Chapter 2 Theory and Calculation method

The propagation of light in a photonic crystal is governed by the four macroscopic Maxwell's equations. [34] Because we are interested in dielectric medium, we assume that the free charge and the electric current are absent. In MKS units they are

$$\nabla \cdot \vec{D}(\vec{r}, t) = 0, \tag{2.1}$$

$$\nabla \cdot \vec{B}(\vec{r}, t) = 0, \tag{2.2}$$

$$\nabla \times \vec{E}(\vec{r}, t) = -\frac{\partial}{\partial t}\vec{B}(\vec{r}, t), \tag{2.3}$$

$$\nabla \times \vec{H}(\vec{r}, t) = \frac{\partial}{\partial t}\vec{D}(\vec{r}, t). \tag{2.4}$$

where **E** and **H** are the macroscopic electric and magnetic fields, **D** and **B** are the displacement and magnetic induction field.

2-1 Introduction [35][36]

In order to solve the wave equations derived from Maxwell's equations, we need the constitution equation between **D** to **E** and **B** to **H**. Since we do not deal with magnetic material, we assume the permeability of the material is equal to that in free space:

$$\vec{B}(\vec{r}, t) = \mu_0 \vec{H}(\vec{r}, t). \tag{2.5}$$

In general, the relation between **D** with **E** can be written as:

$$D = \varepsilon_0 \varepsilon E + 2dE^2 + 4\chi^{(3)} E^3 + \dots \tag{2.6}$$

For simplifying the question, we make four assumptions. First we assume the field strengths are small enough so that they are in the linear regime, or the operation frequency region far away from the resonance frequency region of the photonic materials. Second, we assume the medium is macroscopic and isotropic, so that **E**(**r**,ω) and **D**(**r**,ω) are related by a scalar dielectric constant ε(**r**,ω). Third, we ignore any explicit frequency dependence of the dielectric constant so the materials which construct the photonic crystals are non-dispersive. Four, we assume the material does not absorb the EM wave so the ε(**r**,ω) is treated as a real. According to the last four assumptions, the relation between **D** and **E** can be rewritten as this form:

$$\vec{D}(\vec{r}) = \varepsilon(\vec{r})\vec{E}(\vec{r}). \tag{2.7}$$

If a monochromatic electromagnetic wave is incident, all components of the electric and magnetic fields are harmonic functions of time and the same frequency.

$$\begin{aligned}\vec{H}(\vec{r},t) &= \vec{H}(\vec{r})\cdot e^{i\omega t} \\ \vec{E}(\vec{r},t) &= \vec{E}(\vec{r})\cdot e^{i\omega t}\end{aligned}\ . \tag{2.8}$$

When we substitute (2.8) into (2.1) ~ (2.4), we obtain the following equations:

$$\Theta_E \vec{E}(\vec{r}) \equiv \frac{1}{\varepsilon(\vec{r})}\nabla\times\{\nabla\times\vec{E}(\vec{r})\} = \frac{\omega^2}{c^2}\vec{E}(\vec{r}), \tag{2.9}$$

$$\Theta_H \vec{H}(\vec{r}) \equiv \nabla\times\{\frac{1}{\varepsilon(\vec{r})}\nabla\times\vec{H}(\vec{r})\} = \frac{\omega^2}{c^2}\vec{H}(\vec{r}). \tag{2.10}$$

The (2.9) and (2.10) are the eigen-value problems, and that Θ_H is a Hermitian operator. That means the eigen functions $\mathbf{H_n}$ of Θ_H form an orthonormal complete set. Because ε(**r**) is a period function, we can apply the Bloch's theorem to (2.9) and (2.10). These wave equations can be solved by so-called plane-wave expanding method.

2-2 K.P theory with perfect crystal

2-2.1 One-band model

In photonic crystals, ε (**r**) is periodic function of the spatial coordinate **r**,

$$\varepsilon(\vec{r}+\vec{a})=\varepsilon(\vec{r}), \tag{2.11}$$

where **a** is any lattice vector.

The eigenstates of (2.10) are Bloch functions. According to Bloch theory, we can write $\mathbf{H}_{\mathbf{k}n}$ as the following form:

$$\vec{H}_n(\vec{k},\vec{r})=e^{i\vec{k}\cdot\vec{r}}\vec{u}_{\vec{k}n}(\vec{r}), \tag{2.12}$$

where n is a band index and **k** lies within the first Brillouin zone. The function u(**r**) has the same periodicity with e(**r**), i.e., **u**(**r**+**a**)=**u**(**r**). The Bloch functions $\mathbf{H}_n$(**k**,**r**) form a complete set of the (2.10):

$$\int \vec{H}_n^*(\vec{k}',\vec{r})\vec{H}_m(\vec{k},\vec{r})d\vec{r}=\delta_{nm}\delta_{\vec{k},\vec{k}'}. \tag{2.13}$$

From this orthogonal relation u_n(**k**,**r**) has the follow property:

$$\left\langle \vec{u}_n(\vec{k},\vec{r})\middle|\vec{u}_m(\vec{k},\vec{r})\right\rangle=\delta_{nm}. \tag{2.14}$$

where we define

$$\langle\vec{u}|\vec{v}\rangle=\int_{cell}\vec{u}^*\cdot\vec{v}\,d\vec{r}. \tag{2.15}$$

In order to investigate the properties of photonic crystals, we introduce the new basis as follows:

$$\vec{H}(\vec{r})=\sum_{np}A_n(\vec{k})\vec{H}_{np\vec{k}_0}(\vec{r})\exp(i\vec{S}\cdot\vec{r}), \tag{2.16}$$

S=**k**-$\mathbf{k_0}$,

where $\mathbf{k_0}$ is a specific wave-vector which we are interested, $\mathbf{H}_{np\mathbf{k_0}}$ (**r**) are the eigen-functions of (2.10) at wave-vector $\mathbf{k_0}$ and the corresponding eigenvalues are $\omega_n(\mathbf{k_0})$. The eigenvalue and eigenvector can be derived by the plane-wave expansion method. **S** is the displacement of wave-vector. In our case, we suppose S= |**S** |<<1 and k_0 is near the band edge where the band maximum and minimum occur. A_n(**k**) is the expansion coefficients where n again is a band index and p represents the index of physical solutions ($\omega_n(\mathbf{k_0}) \neq 0$) and unphysical solutions ($\omega_n(\mathbf{k_0}) = 0$).

Now, we introduce a new set of basis:

$$\vec{\chi}_{n\vec{k}}(\vec{r}) \equiv \vec{H}_{np}(\vec{k}_0, \vec{r})\exp(-i\vec{S}\cdot\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\vec{u}(\vec{k}_0, \vec{r}) . \tag{2.17}$$

The properties of orthonormality and completeness can be easily prooved that

$$\int \vec{\chi}^*_{nq}(r)\cdot\vec{\chi}_{mk}(r)dr = \delta_{nm}\delta_{kq} , \tag{2.18}$$

$$\sum_n \int \chi^*_n(k,r)\,\chi_n(k,r')dk = \delta(r-r') . \tag{2.19}$$

From (2.17), we can get $\vec{\chi}_{nk}(\vec{k},\vec{r})$ also obeys the Bloch's theorem for a wave vector ***k***

$$\vec{\chi}_n(\vec{k}, r+a) = \exp(ik\cdot a)\vec{\chi}_n(\vec{k}, r) , \tag{2.20}$$

where ***a*** is lattice constant. For a plane wave $\mathbf{H}_{n\mathbf{k}}(\mathbf{r})$ can be expanded by $\vec{\chi}_n(\mathbf{k}, r)$ as [28]

$$\vec{H}_n(\vec{k},\vec{r}) = \sum_j A_{nj}(\vec{k})\vec{\chi}_j(\vec{k},\vec{r}), \tag{2.21}$$

$$A_{nj} = \int \vec{H}^*_n(\vec{k},\vec{r})\cdot\vec{\chi}_j(\vec{k},\vec{r})d\vec{r} . \tag{2.22}$$

Since $\vec{H}_n(\vec{k},\vec{r})$ must satisfy (2.10), we operate Θ_H at $\vec{\chi}_{n\mathbf{k}}(r)$

$$\begin{aligned}\vec{P}\times\left[\frac{1}{\varepsilon(\vec{r})}\vec{P}\times\vec{\chi}_{j\vec{k}}(\vec{r})\right] = e^{i(\vec{k}-\vec{k}_0)\cdot\vec{r}}\Big\{&\hbar(\vec{k}-\vec{k}_0)\times\left[\frac{\hbar(\vec{k}-\vec{k}_0)}{\varepsilon(\vec{r})}\times\vec{H}_{jk_0}(\vec{r})\right] + \\ &\vec{P}\times\left[\frac{\hbar(\vec{k}-\vec{k}_0)}{\varepsilon(\vec{r})}\times\vec{H}_{jk_0}(\vec{r})\right] + \hbar(\vec{k}-\vec{k}_0)\times\left[\frac{1}{\varepsilon(\vec{r})}\vec{P}\times\vec{H}_{jk_0}(\vec{r})\right] - E_j(\vec{k}_0)\vec{H}_{jk_0}(\vec{r})\Big\}\end{aligned} , \tag{2.23}$$

where $\vec{P} \equiv -i\hbar\vec{\nabla}$, $E \equiv (\hbar\omega/c)^2$. Put (2.23) into (2.10) and multiply the equation by $\vec{u}^*_{l\vec{k}_0}(\vec{r})$ and integrate over a unit cell of the crystal. We can get

$$\Gamma_{lj} - E_n(\vec{k})\delta_{lj} = 0 , \tag{2.24}$$

$$\begin{aligned}\Gamma_{lj} = E_j(\vec{k}_0)\delta_{jl} + \hbar^2(\vec{k}^2 - \vec{k}_0^2)\,\lambda_{lj}(\vec{k}_0) - \hbar^2\sum_{ab}(k^a k^b - k_0^a k_0^b)\theta^{ab}_{lj}(\vec{k}_0) \\ + i\hbar(\vec{k}-\vec{k}_0)\cdot\vec{p}_{lj}(\vec{k}_0)\end{aligned} . \tag{2.25}$$

We define

$$\vec{p}_{lj}(\vec{k}_0)=\vec{P}_{lj}(\vec{k}_0)+\vec{W}_{lj}(\vec{k}_0)-\vec{U}_{lj}(\vec{k}_0)-\vec{V}_{lj}(\vec{k}_0)$$

$$\begin{aligned}
l_{lj}(\vec{k}_0) &= \left\langle \vec{u}_l(\vec{k}_0,\vec{r}) \middle| \frac{1}{\varepsilon(\vec{r})}\vec{u}_j(\vec{k}_0,\vec{r}) \right\rangle \\
P^{\alpha}_{lj}(\vec{k}_0) &= \left\langle \vec{u}_l(\vec{k}_0,\vec{r}) \middle| \frac{\hbar}{i}\partial_{\alpha}\frac{\vec{u}_j(\vec{k}_0,\vec{r})}{\varepsilon(\vec{r})} \right\rangle \\
q^{\alpha\beta}_{lj}(\vec{k}_0) &= \left\langle u^{\alpha}_l(\vec{k}_0,\vec{r}) \middle| \frac{1}{\varepsilon(\vec{r})}u^{\beta}_j(\vec{k}_0,\vec{r}) \right\rangle \\
\vec{U}_{lj}(\vec{k}_0) &= \left\langle \vec{u}_l(\vec{k}_0,\vec{r}) \middle| \frac{\hbar}{i}\nabla\frac{1}{\varepsilon(\vec{r})}\cdot\vec{u}_j(\vec{k}_0,\vec{r}) \right\rangle \\
\vec{V}_{lj}(\vec{k}_0) &= \left\langle \vec{u}_l(\vec{k}_0,\vec{r}) \middle| \frac{\hbar}{\varepsilon(\vec{r})i}\nabla\cdot\vec{u}_j(\vec{k}_0,\vec{r}) \right\rangle \\
\vec{W}_{lj}(\vec{k}_0) &= \int_{cell}\frac{1}{\varepsilon(\vec{r})}\vec{u}^{*}_l\times\left(\frac{\hbar}{i}\nabla\right)\times\vec{u}_j(\vec{k}_0,\vec{r})\,d\vec{r}
\end{aligned} \quad . \qquad (2.26)$$

where $\partial_{\alpha}=\partial/\partial x^{\alpha}$ and $u^{\alpha}_l(\vec{k}_0,\vec{r})$ is the α component of $\vec{u}_l(\vec{k}_0,\vec{r})$. If we make unitary transformation and ignore the term which has the order of $\vec{s}=\vec{k}-\vec{k}_0$ larger than two we can get:

$$\begin{aligned}
E_n(\vec{k}) = {} & E_n(\vec{k}_0)+\hbar^2(\vec{k}^2-\vec{k}_0^2)\,l_{nn}(\vec{k}_0)-\hbar^2\sum_{\alpha\beta}(k^{\alpha}k^{\beta}-k_0^{\alpha}k_0^{\beta})q^{\alpha\beta}_{nn}(\vec{k}_0) \\
& +i\hbar(\vec{k}-\vec{k}_0)\cdot\vec{p}_{nn}(\vec{k}_0)+\hbar^2\sum_j\frac{(\vec{s}\cdot\vec{p}_{nj}(\vec{k}_0))(\vec{s}\cdot\vec{p}_{jn}(\vec{k}_0))}{E_n(\vec{k}_0)-E_j(\vec{k}_0)}
\end{aligned} \quad . \qquad (2.27)$$

If $\vec{k}_0$ is the extreme of the band

$$\frac{dE_n(\vec{k})}{dk^r}\bigg|_{\vec{k}=\vec{k}_0}=0\,, \qquad (2.28)$$

the $E_n(\vec{k})$ can be rewritten as

$$E_n(\vec{k})=E_n(\vec{k}_0)+\hbar^2\,\vec{s}^2\,l_{nn}(\vec{k}_0)-\hbar^2\sum_{\alpha\beta}s^{\alpha}s^{\beta}q^{\alpha\beta}_{nn}(\vec{k}_0)+\hbar^2\sum_j\frac{(\vec{s}\cdot\vec{p}_{nj}(\vec{k}_0))(\vec{s}\cdot\vec{p}_{jn}(\vec{k}_0))}{E_n(\vec{k}_0)-E_j(\vec{k}_0)}. \qquad (2.29)$$

Define a reciprocal effective dielectric tensor equation that has a similar structure of the effective-mass equation in semiconductors:

$$
\begin{aligned}
\left(\frac{1}{\varepsilon^*}\right)_{\alpha\beta} &\equiv \frac{1}{2\hbar^2}\frac{\partial^2 E_n(\vec{k}_0)}{\partial k^\alpha \partial k^\beta} \\
&= \lambda_{nn}(\vec{k}_0)\delta_{\alpha\beta} - \theta^{\alpha\beta}_{nn}(\vec{k}_0) - \theta^{\beta\alpha}_{nn}(\vec{k}_0) + \frac{1}{2}\sum_j \frac{p^\beta_{nj}(\vec{k}_0)p^\alpha_{jn}(\vec{k}_0) + p^\alpha_{nj}(\vec{k}_0)p^\beta_{jn}(\vec{k}_0)}{E_n(\vec{k}_0) - E_j(\vec{k}_0)} . \qquad (2.30)
\end{aligned}
$$

Using the reciprocal effective-dielectric tensor of (2.30), the (2.29) can be written as an eigenvalue equation

$$E_n(\vec{k})A_n(\vec{k}) = [E_n(\vec{k}_0) + \sum_{\alpha\beta}\hbar^2\left(\frac{1}{\varepsilon^*}\right)_{\alpha\beta}\sigma^\alpha\sigma^\beta]A_n(\vec{k}) . \qquad (2.31)$$

(2.30) is the well-known effective-mass equation, written, however, in momentum space. To get more useful formulation, we introduce an envelope function

$$F_n(\vec{r}) = \int e^{i\vec{\sigma}\cdot\vec{r}}A_n(\vec{k})d^3\vec{k} , \qquad (2.32)$$

where the integration being over the first Brillouin zone . Thus, we have

$$\left(\frac{\hbar\omega_n}{c}\right)^2 F_n(\vec{r}) = [\left(\frac{\hbar\omega_n(\vec{k}_0)}{c}\right)^2 - \sum_{\alpha\beta}\hbar^2\left(\frac{1}{\varepsilon^*}\right)_{\alpha\beta}\frac{\partial}{\partial x_\alpha}\frac{\partial}{\partial x_\beta}]F_n(\vec{r}) , \qquad (2.33)$$

where α and β are indices of three different directions of $\mathbf{r}$. We can also transform Eq. (2.33) back to the time space to study the temporal evolution of $F(\vec{r},t)$. We have a tensor equation:

$$-\frac{\partial^2}{\partial t^2}F_n(\vec{r},t) = [\left(\frac{\hbar\omega_n(\vec{k}_0)}{c}\right)^2 - \sum_{\alpha\beta}\hbar^2\left(\frac{1}{\varepsilon^*}\right)_{\alpha\beta}\frac{\partial}{\partial x_\alpha}\frac{\partial}{\partial x_\beta}]F_n(\vec{r},t) . \qquad (2.34)$$

Eq. (2.34) is equivalent to the Maxwell equation of (2.10), under the K.P theory, which is the generalized Klein-Gordon equation and can be reduced to the Klein-Gordon equation in isotropic medium. In this equation, the band interaction is decoupled and the coupling effect is introduced into $(1/\varepsilon^*)$ that can be determined by (2.30) with the simulation result (dispersion relation) of plane-wave wave expansion method. This equation indicates there is an energy-storing mechanism near band edges, thus we can define $m_n=\eta\omega_n(\mathbf{k}_0)/c^2$ as the inertial mass of quasi-particle(QP) of photon. The inertial mass m_n is dependent on the band index n and is quantized. We can extend the one-band approximation to the two-band approximation in next section, if the band mixing has to be considered.

2-2.2 Two-band model

In solid state physics, the theoretical models for calculating the electronic properties of quantum wells and super-lattices fall into two categories: those based on tight-binding methods and those based on K.P theory. [37] Now we introduce the two band model in solid state physics to explain the phenomenon in photonic crystals.

From (2.24), if we consider the wave-vectors are in principle axes this equation can be rewritten as

$$\Gamma_{lj} = E_j(\vec{k}_0)\delta_{jl} + i\hbar(\vec{k}-\vec{k}_0)\cdot\vec{p}_{lj}(\vec{k}_0)\,. \tag{2.35}$$

When we care about the light traveling at the frequency in first and second band, the bands coupling with high order bands can be neglected. (2.35) forms a coupled dielectric and air band model.

$$\begin{bmatrix} E_a & i\hbar^2\vec{s}\cdot\vec{p} \\ i\hbar^2\vec{s}\cdot\vec{p} & E_d \end{bmatrix}\begin{bmatrix} f \\ g \end{bmatrix} = E\begin{bmatrix} f \\ g \end{bmatrix}, \tag{2.36}$$

where E_a and E_d are the air- and dielectric-band-edge energies, f and g are the eigenfunctions of air band and dielectric band, E is the eigen energy, $\vec{p} = \vec{p}/\hbar$. A specific case is considered that the light is normal incident to k_x direction. Thus we may set k_y and k_z equal to zero and Eq(2.36) becomes

$$\begin{bmatrix} E_a - E & i\hbar^2 sp \\ -i\hbar^2 sp & E_d - E \end{bmatrix}\begin{bmatrix} f \\ g \end{bmatrix} = 0\,. \tag{2.37}$$

For a bulk photonic crystal, we can then solve for the square of the wave vector difference in teams of the energy:

$$s^2 = (E - E_a)(E - E_d)/\text{h}^4 p^2 . \qquad (2.38)$$

First, we consider the light traveling in the energy of air band, (2.36) may be written in the form

$$(E - E_a) = s^2 \text{h}^2 / e^* , \qquad (2.39)$$

where the energy-dependent effective dielectric constant ε *(E) in air band is

$$e^*(E) = \frac{E - E_d}{\text{h}^2 p^2} = \frac{E - E_a}{\text{h}^2 p^2} + \frac{E_g}{\text{h}^2 p^2} . \qquad (2.40)$$

In the equation, E_g is the energy gap between air band and dielectric band, i.e., $Eg=E_a-E_d$. For convenience, we define the effective dielectric constant at air-band edge, i.e., $E=E_a$ is

$$e\%0 = \frac{E_g}{\text{h}^2 p^2} \quad \text{or} \quad p = \frac{1}{\text{h}} \sqrt{E_g / e\%0} , \qquad (2.41)$$

then the energy-dependent effective dielectric constant of (2.40) can be expressed in term of the air-band-edge effective dielectric constant as

$$e^*(E) = e\%0 \left(1 + \frac{E - E_a}{E_g}\right) . \qquad (2.42)$$

Inserting (2.41) into (2.37), we can get

$$\begin{bmatrix} E_a - E & i\text{h}s\sqrt{\dfrac{E_g}{e\%0}} \\ -i\text{h}s\sqrt{\dfrac{E_g}{e\%0}} & E_d - E \end{bmatrix} \begin{bmatrix} f \\ g \end{bmatrix} = 0 . \qquad (2.43)$$

Similarity, if we consider the light traveling in dielectric band, (2.38) may be written in the form

$$(E - E_d) = s^2 \text{h}^2 / e^* . \qquad (2.44)$$

The energy-dependent effective dielectric constant ε *(E) in dielectric band is

$$e^*(E) = \frac{E-E_a}{h^2 p^2} = \frac{E-E_d}{h^2 p^2} + \frac{E_g}{h^2 p^2}\,, \tag{2.45}$$

and the effective dielectric constant at the dielectric band-edge is

$$\tilde{e} = \frac{E_g}{h^2 p^2} \quad \text{or} \quad p = \frac{1}{h}\sqrt{E_g / \tilde{e}}\,, \tag{2.46}$$

and (2.45) become

$$e^*(E) = \tilde{e}\left(1 + \frac{E-E_d}{E_g}\right). \tag{2.47}$$

Inserting (2.46) into (2.37), we can still get (2.43). Putting the experiment result or simulation result with plane-wave expansion method into (2.47) and (2.42), we can obtain the energy-dependent effective dielectric constants in all allowed air and dielectric band. In next section, we will introduce the calculated effective dielectric constant into photonic crystal with defect. By the effective dielectric constant, we can expand how light is trapped in the defect potential well.

2-3 K.P theory with localized defect mode

2-3.1 One-band model

If we introduce the defect or disorder perturbation to (2.10), we obtain

$$\nabla \times [\frac{1}{\in(\mathbf{r})}(1+V(\mathbf{r}))\nabla \times \mathbf{H}(\mathbf{r})] = \frac{w^2}{c^2}\mathbf{H}(\mathbf{r})\,, \tag{2.48}$$

where $\in(\vec{r})$ is the periodic dielectric constant. The normalized defect dielectric function is $V(\vec{r}) = -\in'(\vec{r})/(\in(\vec{r})+\in'(\vec{r}))$ and $\in'(\vec{r})$ is the difference of dielectric constant between the bulk and defects or index disorder. By deriving (2.48) as in the section 2-2 (previous section), we can get

$$\begin{aligned}&(E_l(\vec{k}_0)-E)A_n d_{nl} + \sum_n h(\vec{k}-\vec{k}_0)\cdot\vec{p}_{nl}(\vec{k}_0)A_n + \sum_n \int d\vec{k}A_n\left[l\vec{k}\,|\,V\,|\,n\vec{k}_0\right] + \\ &\sum_n \int d\vec{k}A_n\left[l\vec{k}\,|\,\nabla V\,|\,n\vec{k}_0\right] = 0\end{aligned}\,, \tag{2.49}$$

where we define

$$\left[l\vec{k}\,|\,V\,|\,n\vec{k}_0\right] = E_n(\vec{k}_0)\int d\vec{r}\,e^{i(\vec{k}-\vec{k}_0)\cdot\vec{r}}\,V(\vec{r})\,\vec{u}_l^*(\vec{k}_0,r)\cdot\vec{u}_n(\vec{k}_0,r)\,, \tag{2.50}$$

and neglect $\sum_n \int d\vec{k}A_n\left[l\vec{k}\,|\,\nabla V\,|\,n\vec{k}_0\right]$ because we assume the V vary smoothly and the potential well is shallow. The product $\vec{u}_l^*(\vec{k}_0)\cdot\vec{u}_n(\vec{k}_0)$ has the same periodicity with $\varepsilon(\mathbf{r})$ of bulk crystal. So $\vec{u}_l^*(\vec{k}_0)\cdot\vec{u}_n(\vec{k}_0)$ can be expanded by reciprocal lattice vector

$$\vec{u}_l^*(\vec{k}_0,\vec{r})\cdot\vec{u}_n(\vec{k}_0,\vec{r}) = \sum_m B_{nl}(\vec{g}_m)e^{i\vec{g}_m\cdot\vec{r}}\,. \tag{2.51}$$

We get B_{nl} by inversion Fourier transformation

$$B_{nl}(g_m) = \int_{cell}\vec{u}_l^*(\vec{k}_0,\vec{r})\cdot\vec{u}_n(\vec{k}_0,\vec{r})e^{-i\vec{g}_m\cdot\vec{r}}d\vec{r}\,. \tag{2.52}$$

On account of the orthonormality of the $\vec{u}_n(\vec{k}_0,\vec{r})$, we can get

$$B_{nl}(0) = \delta_{nl}\,. \tag{2.53}$$

Inserting (2.51) into (2.50), we get

$$\left[l\vec{k}\,|\,V\,|\,n\vec{k}_0\right] = E_n(k_0)\sum_m B_{nl}(\vec{k}_m)\int e^{i(\vec{k}-\vec{k}_0+\vec{g}_m)\cdot\vec{r}}V(\vec{r})d\vec{r}\,. \tag{2.54}$$

If V(**r**) is varying sufficiently slowly, $\vec{g}_m \neq 0$ can be neglected.

$$\left[l\vec{k}\,|\,V\,|\,n\vec{k}_0\right] = E_n(k_0)\delta_{nl}V(\vec{k}-\vec{k}_0)\,, \tag{2.55}$$

$$V(\vec{k}-\vec{k}_0) = \int e^{i(\vec{k}-\vec{k}_0)\cdot\vec{r}}V(\vec{r})d\vec{r}\,. \tag{2.56}$$

Put (2.55) into (2.49) and neglect the last term of (2.49), we obtain

$$(E_l(\vec{k}_0)-E)A_n\delta_{nl} + \sum_n \hbar(\vec{k}-\vec{k}_0)\cdot\vec{p}_{nl}(\vec{k}_0)A_n + E_n(k_0)\delta_{nl}V(\vec{k}-\vec{k}_0) = 0\,. \tag{2.57}$$

After taking unitary transformation to diagonalize (2.57) in one band approximation and transferring back to real space, we can get

$$\frac{(i\hbar)^2}{c^2}\frac{\partial^2}{\partial t^2}F_n(\vec{r},t) = [E_n(\vec{k}_0) - \sum_{\alpha\beta}(\frac{\hbar^2}{\varepsilon^*})_{\alpha\beta}\frac{\partial}{\partial x^\alpha\partial x^\beta} + U(\vec{r})]F_n(\vec{r},t)\,. \tag{2.58}$$

where U(**r**)= $(m_n c)^2$V(**r**). U(**r**) is a potential produced by the defect. When we add a dielectric defect in the air band, i.e., V(**r**)<0 and $\varepsilon^*>0$, U(**r**) is negative and becomes an attractive potential for the air-band QP (quasi-particle). When we add an air defect in the dielectric band, i.e., V(**r**)>0 and $\varepsilon^*<0$, U(**r**) is still an attractive potential for the dielectric-band QP. When defect potential is given the envelop function $F_n(\vec{r},t)$ can be solved. If we consider an incident harmonic wave, the eigen energy can be solved from (2.58)

When we applied the one-band $\mathbf{k}\cdot\mathbf{p}$ theory to study photons traveling in photonic crystal through the defect, the incident photon excites a QP from the periodic dielectric constant in the crystal. The QP possesses an inertial mass and hence experiences an attractive potential in the defect. It become like quantum mechanics that electron can be trapped by a defect no matter how shallow or narrow the defect is. But an arbitrarily weak attractive potential can bind a state in one dimension, but not in two or three dimensions.

2-3.2 Two-band model

In the present of an external disorder, when we consider defect energy is located between air band and dielectric band, i.e., with in the band gap, (2.57) is written as

$$\begin{bmatrix} E_a(1+V)-E & \hbar\vec{p}\cdot\vec{s} \\ -\hbar\vec{p}\cdot\vec{s} & E_d(1+V)-E \end{bmatrix}\begin{bmatrix} f \\ g \end{bmatrix}=0. \qquad (5.59)$$

As the same definition in section 2-2.2 , (5.59) becomes

$$\begin{bmatrix} E_a(1+V)-E & i\hbar^2\vec{s}\cdot\vec{p} \\ -i\hbar^2\vec{s}\cdot\vec{p} & E_d(1+V)-E \end{bmatrix}\begin{bmatrix} f \\ g \end{bmatrix}=0. \qquad (5.60)$$

For concreteness, when we let light travel in x direction or just calculate the 1D photonic crystal the vector in (5.60) will become scalar. After transferring it to real space, we can get

$$\begin{bmatrix} E_a(1+V) & \hbar\sqrt{\dfrac{E_g}{\varepsilon^*}}\dfrac{d}{dx} \\ -\hbar\sqrt{\dfrac{E_g}{\varepsilon^*}}\dfrac{d}{dx} & E_d(1+V) \end{bmatrix}\begin{bmatrix} f \\ g \end{bmatrix} = E\begin{bmatrix} f \\ g \end{bmatrix}. \tag{2.61}$$

As we discuss in section 2-3.1, when we add air defect in bulk photonic crystals, the eigen-energy (E) will rise from dielectric band energy (E_d). On the other hand, when we add dielectric in bulks, the eigen-energy will decrease from air band energy. This phenomenon still can be expanded well in two-band model. In dielectric defect, the normalized defect constant (V) is negative and the band-edge effective dielectric constant ($e*$) is positive. It is an attractive potential. The larger the disorder the more negative V is and the eigen energy will be lower. However, when we add air defect in bulk PCs, V is positive and $e*$ is negative. It is also an attractive potential. The larger the disorder the more positive V is . The eigen energy will become higher. From (2.61), we can qualitatively explain the localized defect mode. In next chapter, we will try to solve (2.61) in 1-D case and 2-D case. With small defect perturbation, the simulation result of two-band model will match well with the exact solution which is solved directly from the Plane-wave expansion method.

2-4 Finite different time domain method

The finite-difference time-domain method is introduced by Yee in 1966. [38] [39] During the 1970s and 1980s, several defense agencies working in the areas motivated large-scale solutions of Maxwell's equations. The entire field of computation electrodynamics is shifting rapidly in high-speed communications and computing. In 1990, engineers in the general electromagnetic community became aware of the modeling capabilities afforded by FDTD and related techniques and the interest in this area has expanded well beyond defense technology. The main reason we introduce FDTD method to solve photonic crystal is that when the structure is too complex, it is hard to solve Maxwell's equation in frequency domain. FDTD provide a straight forward to solve it in time domain. With this method, we can see the field distribution in photonic crystals. In addition, there are several advantages in FDTD method. First, FDTD is accurate and robust. The sources of error are well known. Second, being a time domain technology, FDTD treats impulsive behavior and nonlinear behavior naturally. Third, FDTD uses no linear algebra. Being a fully explicit computation, FDTD avoids the difficulties with linear algebra that limit the size of frequency-domain integral-equation.

One-dimensional photonic crystal formulation

The time-dependent Maxwell's curl equations in dielectric medium are

$$\frac{\partial \vec{E}}{\partial t} = \frac{1}{\varepsilon(r)\varepsilon_0}\nabla \times \vec{H}, \tag{2.62}$$

$$\frac{\partial \vec{H}}{\partial t} = -\frac{1}{\mu_0}\nabla \times \vec{E}. \tag{2.63}$$

E and **H** are vectors in three dimensions. When we start with a 1-D simple case, we can let **E** in x direction and **H** in y direction. (2.62) and (2.63) become

$$\frac{\partial E_x}{\partial t} = -\frac{1}{\varepsilon(r)\varepsilon_0}\frac{\partial H_y}{\partial z} \tag{2.64}$$

$$\frac{\partial H_y(t)}{\partial t} = -\frac{1}{\mu_0}\frac{\partial E_x(t)}{\partial z} \tag{2.65}$$

(2.64) and (2.65) are very similar, but because ε_0 and μ_0 differ by several orders of magnitude. This is circumvented by making the following change of variables:

$$\tilde{E} = \sqrt{\frac{\varepsilon_0}{\mu_0}}E \tag{2.66}$$

Substituting this in to (2.64) and (2.65) gives

$$\frac{\partial \tilde{E}_x}{\partial t} = -\frac{1}{e(r)\sqrt{e_0 m_0}}\frac{\partial H_y}{\partial z}, \qquad (2.67)$$

$$\frac{\partial H_y(t)}{\partial t} = -\frac{1}{\sqrt{e_0 m_0}}\frac{\partial \tilde{E}_x(t)}{\partial z}, \qquad (2.68)$$

and then go to the finite difference approximations

$$\frac{\tilde{E}_x^{n+1/2}(k) - \tilde{E}_x^{n-1/2}(k)}{\Delta t} = \frac{-1}{e\sqrt{e_0 m_0}}\frac{H_y^n(k+1/2) - H_y^n(k-1/2)}{\Delta t}\ , \qquad (2.69)$$

$$\frac{H_y^{n+1}(k+1/2) - H_y^n(k+1/2)}{\Delta t} = \frac{-1}{\sqrt{e_0 m_0}}\frac{\tilde{E}_x^{n+1/2}(k+1) - \tilde{E}_x^{n+1/2}(k)}{\Delta x}. \qquad (2.70)$$

Let us return to discuss the stability. An electromagnetic wave propagating in free space cannot go faster than the speed of light. So the relationship between Δx and Δt can be written as the well-known “Courant Condition”

$$\Delta t \le \frac{\Delta x}{\sqrt{d}\,c}, \qquad (2.71)$$

where d is the dimension of the simulation and c is the speed of light. In this section, we will determine Δt by

$$\Delta t = \frac{\Delta x}{2c}. \qquad (2.72)$$

Substituting (2.72) into (2.69) and (2.70), those Equations become

$$\tilde{E}_x^{n+1/2}(k) = \tilde{E}_x^{n-1/2}(k) - \frac{0.5}{e}(H_y^n(k+1/2) - H_y^n(k-1/2))\ , \qquad (2.73)$$

$$H_y^{n+1}(k+1/2) = H_y^n(k+1/2) - 0.5[\tilde{E}_x^{n+1/2}(k+1) - \tilde{E}_x^{n+1/2}(k)]\,. \qquad (2.74)$$

Besides the last two iterative equations, we still need to add incident wave source condition and absorbing boundary condition. It is a great subject in dealing with the wave source condition. For simplicity, we divide it into two categories in 1-D case: hard source and soft source. In a hard source, a propagation wave will see that value and be reflected, because the hard value of E_x looks like a metal wall to FDTD. However a soft source is added to E_x at a certain point and a propagating pulse will just pass through. In calculating photonic crystal, we must consider the field scattering from the material. Therefore we use a soft source.

$$\begin{aligned} pulse &= \sin(2\pi f * dt * t) \\ E_x &= E_x + pulse \end{aligned} . \tag{2.75}$$

Absorbing boundary conditions are necessary to keep outgoing **E** and **H** fields from being reflected. From (2.72), the traveling distance in one time step of the FDTD algorithm is

$$disatnce = c \cdot \Delta t = c \cdot \frac{\Delta x}{c} = \frac{\Delta x}{2} . \tag{2.76}$$

This equation basically explains that it takes two steps for a wave front to cross one cell. So the boundary conditions might be

$$\begin{aligned} E_x^n(0) &= E_x^{n-2}(1) \\ E_x^n(k) &= E_x^{n-2}(k-1) \end{aligned} , \tag{2.77}$$

where 0 and k are the end points and n is a time step. With the iterative equation, wave source and absorbing boundary condition, the electric field or magnetic field in 1-D photonic crystals can be solved easily.

Two-dimensional photonic crystal formulation

When we start with the Maxwell's equation in (2.3) and (2.4) and normalize it by these equations

$$\begin{aligned} \tilde{E} &= \sqrt{\frac{\varepsilon_0}{\mu_0}} \vec{E} \\ \tilde{D} &= \sqrt{\frac{1}{\varepsilon_0 \mu_0}} \vec{D} \end{aligned} , \tag{2.78}$$

we will get the normalized Maxwell's equations

$$\frac{\partial \tilde{D}}{\partial t} = \frac{1}{\sqrt{e_0 m_0}} \nabla \times \vec{H} \,, \tag{2.79}$$

$$\tilde{D}(w) = e\,(w)\tilde{E}(w)\,, \tag{2.80}$$

$$\frac{\partial \vec{H}}{\partial t} = -\frac{1}{\sqrt{e_0 m_0}} \nabla \times \tilde{E}. \tag{2.81}$$

In simulation a two dimensional case, the six different fields can be divided into two groups: (1) the transverse magnetic (TM) modes ($\tilde{E}_z, H_x, H_y$) and (2) transverse electric (TE) mode ($\tilde{E}_x, \tilde{E}_y, H_z$). We will work with TM mode and TE mode can be deal with the similar method. In TM mode, (2.79) ~ (2.81) are now reduced to

$$\frac{\partial D_z}{\partial t} = \frac{1}{\sqrt{e_0 m_0}} \left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right), \tag{2.82}$$

$$D_z(w) = e(w) E_z(w)\,, \tag{2.83}$$

$$\frac{\partial H_x}{\partial t} = -\frac{1}{\sqrt{e_0 m_0}} \frac{\partial E_z}{\partial y}\,, \tag{2.84}$$

$$\frac{\partial H_y}{\partial t} = \frac{1}{\sqrt{e_0 m_0}} \frac{\partial E_z}{\partial x}\,. \tag{2.85}$$

Put (2.82), (2.84) and (2.85) into the finite difference scheme, and take equivalent incremental step in x and y direction, these equation become

$$\begin{aligned} \frac{D_z^{n+1/2}(i,j) - D_z^{n-1/2}(i,j)}{\Delta t} = \frac{1}{\sqrt{e_0 m_0}} \bigg(& \frac{H_y^n(i+1/2,j) - H_y^n(i-1/2,j)}{\Delta x} \\ & - \frac{H_x^n(i,j+1/2) - H_x^n(i,j-1/2)}{\Delta x} \bigg) \end{aligned}, \tag{2.86}$$

$$\frac{H_x^{n+1}(i,j+1/2) - H_x^n(i,j+1/2)}{\Delta t} = -\frac{1}{\sqrt{e_0 m_0}} \frac{E_y^{n+1/2}(i,j+1) - E_y^{n+1/2}(i,j)}{\Delta x}\,, \tag{2.87}$$

$$\frac{H_y^{n+1}(i+1/2,j)-H_y^{n}(i+1/2,j)}{\Delta t}=\frac{1}{\sqrt{e_0 m_0}}\frac{E_z^{n+1/2}(i+1,j)-E_z^{n+1/2}(i,j)}{\Delta x}. \tag{2.88}$$

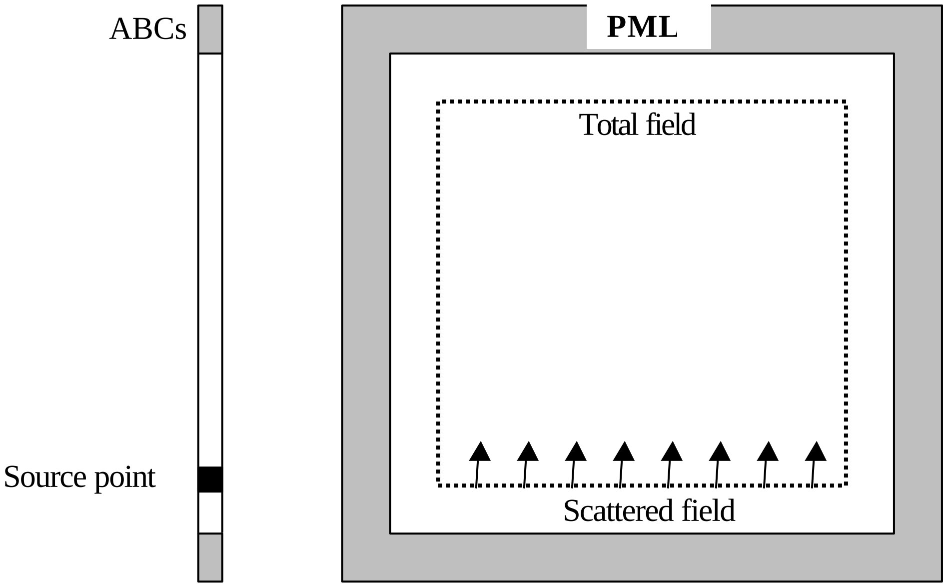

Fig. 2-1 Total fields/scattered field of the 2-D problem space

The size of the area that can be simulated using FDTD is limited by computer resources. In order to decrease the computing time, simulation area must be limited. At the boundary of the simulation area, we use the perfectly matched layer (PML) method to minimize the reflection from boundary. If we want to simulate a plane wave in a 2-D FDTD program, we must use the total field and the scattered field (TF/CF) method to divide the problem space into two regions. The primary reasons for doing this is: (1) The propagating plane wave should not interact with the absorbing boundary condition; (2) the load on the absorbing boundary conditions should be minimized.

By subtracting the incident field, the amount of the radiating field hitting the boundary is minimized, thereby reducing the amount of error.

2-5 Transfer matrix method

Let’s consider the propagation of a wave through 1-D PCs consisting of N layers with thicknesses a and b and refractive indices n_a and n_b.[40]

$$n_j = \begin{cases} n_i, & j = 0 \\ n_a, & j = 1,3,5,....,N(N-1) \\ n_b, & j = 2,4,6,....,N(N-1) \\ n_o, & j = N+1 \end{cases} , \tag{2.89}$$

$$d_j = \begin{cases} a, & j = 1,3,5,....,N(N-1) \\ b, & j = 1,3,5,....,N(N-1) \end{cases} . \tag{2.90}$$

The wave vector in j layer can be written as $k_j = n_j k_0$, where $k_0 = w/c$. We search for the field amplitude E_j in the jth layer as a superposition of incident and reflected wave:

$$E_j = A_j e^{i(k_j x - wt)} + B_j e^{i(-k_j x - wt)} , \tag{2.91}$$

where A_j and B_j are the amplitudes of the forward and backward waves, respectively. When we match the boundary conditions which require that the tangential components of electric field and magnetic field must be continuous, we can get the relationship layer by layer.

$$\begin{aligned} & E_r - A_1 - B_1 = -E_{i,} \quad k_i E_r + k_1 A_1 - k_1 B_1 = -k_i E_{i,} \\ & A_1 e^{ik_1 a} + B_1 e^{-ik_1 a} - A_2 - B_2 = -E_{i,} - k_1 A_1 e^{ik_1 a} + k_1 B_1 e^{-ik_1 a} + k_2 A_2 - k_2 B_2 = 0,... \\ & A_N e^{ik_N d_N} + B_N e^{-ik_N d_N} - E_t = 0, -k_N A_N e^{ik_N d_N} + k_N B_N e^{-ik_N d_N} - k_o E_t = 0 \end{aligned} \tag{2.92}$$

where E_0, E_t, and E_r are the amplitude of incident, transmission and reflection field.(2.92) can be written as a matrix form:

$$\begin{aligned} & T_{2N+2,2N+2} E_{2N+2} = S_{2N+2} \\ & E^T_{2N+2} = \begin{pmatrix} E_t & A_1 & B_1 & A_2 & B_2 & ... & A_N & B_N & E_t \end{pmatrix} . \\ & S^T_{2N+2} = \begin{pmatrix} -1 & k_i & 0 & ... & 0 \end{pmatrix} \end{aligned} \tag{2.93}$$

$$T=\begin{pmatrix} 1 & -1 & -1 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ k_i & k_1 & -k_1 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & e^{ik_1a} & e^{-ik_1a} & -1 & -1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & -k_1e^{ik_1a} & k_1e^{ik_1a} & k_2 & -k_2 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{ik_2b} & e^{-ik_2b} & -1 & -1 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & -k_2e^{ik_2b} & k_2e^{-ik_2b} & k_1 & -k_1 & \dots & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & e^{ik_Nd_N} & e^{-ik_Nd_N} & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & -k_Ne^{ik_Nd_N} & k_Ne^{-ik_Nd_N} & k_0 \end{pmatrix}$$

Substituting E_{2N+2} into Eq. (2.91), we will get the electric field distribution in each layer. From the solutions of these equations, i.e., E_r and E_t, transmittance and reflection rate of the electric field will be find.

$$t=\left|E_t\right|, \tag{2.94}$$

$$r=\left|E_r\right|. \tag{2.95}$$

In 1-D case, transfer matrix method (TMM) is an exact solution so it can get more correct solution than FDTD method. Especially, when we calculate the defect mode, the line width of frequency is very narrow. If we want to get more correct result in FDTD method, the calculating time and space interval must be very small. It is time consuming. So TMM is a better way in calculating 1-D PCs. But in 2-D PCs, to construct the matrix T is more difficult and the solution is not an exact solution because the dielectric constant must transfer to K space. On the contrary, FDTD method is an easy way in calculating 2-D PCs.