Chapter 2

Theoretical Framework

Recently various methods have been proposed to calculate band structures of photonic crystals such as the plane-wave expansion method (PWEM),[44,45] the transfer matrix method,[46,47] the finite-difference time-domain (FDTD) method,[48] scattering matrix method,[49] and the finite element method.[50] Among these methods, the band structures of photonic band gap material have almost exclusively been obtained from the PWEM.

Plane-wave expansion method is a frequency domain for calculations of band structure and mode field in the general periodic structure. This full-vector method can treat macroscopic electromagnetic problems by applying periodic boundary, and the non-periodic (defect structure) system can also be solved by applying the super-cell technique. This method has been showing great promise to treat complicated PBG structures and real PBG devices. In this thesis, the plane-wave expansion method is employed to calculate band structures and mode fields, allowing us to investigate the optical properties of 2D photonic crystals.

Theory and features of PWEM will be formulated in this chapter. The issues and limitations of PWEM in obtaining accurate predictions of the optical properties of photonic crystal will also be briefly discussed. The propagation of electromagnetic waves in periodic structures will be formalized for models and arrangement. We will formulate the eigenvalue problem of the wave equation in the photonic crystal and give a general numerical method to solve it. Additionally, the structure factor plays an important role in the PWEM and it has a strong relation with the structural design of

photonic crystal. The structure factor for a given column will be described and proofed, and the transformation of structural factors with regard to a single rod will be interpreted and discussed in detail. The aim of this chapter is to provide us with the background necessary to support the theoretical investigations and views presented in following chapters.

2.1 Maxwell Equation

The photonic band gap can be obtained by solving Maxwell's equations. In a source-free space ($\rho = 0,\ J = 0$), time-invariant, lossless medium (dielectric constant is real) and nonpermeable $(\mu = \mu_0)$ space, Maxwell's equations in the most general form are given in SI units as follows,

$$\begin{aligned}
&\nabla \cdot \vec{D}(\vec{r},t) = 0, \\
&\nabla \cdot \vec{B}(\vec{r},t) = 0, \\
&\nabla \times \vec{E}(\vec{r},t) = \frac{-\partial}{\partial t}\vec{B}(\vec{r},t) \\
&\nabla \times \vec{H}(\vec{r},t) = \frac{\partial}{\partial t}\vec{D}(\vec{r},t)
\end{aligned} \tag{2.1}$$

The notations for electric field (***E***), magnetic field (***H***), electric displacement (***D***), and magnetic flux density (***B***) are used in these equations. Assuming the fields oscillate sinusoidal with time, so the fields can be written as $\vec{E}(\vec{r},t) = E(\vec{r}) \cdot \exp[i(\omega t - \vec{k} \cdot \vec{r})]$ and $\vec{H}(\vec{r},t) = H(\vec{r}) \cdot \exp[i(\omega t - \vec{k} \cdot \vec{r})]$.

Using $D(r) = \varepsilon_0 \varepsilon_r E(r)$, $B(r) = \mu_0 H(r)$ and $\partial/\partial t \to j\omega$, the time derivatives of Maxwell equations can be eliminated as,

$$\begin{aligned}
&\nabla \cdot \varepsilon(\vec{r})\vec{E}(\vec{r}) = 0, \\
&\nabla \cdot \vec{H}(\vec{r}) = 0, \\
&\nabla \times \vec{E}(\vec{r}) = -j\omega\mu_0 \vec{H}(\vec{r}), \\
&\nabla \times \vec{H}(\vec{r}) = j\omega\varepsilon_0 \varepsilon(\vec{r})\vec{E}(\vec{r}),
\end{aligned} \tag{2.2}$$

where ω is the eigen-angular frequency. We denote the dielectric constant of free space by ε_0 and the relative dielectric constant of the photonic crystal by $\varepsilon(r)$. When we eliminate $\vec{E}(\vec{r})$ or $\vec{H}(\vec{r})$ in equation (2.2), we obtain the following wave equations,

$$\vartheta_H \vec{H}(\vec{r}) = \nabla \times [\frac{1}{\varepsilon(\vec{r})} \nabla \times \vec{H}(\vec{r})] = \frac{\omega^2}{c^2} \vec{H}(\vec{r}), \tag{2.3}$$

$$\vartheta_E \vec{E}(\vec{r}) = \frac{1}{\varepsilon(\vec{r})} \nabla \times [\nabla \times \vec{E}(\vec{r})] = \frac{\omega^2}{c^2} \vec{E}(\vec{r}), \tag{2.4}$$

Equations (2.3) and (2.4) are so-called master equations. The transverse condition in (2.2) shows that ***H*** and ***D*** fields continue everywhere, but ***E*** field is discontinuous. For $\varepsilon(r)$ is a highly discontinuous function, so ***E*** field is not proper for calculation. For this reason, it is more convenient to use ***H*** to get ***E***, instead of using ***E*** to get ***H***, i.e. we use equation (2.3) to calculate band structure of photonic crystal. When we solve the master equation in equation (2.3), the allowable modes ***H(r)*** can be found for a given frequency. Then ***E(r)*** can be obtained by following relation,

$$\vec{E}(\vec{r}) = \frac{1}{j\omega\varepsilon_0\varepsilon(\vec{r})} \nabla \times \vec{H}(\vec{r}) \tag{2.5}$$

Equation (2.3) is a standard eigenvalue problem. The operator ϑ_H acts on eigenvector ***H(r)***, and the eigenvalue $\frac{\omega^2}{c^2}$ are proportional to the squared frequencies of those modes. Note that the operator ϑ_H has some important features,

1. ϑ_H is a linear operator. If ***H₁(r)*** and ***H₂(r)*** are both modes with the same frequency, then linear combination of (α ***H₁(r)***+ β ***H₂(r)***) is also a mode, where α and β are constants.

2. ϑ_H is a Hermitian operator. We know $(f, \vartheta_H g) = (\vartheta_H f, g)$ for any vector fields f and g. The operator ϑ_H acts on ***H(r)*** must have real eigenvalues. Moreover, we consider ϑ_H forces any two normalized modes ***H₁(r)*** and ***H₂(r)*** with different frequency ω_1 and ω_2. Using the relations of $\vartheta_H H(\vec{r}) = (\frac{\omega}{c})^2 H(\vec{r})$ and

$(H, \vartheta_H H) = (\frac{\omega}{c})^2 (H, H)$, we can obtain,

$$\begin{aligned} &(H_1, \vartheta_H H_2) = (\frac{\omega_2}{c})^2 (H_1, H_2) = (\vartheta_H H_1, H_2) = (\frac{\omega_1}{c})^2 (H_1, H_2) \\ &\Rightarrow (\omega_1^2 - \omega_2^2)(H_1, H_2) = 0 \end{aligned} \tag{2.6}$$

(1). If two modes have different frequencies ($\omega_1 \neq \omega_2$), then we must have $(H_1, H_2) = 0$. That is ***H₁(r)*** and ***H₂(r)*** orthogonal to each other.

(2). If two modes have the same frequencies ($\omega_1 = \omega_2$), then we say these modes are the degenerate modes.

2.2 Periodicity of Dielectric Function

To solve the electromagnetic problem for a photonic crystal, it is necessary to impose that the dielectric function is periodic. The periodicity can be in one, two or three dimensions and the photonic crystal correspondingly is one-, two-, or three dimensions. Notice that the dielectric function of a photonic crystal is made of a unit cell repeated in space according to a well defined pattern. In this framework, the periodicity of the dielectric function implies,

$$\varepsilon(\vec{r} + \vec{T}) = \varepsilon(\vec{r}), \qquad \vec{T} = \ell_1 \vec{a}_1 + \ell_2 \vec{a}_2 + \ell_3 \vec{a}_3 \tag{2.7}$$

where $\vec{T}$ is translation vector, $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$ are elementary lattice vectors, $\{\ell_i\}$ are arbitrary integers. Because of the spatial periodicity, the inverse of dielectric function in the master equation can be expanded in a Fourier series.

$$\varepsilon(\vec{r}) = \sum_G \varepsilon(\vec{G}) \exp(i\vec{G} \cdot \vec{r}), \qquad \vec{G} = h_1 \vec{b}_1 + h_2 \vec{b}_2 + h_3 \vec{b}_3 \tag{2.8}$$

where $\vec{G}$ is reciprocal vector, $\vec{b}_1$, $\vec{b}_2$ and $\vec{b}_3$ are elementary reciprocal lattice vectors. $\{h_i\}$ are arbitrary integers. Two sets of basic vectors are orthogonal to each other, and they are related by,

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$$

$$\begin{cases} \vec{b}_1 = 2\pi \dfrac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \\ \vec{b}_2 = 2\pi \dfrac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \\ \vec{b}_3 = 2\pi \dfrac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \end{cases} \tag{2.9}$$

The expansion coefficient $\varepsilon(\vec{G})$ in equation (2.8) can be solved by calculating the inverse Fourier transform,

$$\varepsilon(\vec{G}) = \frac{1}{\mathrm{V}_0} \int_{\mathrm{V}_0} dr \ \varepsilon(\vec{r}) \exp(-i\vec{G} \cdot \vec{r}) \tag{2.10}$$

where V_0 denotes the volume of the unit cell of the photonic crystal. From equaiton (2.10), it is obviously that the coefficient $\varepsilon(\vec{G})$ is mainly dominated by the dielectric function (related to the geometry and arrangement of rods) and lattice vectors (related to the lattice types).

2.3. Bloch Theorem for Periodic Structure

In periodic structure, the plane waves propagated in the periodic structure will be modulated by periodicity. According to the Bloch theorem, the magnetic field in equation (2.3) can be expressed as,

$$\vec{H}(\vec{r}) = h(\vec{r}) \exp(i\vec{k} \cdot \vec{r}) \hat{\mathrm{e}}_k$$

where $h(\vec{r})$ is a periodic function that satisfy the relation of $h(\vec{r} + \vec{T}) = h(\vec{r})$. $\vec{k}$ is a wave vector in the first Brillouin zone. $\hat{\mathrm{e}}_k$ is an unit vector parallel to the ***H(r)*** and perpendicular to the wave vector $\vec{k}$. Like the expression of $\varepsilon(\vec{r})^{-1}$ in equation (2.8), the periodic function $h(\vec{r})$ can also be expanded in Fourier series,

$$h(\vec{r}) = \sum_G h(\vec{G}) \exp(i\vec{G} \cdot \vec{r})$$

So, the magnetic field can be expressed as,

$$\vec{H}(\vec{r}) = \sum_{G,\lambda} h(\vec{G},\lambda)\exp[i(\vec{k}+\vec{G})\cdot\vec{r}]\hat{e}_\lambda, \tag{2.11}$$

Two independent polarizations characterized by the unit vectors $\hat{e}_\lambda(\lambda = 1,2)$ are perpendicular to the propagation vector $(\vec{k}+\vec{G})$. Considering light to propagate perpendicularly to the rods, we can decouple light propagation from H-polarization and E-polarization modes whose magnetic and electric fields, respectively, are parallel to the rods.

Putting equations (2.8) and (2.11) into (2.3), then the wave equation can be transformed to linear matrix equations,

$$\sum_{G'}\left|\vec{k}+\vec{G}\right|\left|\vec{k}+\vec{G}'\right|\begin{bmatrix}\hat{e}_2\cdot\varepsilon^{-1}_{G,G'}\cdot\hat{e}_2' & -\hat{e}_2\cdot\varepsilon^{-1}_{G,G'}\cdot\hat{e}_1' \\ -\hat{e}_1\cdot\varepsilon^{-1}_{G,G'}\cdot\hat{e}_2' & \hat{e}_1\cdot\varepsilon^{-1}_{G,G'}\cdot\hat{e}_1'\end{bmatrix}\begin{bmatrix}h_{1,G'} \\ h_{2,G'}\end{bmatrix} = \frac{\omega^2}{c^2}\begin{bmatrix}h_{1,G} \\ h_{2,G}\end{bmatrix}, \tag{2.12}$$

where $\varepsilon^{-1}_{G,G'} = \varepsilon^{-1}(\vec{G}-\vec{G}')$ represents the inverse of the matrix $\varepsilon(\vec{G}-\vec{G}')$. The eigenvalue equation (2.12) is real and symmetric, then it can be solved using the matrix diagonalization technique. For two-dimensional photonic crystal, the dielectric constant is periodicity in the x-y plane and invariant along the z direction. For the condition of in-plane propagation, i.e. $\vec{k}_z = 0$, the unit vectors $\hat{e}_2 = \hat{e}_z$ and $\hat{e}_1$ are in the x-y plane, the polarization modes $h_{1,G'}$ and $h_{2,G'}$ become decoupled. Furthermore, the master equation (2.12) can be decomposed separately into H-polarization and E-polarization modes,

$$\sum_{G'}\left|\vec{k}+\vec{G}\right|\left|\vec{k}+\vec{G}'\right|\varepsilon^{-1}(\vec{G}-\vec{G}')h_{1,G'} = \frac{\omega^2}{c^2}h_{1,G'}, \quad \text{for E-polarization mode} \tag{2.13}$$

$$\sum_{G'}(\vec{k}+\vec{G})\cdot(\vec{k}+\vec{G}')\varepsilon^{-1}(\vec{G}-\vec{G}')h_{2,G'} = \frac{\omega^2}{c^2}h_{2,G'}, \text{ for H-polarization mode} \tag{2.14}$$

Theoretically, the number of ***G*** vectors should be set infinitely. However, this is difficult to set infinite number of ***G*** vectors in the calculation. In the actual numerical calculation of the photonic bands, the summation in equation (2.13) and (2.14) need

to be calculated up to a sufficiently large number ***N*** of reciprocal lattice vectors ***G***, and an eigenvalue problem for each $\vec{k}$ can be solved, which is equivalent to the diagonalization of the matrix defined by the left-hand side equations. In short, the lower-frequency bands of interest can be approached very well when the number of ***G*** vectors is large enough.

The band structure in the photonic crystal is presented as a $\vec{k}-\omega$ relation. Only $\vec{k}$ points in the first Brillouin zone are considered to calculate the band structures. Because of the periodicity in the photonic crystal, the frequencies correspond to $\vec{k}$ points outside the Brillouin zone will fall inside the first Brillouin zone by considering the translation property.

2.4. Dielectric Function

The plane-wave expansion method is based on the Bloch theorem, which states that the eigenvalue equations with periodic coefficient may be expressed as a product of plane waves and lattice-periodic functions. Thus, the periodic functions can be expanded into appropriate Fourier series. Since the eigenvalue problem of equations (2.13) and (2.14) is a standard problem, the difficulty lies in evaluating the Fourier transforms of different structures. Such columns' shape, lattice geometry and dimensionality have the different Fourier transforms. As seen in equation (2.10), the inverse Fourier transform is strong related to the shape of rods and should be prior to derive before solving the master equation. The most common shapes of column such as the cross sections of cylinder, hexagonal, square and diamond are extensively studied in the photonic crystals.[29,36,42] Here we only show a simple case of circular cross-section organized in a square lattice to get its Fourier coefficients. Generally, there are only two media in a PBG structure, the rod and the background material,

and very often one material in air, so actually only one material is used. In the case, we denote the radius and the dielectric constant of the circular column by r_a and ε_a, respectively, and the dielectric constant of the background material by ε_b. The dielectric constant $\varepsilon(\vec{r})$ is a position-dependent function, and it can be written with the concept of spatial position. As shown in Fig. 2.1, the dielectric constant can be written as,

$$\varepsilon(\vec{r}) = \varepsilon_b + \varepsilon_a \cdot S(\vec{r}) - \varepsilon_b \cdot S(\vec{r}) = \varepsilon_b + (\varepsilon_a - \varepsilon_b) \cdot S(\vec{r}) \tag{2.15}$$

where $S(\vec{r})$ is a function for the rod and is defined such that,

$$S(r) = \begin{cases} 1 & for \quad |r| \le r_a, \\ 0 & for \quad |r| > r_a, \end{cases}$$

Substituting (2.15) into equation (2.10), the Fourier coefficient can be expressed as,

$$\varepsilon(\vec{G}) = \frac{1}{V_0}\int_{V_0} \varepsilon_b e^{-i\vec{G}\cdot\vec{r}}\,dr + \frac{1}{V_0}\int_{V_0} (\varepsilon_a - \varepsilon_b)\cdot S(r) e^{-i\vec{G}\cdot\vec{r}}\,dr$$

Now we evaluate the first integral $I_1(\vec{G})$ and the second integral $I_2(\vec{G})$ separately,

Evaluation of $I_1(\vec{G})$,

The first integral is easily evaluated as:

$$I_1(\vec{G}) = \begin{cases} \varepsilon_b & if \quad \vec{G}_p = 0 \\ 0 & elsewhere \end{cases}$$

Evaluation of $I_2(\vec{G})$,

$$If \quad \vec{G}_p = 0, \quad I_2(\vec{G}) = (\varepsilon_a - \varepsilon_b)\frac{\pi r_a^2}{V_0} = (\varepsilon_a - \varepsilon_b)\cdot f$$

$$If \quad \vec{G}_p \neq 0, \quad I_2(\vec{G}) = \frac{(\varepsilon_a - \varepsilon_b)}{V_0}\int_{V_0} S(r) e^{-i\vec{G}\cdot\vec{r}}\,dr = (\varepsilon_a - \varepsilon_b)\cdot S(\vec{G})$$

Here, we denote the volume fraction of the circular rods by $f = \frac{\pi r_a^2}{V_0}$ and the structure factor of this structure by $S(\vec{G}) = \frac{1}{V_0}\int_{V_0} S(r) e^{-i\vec{G}\cdot\vec{r}}\,dr = \frac{1}{V_0}\int_{Rod} e^{-i\vec{G}\cdot\vec{r}}\,dr$.

For this case, we use the polar coordinate (r,φ) in the system and the integral can

be modified to,

$$\int_{V_0} S(r)e^{-i\vec{G}\cdot\vec{r}}dr = \int_0^{r_a} dr \int_0^{2\pi} d\varphi\, r \exp[iGr\sin(\varphi - \frac{\pi}{2})]$$

$$= \int_0^{r_a} dr \int_0^{2\pi} d\varphi\, r \sum_{\ell=-\infty}^{\infty} J_\ell(Gr)\exp[i\ell(\varphi - \frac{\pi}{2})]$$

where $G = |\vec{G}|$ and $J_\ell(Gr)$ is the Bessel function of the ℓ_{th} order. Upon using $\int xJ_0(\alpha x)dx = x/\alpha\, J_1(\alpha x)$ and $\exp[i\omega\sin(\varphi)] = \sum_{\ell=-\infty}^{\infty} J_\ell(\omega)\exp(i\ell\varphi)$, we continue with,

$$\int_{V_0} S(r)e^{-i\vec{G}\cdot\vec{r}}dr = 2\pi\int_0^{r_a} rJ_0(Gr)dr = \frac{2\pi r_a}{G}J_1(Gr_a)$$

and,

$$I_2(\vec{G}) = \frac{(\varepsilon_a - \varepsilon_b)}{V_0}\frac{2\pi r_a}{G}J_1(Gr_a) = (\varepsilon_a - \varepsilon_b)\frac{2f}{Gr_a}J_1(Gr_a)$$

This lead to the final result that:

$$\varepsilon(\vec{G}) = \begin{cases} \varepsilon_a \cdot f + \varepsilon_b \cdot (1-f) & \text{for G=0} \\ (\varepsilon_a - \varepsilon_b)\cdot\dfrac{2f}{Gr_a}J_1(Gr_a) & \text{elsewhere} \end{cases} \qquad (2.16)$$

The expressions of dielectric function for various columns are shown as follows. Here we only consider the two-dimensional photonic crystal.

1. Square Rod

$$\varepsilon(\vec{G}) = \begin{cases} \varepsilon_a \cdot f + \varepsilon_b \cdot (1-f) & \text{for } G_x = 0,\ G_y = 0 \\ \dfrac{(\varepsilon_a - \varepsilon_b)}{A_u}\cdot\dfrac{4}{G_xG_y}\cdot\sin(\dfrac{G_xd}{2})\sin(\dfrac{G_yd}{2}) & \text{for } G_x \neq 0,\ G_y \neq 0 \\ \dfrac{(\varepsilon_a - \varepsilon_b)}{A_u}\cdot\dfrac{2d}{G_y}\cdot\sin(\dfrac{G_yd}{2}) & \text{for } G_x = 0,\ G_y \neq 0 \\ \dfrac{(\varepsilon_a - \varepsilon_b)}{A_u}\cdot\dfrac{2d}{G_x}\cdot\sin(\dfrac{G_xd}{2}) & \text{for } G_x \neq 0,\ G_y = 0 \end{cases}$$

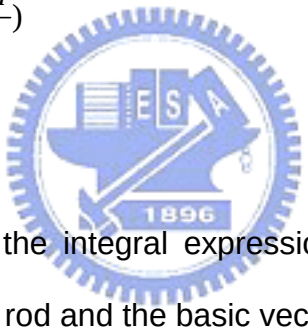
where A_u is the cross-section area of a unit lattice, d is the length of each side of the square; and G_x and G_y are the x and y component of $\vec{G}$, respectively.

2. Hexagonal Rod

$$\varepsilon(\vec{G}) = \begin{cases} \varepsilon_a \cdot f + \varepsilon_b \cdot (1-f) & \text{for } G_x = 0,\ G_y = 0 \\ \dfrac{(\varepsilon_a - \varepsilon_b)}{A_u} \cdot \dfrac{4}{G_y^2 - 3G_x^2} \cdot [\sqrt{3}\cos(\dfrac{\sqrt{3}G_x d}{2})\cos(\dfrac{G_y d}{2}) & \\ -\sqrt{3}\ \cos(G_y d) - 3\dfrac{G_x}{G_y}\sin(\dfrac{\sqrt{3}G_x d}{2})\sin(\dfrac{G_y d}{2}) & \text{for } G_x \neq 0,\ G_y \neq 0 \\ \dfrac{(\varepsilon_a - \varepsilon_b)}{A_u} \cdot \dfrac{1}{\sqrt{3}G_x^2} \cdot [1 - \cos(\sqrt{3}G_x d) & \\ +\sqrt{3}G_x \cdot d\sin(\sqrt{3}G_x d)] & \text{for } G_x \neq 0,\ G_y = \pm\sqrt{3}G_x \end{cases}$$

3. Diamond Rod

$$\varepsilon(\vec{G}) = \begin{cases} \varepsilon_a \cdot f + \varepsilon_b \cdot (1-f) & \text{for } G_x = 0,\ G_y = 0 \\ \dfrac{(\varepsilon_a - \varepsilon_b)}{A_u} \cdot \dfrac{4}{G_x^2 - G_y^2} \cdot [\cos(\dfrac{G_x d}{2}) - \cos(\dfrac{G_y d}{2})] & \text{for } G_x \neq 0,\ G_y \neq 0 \\ \dfrac{(\varepsilon_a - \varepsilon_b)}{A_u} \cdot \dfrac{d}{G_x} \cdot \sin(\dfrac{G_x d}{2}) & \text{for } G_x = 0,\ G_y = \pm G_x \end{cases}$$



From above mentions, the integral expressions of structure factor are mainly determined by the shapes of rod and the basic vectors of lattice. The structure factors for regular rods are easy to derive, but that for the irregular rods are complex and difficult to derive. In last chapter, we have described that the shape of rod and the type of lattice strongly affect the photonic band structure. Moreover the degenerated band in the Brillouin zone may be split by reducing the symmetry of photonic crystal. The deformation and rotation are the common and immediate methods to change the symmetry of photonic crystal. When the rods or lattices are designed into the irregular shapes with deformation and rotation, it may provide an opportunity to increase the PBG width for either the E-polarization or H-polarization modes and to increase the PBG overlapping the E-polarization and H-polarization photonic band gaps. In order to construct the structure factor of irregular rods easily, some features of operation in

the PWEM need to evaluate. These operations include translation, rotation and scaling and are described as follows.

1. Translation Operation

When the coordinate of system is transformed by a displacement of r_0, the new structure factor $S'(\vec{G})$ can be obtained by applying the translation operation,

$$S'(\vec{G}) = T_t[S(\vec{G})] = \exp(-i\vec{G}\cdot\vec{r}_0)S(\vec{G}) \tag{2.17}$$

This translation property is also useful to the Fourier transform for the supercell.

2. Rotation Operation

When the rods in the photonic crystal are rotated by an arbitrary angle θ, it is equivalent to rotate the coordinate of the system by an arbitrary angle θ. Therefore, the original $\vec{G}$ vectors in the x-y plane can be transformed by a matrix,

$$\begin{pmatrix} G'_x \\ G'_y \end{pmatrix} = T_r \begin{pmatrix} G_x \\ G_y \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} G_x \\ G_y \end{pmatrix} \tag{2.18}$$

where G_x and G_y are the components of original $\vec{G}$ vectors. G'_x and G'_y are the $\vec{G}'$ vectors in the new system. Under this rotation operation, the structure factor can be transformed as,

$$S'(\vec{G}) = T_r[S(\vec{G})] = S(T_r[\vec{G}]) \tag{2.19}$$

3. Scaling Operation

When the shape or dimension of rods is changed, it is equivalent to change the dimension of coordinate of the system. Assuming the dimensions of original rods in x- and y-axis are ℓ_x and ℓ_y respectively. Now we deform the rods and their dimensions in x- and y-axis are $\ell_x' = \lambda_x \ell_x$ and $\ell_y' = \lambda_y \ell_y$ respectively. We can write,

$$\begin{pmatrix} \ell'_x \\ \ell'_y \end{pmatrix} = T_r \begin{pmatrix} \ell_x \\ \ell_y \end{pmatrix} = \begin{pmatrix} \lambda_x & 0 \\ 0 & \lambda_y \end{pmatrix} \begin{pmatrix} \ell_x \\ \ell_y \end{pmatrix}$$

Under this operation,

$$T_s[\vec{G}\cdot\vec{r}] = \vec{G}\cdot T_s[\vec{r}] = T_s[\vec{G}]\cdot\vec{r} \qquad \text{and} \qquad dA'_{rod} \to \lambda_x\lambda_y dA_{rod}$$

Thus, the new structure factor under the scaling operation is,

$$S'(\vec{G}) = T_s[S(\vec{G})] = \lambda_x\lambda_y S(T_s[\vec{G}]) \tag{2.20}$$

2.5. Mode Field Calculation

The mode-field calculation for a given band and a specific k point is helpful to understand and evaluate the formed photonic band gap. After the eigenvalue problem is solved, the eigenvalue and associated eigenvector can be obtained, allowing us to calculate the field pattern. The eigenvalue is real for eiegnvalue solution, but the real and imaginary parts are both solutions for mode-field calculation. The analytical forms for calculating field pattern are described as follow.

For the E-polarization modes, the displacement field $\vec{D}$ is along z axis and it can be written as,

$$\begin{aligned}\vec{D}_{n,\bar{k}}(\vec{r}) &= \varepsilon(\vec{r})\vec{E}(\vec{r}) = \varepsilon(\vec{r})\frac{-ic}{\omega\varepsilon(\vec{r})}\nabla\times\vec{H}_{n,\bar{k}}(\vec{r}) \\ &= \frac{-ic}{\omega}\sum_G h_1(\vec{G})i(\vec{k}+\vec{G})\times\hat{e}_1 e^{i(\bar{k}+\vec{G})\cdot\vec{r}} \\ &= \frac{1}{|\vec{k}|}\sum_G |\vec{k}+\vec{G}| h_1(\vec{G}) e^{i(\bar{k}+\vec{G})\cdot\vec{r}}\ \hat{e}_z\end{aligned} \tag{2.21}$$

For the H-polarization modes, the displacement field $\vec{D}$ is in x-y axis. In fact, the displacement field in in-plane is not easy to find the difference in field patterns between dielectric and air bands at the same k point. The displacement field for the H-polarization modes is,

$$\vec{D}_{n,\vec{k}}(\vec{r}) = \varepsilon(\vec{r})\vec{E}(\vec{r}) = \varepsilon(\vec{r})\frac{-ic}{\omega\varepsilon(\vec{r})}\nabla\times\vec{H}_{n,\vec{k}}(\vec{r})$$
$$= \frac{-ic}{\omega}\sum_{G} i(\vec{k}+\vec{G})\times\hat{e}_z e^{i(\vec{k}+\vec{G})\cdot\vec{r}} h_1(\vec{G}) \qquad (2.22)$$
$$= \frac{1}{\left|\vec{k}\right|}\sum_{G}\left|\vec{k}+\vec{G}\right| h_1(\vec{G}) e^{i(\vec{k}+\vec{G})\cdot\vec{r}}\ \hat{e}_2$$

Here the subscript n labels the bands. Finally, it follows from the orthonormality of equation (2.12) that the Bloch functions $\vec{H}_{n,\vec{k}}$ and $\vec{E}_{n,\vec{k}}$ obey the orthonormality relations,

$$\int \vec{H}_{n,\vec{k}}(\vec{r})\cdot\vec{H}^{*}_{n',\vec{k}'}(\vec{r})dr = \delta(\vec{k}-\vec{k}')\delta_{n,n'}$$
$$\int \varepsilon(\vec{r})\vec{E}_{n,\vec{k}}(\vec{r})\cdot\vec{E}^{*}_{n',\vec{k}'}(\vec{r})dr = \delta(\vec{k}-\vec{k}')\delta_{n,n'}$$

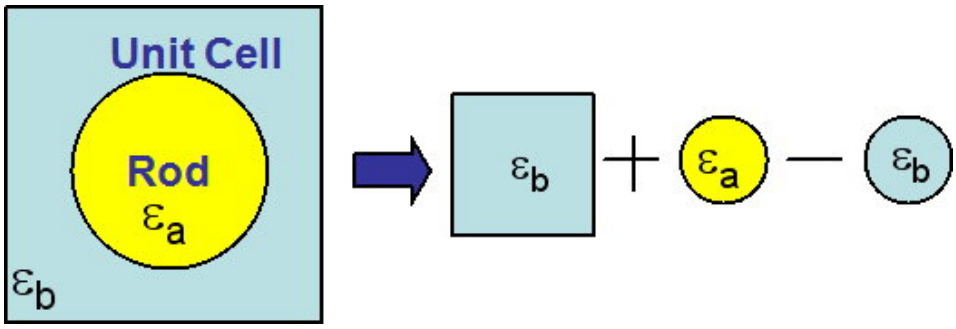


Figure 2.1 Schematic illustration of the unit cell construction for the circular dielectric rod.