplitude of initial exiting field to be unity
(this does not impose any restriction to the problem), one can conclude that the effective plane waves have the following forms,

\[
E_{x,e}^{\text{eff}}(k, d_{ix}) = \frac{1 - \text{Re}\{r_{\text{right},e}(d_{ix})r_{\text{left},e}(d_{ix})\exp(-2ik_{ix}d_{ix})\}}{1 + |r_{\text{right},e}(d_{ix})r_{\text{left},e}(d_{ix})|^2 - 2\text{Re}\{r_{\text{right},e}(d_{ix})r_{\text{left},e}(d_{ix})\exp(-2ik_{ix}d_{ix})\}}
\]

\[
E_{y,e}^{\text{eff}}(k, d_{iy}) = \frac{1 - \text{Re}\{r_{\text{up},e}(d_{iy})r_{\text{down},e}(d_{iy})\exp(-2ik_{iy}d_{iy})\}}{1 + |r_{\text{up},e}(d_{iy})r_{\text{down},e}(d_{iy})|^2 - 2\text{Re}\{r_{\text{up},e}(d_{iy})r_{\text{down},e}(d_{iy})\exp(-2ik_{iy}d_{iy})\}}
\]

For finding the mode density \(\rho_e(d, k)\), it is necessary to subtract the initial exciting plane wave from the effective fields because in doing the above summations, there are extra terms related to exiting plane wave. So, the eigen-values for two spatially
perpendicular FP resonators, can be calculated for both $x$ and $y$ components of mode density as the following expressions

$$
\rho_x,\epsilon(k, d_x) = E_{x,\epsilon}^{\text{eff}}(k, d_x) - 1
\quad \frac{1 - |r_{\text{right},\epsilon}(d_x)r_{\text{left},\epsilon}(d_x)|^2}{1 + |r_{\text{right},\epsilon}(d_x)r_{\text{left},\epsilon}(d_x)|^2 - 2\Re\{r_{\text{right},\epsilon}(d_x)r_{\text{left},\epsilon}(d_x)\exp(-2ik_xd_x)\}} \quad \text{(30)}
$$

$$
\rho_y,\epsilon(k, d_y) = E_{y,\epsilon}^{\text{eff}}(k, d_y) - 1
\quad \frac{1 - |r_{\text{up},\epsilon}(d_y)r_{\text{down},\epsilon}(d_y)|^2}{1 + |r_{\text{up},\epsilon}(d_y)r_{\text{down},\epsilon}(d_y)|^2 - 2\Re\{r_{\text{up},\epsilon}(d_y)r_{\text{down},\epsilon}(d_y)\exp(-2ik_yd_y)\}} \quad \text{(31)}
$$

Therefore, the mode density in the 2D structure can be calculated using the following expression

$$
\rho_\epsilon(d, k) = A\rho_x,\epsilon(d_x, k_x)\rho_y,\epsilon(d_y, k_y) \quad \text{(32)}
$$

The constant $A$ is the normalisation coefficient. It can be found using the mode density in free space, where $\rho_x,\epsilon(d_x, k_x) = \rho_x,\epsilon(d_y, k_y) = 1$. For calculating the number of modes $N$ at the position of $d$ in the system we can use the following relation

$$
\sum_{k,\epsilon} \rho_\epsilon(d, k) = N(d) \quad \text{(33)}
$$

We intend to investigate a finite structure in which there are probably some disorders so, instead of making use of periodic boundary condition we impose boundary condition in the edges of the structure in contact with background material as

$$
E_\epsilon(x + n_xL_x, y) = E_\epsilon(0, y) \quad \text{(34)}
$$

$$
E_\epsilon(x, y + n_yL_y) = E_\epsilon(x, 0) \quad \text{(35)}
$$

where $n_x$ and $n_y$ are the number of unit cells defined in Figure 1 in the $x$ and $y$ directions, respectively.

For calculating the number of modes ‘$N$’ according to Equation (33) which is to calculate the number of $k$-states lying in an annulus of radius $k$ to $k + dk$, we need to do the summation over $k$-space. With the boundary conditions mentioned in Equations (34) and (35), the area occupied by each state in two-dimensional $k$-space will be equal to $(2\pi)^2/S$. In this expression $S$ is the area of the structure and is equal to $n_xn_yL_xL_y$. So, knowing the area occupied by each state, we can replace the summation into the integral over the $k$-space which is

$$
\sum_k \rightarrow \frac{S}{(2\pi)^2} \int \int dk^2 \quad \text{(36)}
$$

In the polar coordinates the area differential reads as $dk^2 = dk \, d\theta$; therefore, one can find an expression for the number of modes $N$, and hence the local density of
states \( g(d, k) \), in terms of the mode density \( \rho_s(d, k) \). This results in

\[
N(d) = \sum_s \frac{n_s n_i L_x L_y}{4\pi^2} \int \int \rho_s(d, k, \theta) k \, dk \, d\theta
\]  

\[
g(d, k)dk = \frac{1}{S} dN(d, k) = \frac{1}{4\pi^2} \sum_s k \, dk \int \theta \rho_s(d, k, \theta).
\]

So, we can write an expression for calculating of LDOS in SPP PC, using Equation (32) and inserting into Equation (38) as

\[
g(d_i, k) = \frac{k}{4\pi^2} \int_0^\pi d\theta \sum_s \left( \frac{1 - |r_{right,s}(d_{ix}, \theta) r_{left,s}(d_{ix}, \theta)|^2}{1 + |r_{right,s}(d_{ix}, \theta) r_{left,s}(d_{ix}, \theta)|^2} \right)
\]

\[
\quad \times \frac{1 - |r_{up,s}(d_{iy}, \theta) r_{down,s}(d_{iy}, \theta)|^2}{1 + |r_{up,s}(d_{iy}, \theta) r_{down,s}(d_{iy}, \theta)|^2} \exp(-2ik_{ix}d_{ix}) \exp(-2ik_{iy}d_{iy})
\]\n
\[
(39)
\]

The radiating source for calculating the 2D LDOS is a line source placed in the desired position perpendicular to the plane of structure.

4.1. Calculation of boundary conditions

We consider a 1D photonic crystal as a one Fabry–Perot resonator consisting of two multilayer Bragg reflectors as mirrors, where the mirror reflection coefficients is computed by the method of unit cell translation operator [38]. The structure that has been used is illustrated in Figure 2.

This structure build of alternating layers of linear, uniform and isotropic material of different refractive indices \( n_i \) with thickness of \( d_{x,i} \) respectively. The layers are indicated with subscript \( i \). The number of layers in the right and the left of the resonator are \( N_R \) and \( N_L \), respectively. Moreover, \( A_i \) and \( B_i \) are the field amplitudes for the right and the left travelling waves, respectively. The geometry and definitions of the parameters are shown in Figure 3. The field in this stratified medium can be considered as the following formulae

\[
E(x, y) = A(x) \exp[i(\omega t - \beta y)]
\]

\[
A(x) = \begin{cases} 
A_o \exp[-ik_{ox}(x - x_o)] + B_o \exp[ik_{ox}(x - x_o)] & x < x_o \\
A_i \exp[-ik_{ix}(x - x_i)] + B_i \exp[ik_{ix}(x - x_i)] & x_{i-1} < x < x_i \\
A_s \exp[-ik_{sx}(x - x_N)] + B_s \exp[ik_{sx}(x - x_N)] & x_N < x
\end{cases}
\]

\[
k_{ix} = \frac{n_i \omega}{c} \sin \theta_i
\]

where \( \theta_i \) is the angle of incidence with respect to the y-axis.
The left layers constitute the back mirror of the Fabry–Perot resonator and the right layers do the front mirror. For calculating the reflection coefficients of the mirrors we use the method of matrix formulation for isotropic layered media. By this formalism it becomes possible to relate the amplitude of forward and backward field in one layer to its neighbouring layers. The relations are expressed in the matrix form given by

\[
\begin{pmatrix}
A_i \\
B_i
\end{pmatrix} = \begin{pmatrix}
\exp(ik_{ix}d_{ix}) & 0 \\
0 & \exp(-ik_{ix}d_{ix})
\end{pmatrix} \begin{pmatrix}
M_{R_{i1}} & M_{R_{i2}} \\
M_{L_{i1}} & M_{L_{i2}}
\end{pmatrix} \begin{pmatrix}
A_s \\
B_s
\end{pmatrix}
\]

(43)

\[
\begin{pmatrix}
A_o \\
B_o
\end{pmatrix} = \begin{pmatrix}
M_{L_{i1}} & M_{L_{i2}} \\
M_{L_{i1}} & M_{L_{i2}}
\end{pmatrix} \begin{pmatrix}
A_i \\
B_i
\end{pmatrix}
\]

(44)

\[
\begin{pmatrix}
M_{R_{i1}} & M_{R_{i2}} \\
M_{R_{i1}} & M_{R_{i2}}
\end{pmatrix} = D_i^{-1} \left[ \prod_{i=0}^{N_d} D_i P_i D_i^{-1} \right] D_s
\]

(45)

\[
\begin{pmatrix}
M_{L_{i1}} & M_{L_{i2}} \\
M_{L_{i1}} & M_{L_{i2}}
\end{pmatrix} = D_o^{-1} \left[ \prod_{i=0}^{N_d} D_i P_i D_i^{-1} \right] D_i
\]

(46)

\[
P_i = \begin{pmatrix}
\exp(ik_{ix}d_{ix}) & 0 \\
0 & \exp(-ik_{ix}d_{ix})
\end{pmatrix}
\]

(47)

\[
D_i = \begin{cases}
\left( \frac{\cos \theta_i}{\sqrt{\mu_i}} \frac{-\cos \theta_i}{\sqrt{\mu_i}} \right) & \text{For TE-Polarised light} \\
\left( \frac{\sqrt{\mu_i} \cos \theta_i}{\sqrt{\mu_i}} \frac{-\sqrt{\mu_i} \cos \theta_i}{\sqrt{\mu_i}} \right) & \text{For TM-Polarised light.}
\end{cases}
\]

(48)

The reflection coefficients of the right \( r_R \) and left \( r_L \) mirrors of FP resonator can be defined using these matrix translation operators as follows

\[
r_R = \left. \frac{B_i}{A_i} \exp(2ik_{ix}d_{ix}) \right|_{\substack{B_i = 0 \\ M_{R_{i1}} \neq 0}} = \frac{M_{R_{i1}}}{M_{R_{i1}}}
\]

(49)

\[
r_L = \left. \frac{A_i}{B_i} \right|_{\substack{A_i = 0 \\ M_{L_{i1}} \neq 0}} = -\frac{M_{L_{i2}}}{M_{L_{i1}}}
\]

(50)

where \( M_{L_{i1}} \) and \( M_{R_{i1}} \) are the matrix elements of left and right matrix translation operators. In the same fashion one can consider the stratified medium in the \( y \) direction to constitute a FP resonator with the upper layers and bottom layers as upper and bottom mirrors of the resonator denoted by indices U and D, respectively.
5. Results and discussion

In this section the calculation results are presented. A specific structure with definite parameters is defined in beginning of the section. After defining the structure parameters, its in-plane band structure is calculated for both E- and H-polarisations through the PWE method. Moreover, the LDOS results for both polarisations are presented with respect to frequency for five structures whose clusters differ in number of unit cells from one to nine. In the next, we verify the results by comparing LDOS result with what is obtained from band structure calculation through PWE method as a standard method for investigating the band gap formation. Since, the results of band gap calculation through the PWE method is for an infinite structure, we consider a larger structure consisting of 33 unit cells in order that the comparison between these two methods may be reasonable. In addition, the LDOS are illustrated versus the spatial coordinate in plane of the 2D structure for frequency placed within the gap region and out of the gap region. Furthermore, having introduced defect in SPP structure as a reduction or increase in width of the layers, we present a integrated structure consist of a point-like defect in the vicinity of a waveguide-like defect and analyse the variation of LDOS in the gap region.

Since Equation (39) is an analytical expression for calculating of the local density of states one can simply overcome the intractable problem which occurs at the critical points in a band. By solving Equation (39) numerically, the LDOS of the structure for E-Polarisation and H-Polarisation have been shown in the next figures. The clusters of rectangular rods are arranged in a square lattice with period \( L \) as illustrated in Figure 1. The fraction of \( d_i/L \) and \( d_{i-1}/L \) are considered to be 0.5 and the permittivity contrast of the layers in horizontal and the vertical direction is 0.5/5.78. This choice for index contrast causes to build a 2D structure with permittivity of \( n_2 = \epsilon_2 + \epsilon_4 = 3.4^2 \) at the centre of the unit cells, \( n_1^2 = \epsilon_1 + \epsilon_3 = 1^2 \) at the corners, \( n_2^2 = \epsilon_1 + \epsilon_4 = 2.5^2 \) and \( n_3^2 = \epsilon_2 + \epsilon_3 = 2.5^2 \) at the middle sides of the unit cells, respectively. Here, \( n_1, n_2, n_3 \) and \( n_4 \) are the refractive indices of the respective location in the structure. The geometry of the resulting structure consisting of \( 7 \times 7 \) unit cells is shown in Figure 4.

The computed in-plane band structure for the lattice through plane wave expansion (PWE) method is shown in Figure 5. We used \( 11 \times 11 \) harmonic plane waves in computing the band structure. Both TE- and TM-bands have been considered in solid and dashed lines in the figure, respectively. The 2D PC reveals two TE-gaps and one TM-gap in the in-plane band structure. Because of the harmonic expansion-based calculation in the PWE method, only the first several bands can be expected to be accurate. The first TE-gap is in the normalised frequency range \( \omega d/2\pi c = 0.258 - 0.28 (\Delta \omega/\omega_0 = 8.2\%) \) and the second one is very narrow in the range of \( \omega d/2\pi c = 0.452 - 0.466 (\Delta \omega/\omega_0 = 3\%) \). The only TM-gap is in the normalised frequency range \( 0.337 - 0.353 (\Delta \omega/\omega_0 = 4.6\%) \). It shows that the first TE-gap is about two times larger than the TM-gap and they do not have any overlap to each other so there is no complete gap but for specific polarisation.

The normalised LDOS, \( 2\pi g(d_i,k)/k \) for E-polarisation and H-polarisation are separately depicted in Figure 6(a) and (b) at the left edge of the central square for the clusters consist of 1, 3, 5, 7 and 9 unit cells in each direction. As shown
in these figures, there are only one strong optical mode suppression region $2.5 < \frac{c_0 d}{2\pi c} < 0.3$ for E-polarisation and one $3.2 < \frac{c_0 d}{2\pi c} < 4.2$ for H-polarisation and the suppression grows exponentially with cluster size. The 2D LDOS in the frequency region of the second TE-gap does not decrease with increasing the cluster size and it is maximum suppressed by a factor of about 10 with respects to the free space value.
For justifying the LDOS results, one can compare the region of low optical density in the LDOS figure with the gap formation through the PWE method. Note that unit cells in Figure 5 are infinite but in Figure 6 we have a limited number of unit cells. Even though the structure is finite but with increasing the number of unit cells to construct a larger 2D structure we can compare them to understand the LDOS results, although for an exact comparison one must do the sum over all LDOS quantity through the different sites to calculate the DOS quantity. Figure 7(a) and (b) show the normalised LDOS for a large cluster consist of 33 unit cells in each direction at the same location as Figure 6 for E- and H-polarisation, respectively.

As it has been shown in Figure 7, with increasing the size of the cluster up to 33 unit cells the LDOS in the first gap regions tend to zero. But, for the second TE-gap the LDOS does not vary with increasing the number of unit cell in the structure. The reason can be understood as follows. In the region of strong suppression the 2D LDOS sharply decrease with increasing the frequency and reaches to a minimum value at the top of the band gap followed by an abrupt jump above the gap. However, in the region of weak suppression the 2D LDOS decrease gently with increasing the frequency and then jump above the gap region. This saturation in the suppression grows might be happen towing to its small gap region.

The normalised LDOS in a specific normalised frequency has been calculated in Figures 8 and 9 so that the spatial variation of the LDOS would investigate at different sites within the structure. The results have been shown for a cluster of seven unit cells in each direction.
The spatial variation of LDOS in the frequency above the upper band of the first band gap region has been illustrated in Figure 8(b). Although the LDOS has been calculated outside the frequency band gap, suppression still occurs in the air regions inside the structure by a factor of 0.003 respects to the free space. This moderate suppression in LDOS is understood due to the defect-like air square regions that

Figure 6. (Colour online) 2D normalised LDOS located at left surface of the central square of the cluster versus normalised frequency is illustrated for different unit cells for (a) E-polarisation and (b) H-polarisation.
have been surrounded by high index rectangular rods. The LDOS varies around the air value of 1 inside the rectangular rods and can be enhanced within the outermost rods.

For the frequencies inside the band gap there would be a large area at the middle of the structure that LDOS suppression takes place. Specifically, the four square corner of the middle of the structure have the largest suppression. Therefore, one

Figure 7. 2D normalised LDOS versus normalised frequency for a cluster consist of 33 unit cells in each direction at the left edge of the central square for (a) TE-polarisation and (b) TM-polarisation.
Figure 8. The normalised LDOS, $2\pi g(d, k)/k$ for $E$-polarisation in the plane of the cluster consist of 7 unit cells in each direction in $x$–$y$ coordinates for (a) $\omega \alpha/2\pi c = 0.27$, that is in the middle of the first gap region and (b) $\omega \alpha/2\pi c = 0.3$, above the upper band of the first gap region.

Figure 9. The normalised defect LDOS, $2\pi g(d, k)/k$ for $E$-polarisation for the cluster consist of 7 unit cells in each direction in $x$–$y$ coordinates (a) versus normalised frequency (b) versus spatial coordinates in the plane of the structure in the onset of the first gap region at $\omega \alpha/2\pi c = 0.261$. The defect has been introduced by decreasing the width of the mid-layers located at the coordinates (12, 12) to (13, 13) by 200 nm.
would expect that the centre of the structure as well as its corners suppress the modes density that leads to the strong decrease of the rate of atomic spontaneous emission.

For calculating the defect Eigen frequencies, we introduce defect in the structure as a reduction or increase in the size or refractive index of one or several of the layers in the 1D resolved stepwise structure. The normalised LDOS at the middle of the structure as a function of normalised frequency has been illustrated in Figure 9(a) for defect and non-defect one. Also, Figure 9(b) shows the spatial variation of LDOS in the plane of the corresponding defect 2D structure at normalised frequency equal to 0.261. This frequency is the defect Eigen frequency of the structure which is placed in the gap region just above the dielectric band as illustrated in Figure 9(a). In this figure the defect was introduced through decreasing the width of the layer at the middle of the vertical and horizontal staircase profile by 200 nm which is corresponding to the reduction of the wide of the mid-layers of the 2D structure. The LDOS enhance by a factor of about 12 in the centre of the 2D structure. So, the spontaneous emission rate of an atom that placed in the defect can enhance by a factor of 12 with respect to its free space value. Introducing such a defect in middle of this structure causes to form localised defects mode in region in which there was a strong suppression in optical density and get it enhance the mode density by a factor of 12 related to the density of state in free space.

The significance of thickness of layers in formation of localised defect mode is also illustrated in Figure 10. The defect has been introduced through increasing the width of the layers in the middle of the resolved staircase profile by 200 nm and the corresponding of the 2D structure has been shown in the figure. The normalised LDOS versus the normalised frequency has been depicted in Figure 10(a) for the

![Figure 10](https://example.com/figure10.png)

Figure 10. (Colour online) The normalised LDOS, $2\pi g(d, k)/k$ for E-polarisation for the cluster consist of 7 unit cells in each direction in $x$–$y$ coordinates for (a) versus normalised frequency (b) versus spatial coordinates in the plane of the structure in the first gap region at $\omega_d / 2\pi c = 0.263$. The defect has been introduced by increasing the wide of the mid-layers located at the coordinates (12, 12) to (13, 13) by 200 nm.
central square rod in the 2D structure. The localised defect frequencies which have been created in band gap region (air band mode) have a peak in the LDOS at normalised frequency equal to 0.263. The enhancement drastically increases by a factor of 16 respects to its free space value. The variation of LDOS in the plane of the 2D structure has been illustrated in Figure 10(b).

As illustrated in Figures 9(b) and 10(b), the enhanced LDOS at the central square rod spread to the neighbouring rods in vertical and horizontal directions. Specially, it is quite considerable in the two vertical and horizontal mid-layers of the 2D structure crossing at the central square rod. The enhancement spread can be understood as follows. Introducing the defect into this 2D structure which is constructed through the two perpendicular staircase profiles cannot be a point-wise defect, but it extends to the 2D structure through a vertical or horizontal strips. After passing two layers in oblique directions of the central square except for those perpendicular strips the suppression takes place equal to 0.02 of its free space value in Figures 9(b) and 10(b). The enhancement that takes place at the central square rod of the 2D structure and spread to the two perpendicular mid-layers crossing the central square rod remains constant along the mid-layers in Figure 10(b) but decreases smoothly along the mid-layers in Figure 9(b) as moving away from the central square rod. The enhancement spread introduces a limit in decreasing the optical mode volume in the cavity. It is proportional to the area of the unit cell in the structure. This limitation can be considered as a deficiency in designing a cavity resonator.

The results gained from Figures 9 and 10 in the previous section suggest ideas to introduce some application using the defect SPP structure. As illustrated from Figure 10(b), the defect which has been introduced to the structure causes to form a region of enhanced LDOS with stable profile along the extended middle strips. This can be utilised as a line defect for propagation of electromagnetic radiation with frequency inside the gap region. The enhanced LDOS spread into the neighbouring layers is a key idea for coupling of optical modes in such a dielectric waveguides to the other neighbouring defect involving exchange of energy between modes which applies to design optical modulation, switching and power division in integrated optical system. Figure 11 shows the possibility of designing of a cavity resonator next to a waveguide which can be created inside a SPP structure consist of 9 unit cells in each direction. This component can act as a channel filter in optical communication [39,40].

The normalised LDOS has been shown at the centre of the cavity in Figure 11(a) as a function of normalised frequency for both defect and nondefect structure. The defects have been introduced through increasing the wide of the 15th layer of the horizontal resolved staircase profile and decreasing of the 11th layers of the horizontal and vertical resolved stair case profile by 200 nm. The incoming structure is a one cavity-like defect in the vicinity of a horizontal waveguide-like defect that has been introduced in SPP structure. A strong enhancement takes place just above the first band edge at normalised frequency $\omega a/2\pi c = 0.262$, with a value about four times greater than that of free space. The spatial variation of the LDOS in the plane of the defect SPP structure has been shown in Figure 11(b). The large value of LDOS can be consider as a attraction of electromagnetic wave to propagates through the area having large LDOS value. So, the large LDOS value in the defect area which is
illustrated in Figure 11(b), shows that coupling of available modes can be happen between the cavity-like defect and the line-like defect in the SPP structure.

6. Conclusions

The method of effective resonance in a resonator can be an appropriate way in which to calculate the local density of states as well as an efficient way in investigating of disorders in the finite structure. Using this approach, we calculate the LDOS in a SPP structure that is a rectangular-lattice PC with separable profile of permittivity. The LDOS have been calculated in different sites for the case of a finite-sized SPP structure with a cluster consist of 7 unit cells in each direction. We have shown that it is possible to design a microstructure which consists of a cavity in vicinity of a waveguide by introducing some defects in the SPP structure. It has been shown that the enhancement of LDOS takes place in the both cavity- and waveguide-like defect so that it may be used in the design of a channel drop filter.

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