Chapter 2 Theory and Calculation Method

The same as all studies of the electromagnetism, analyses to the propagation of light in a photonic crystal start with four macroscopic Maxwell equations. In cgs units, they are

$$\begin{aligned} \nabla \cdot B &= 0 & \nabla \times E + \frac{1}{c}\frac{\partial B}{\partial t} &= 0 \\ \nabla \cdot D &= 4\pi\rho & \nabla \times H - \frac{1}{c}\frac{\partial D}{\partial t} &= \frac{4\pi}{c} J, \end{aligned} \tag{2.1}$$

where ***E*** and ***H*** are the macroscopic electric and magnetic fields, ***D*** and ***B*** are the displacement and magnetic induction fields, and ***ρ*** and ***J*** are the free charge and current densities. Without free charges and currents in our calculation in periodic dielectric medium, the ***ρ*** and ***J*** in Eq. (2.1) are all set to be zero.

2-1 Introduction

Generally, the components $\boldsymbol{D_i}$ of the displacement field **D** are related to the components $\boldsymbol{E_i}$ of the electric field ***E*** via a complicated power series, as follows [3]:

$$D_i = \sum_j \varepsilon_{ij} E_j + \sum_j k\chi_{ijk} E_j E_k + \mathrm{O}(E^3). \tag{2.2}$$

For many dielectric materials, we usually assume the field strengths are small enough so that we are in the linear regime, it means $\boldsymbol{\chi}$ and all higher terms can be ignored. Besides, we also assume the material is macroscopic and isotropic, so that $E(r,\omega)$ and $D(r,\omega)$ are related by a scalar dielectric constant $\varepsilon(r,\omega)$. Any explicit frequency dependence of the dielectric

constant are also been ignored. The last assumption is that we focus only on low-loss dielectrics, which means we treat $\varepsilon(r)$ as pure real. Hence, we have a brief expression as relating ***D*** and ***E*** fields

$$D(r) = \varepsilon(r)E(r). \tag{2.3}$$

Such a simplification process can also be performed in ***B*** and ***H***. For most dielectric materials of interest, the magnetic permeability $\mu(r)$ is very close to unity and we may set $B = H$.

With four assumptions above, the Maxwell equations Eq. (2.1) become

$$\begin{aligned} &\nabla \cdot H(r,t) = 0 \\ &\nabla \cdot \varepsilon(r)E(r,t) = 0 \end{aligned} \qquad \begin{aligned} &\nabla \times E(r,t) + \frac{1}{c}\frac{\partial H(r,t)}{\partial t} = 0 \\ &\nabla \times H(r,t) - \frac{\varepsilon(r)}{c}\frac{\partial E(r,t)}{\partial t} = 0. \end{aligned} \tag{2.4}$$

In general both ***E*** and ***H*** are complicated functions of time and space, and the Maxwell equations are linear. We can separate out the time dependence by expanding the fields into a set of harmonic modes. We employ the familiar trick of using a complex-valued field for mathematical convenience, and the physical fields can be obtained by taking the real part. Hence we write a harmonic mode as a certain field pattern times a complex exponential.

$$\begin{aligned} H(r,t) &= H(r)e^{i\omega t} \\ E(r,t) &= E(r)e^{i\omega t} \end{aligned} \tag{2.5}$$

Because there is no free charge and current, the electromagnetic waves considered to be

transverse. By eliminating Eq. (2.5) in Eq. (2.4) we can obtain the following equations:

$$\Theta_E \vec{E}(\vec{r}) \equiv \frac{1}{\varepsilon(\vec{r})} \nabla \times \{\nabla \times \vec{E}(\vec{r})\} = \frac{\omega^2}{c^2} \vec{E}(\vec{r}) \tag{2.6}$$

$$\Theta_H \vec{H}(\vec{r}) \equiv \nabla \times \{\frac{1}{\varepsilon(\vec{r})} \nabla \times \vec{H}(\vec{r})\} = \frac{\omega^2}{c^2} \vec{H}(\vec{r}) \tag{2.7}$$

Solving Eqs. (2.6) and (2.7) are the eigen-value problems, and we can easily prove that Θ_H is a special type of linear operator known as a *Hermitian* operator. The eigenvectors ***H(r)*** and $\widetilde{E}(r)$ (where $\widetilde{E}(r) = \sqrt{\varepsilon(r)} E(r)$) are the field patterns of the harmonic modes, and the eigenvalues $(\frac{\omega}{c})^2$ are proportional to the squared frequencies of those modes.

The Maxwell equations are th most important kernel of following calculations (both PWE and FDTD) and analyses in the next chapter except only the tight-binding approximation by solid-state physics we'll discuss later.

2-2 Plane-wave expansion method

Photonic crystals have structural periodicity (i.e. the dielectric constant is periodic distribution), hence we can write its dielectric function as

$$\varepsilon(\vec{r}) = \varepsilon(\vec{r} + \vec{a}_i) \qquad i = 1,2,3, \tag{2.8}$$

where $\{\vec{a}_i\}$ are the primitive lattice vectors of the photonic crystal. Because of the spatial periodicity, we introduce the primitive reciprocal lattice vectors $\{\mathbf{b}_i$; i=1,2,3$\}$ and the reciprocal lattice vector can be defined as $\{\mathbf{G}\}$:

$$a_i \cdot b_j = 2\pi\delta_{ij}$$

and $G = l_1 b_1 + l_2 b_2 + l_3 b_3$, (2.9)

where $\{l_i\}$ are arbitrary integers and δ_{ij} is the Kronecker's delta function. We can expand $\varepsilon^{-1}(\vec{r})$ into Fourier series as

$$\frac{1}{\varepsilon(r)} = \sum_G \kappa(G)\exp(iG \cdot r). \tag{2.10}$$

Due to the dielectric function is real, we have $\kappa(-G) = \kappa^*(G)$. As we discussed in section 2-1, the eigenfunctions which were derived from Maxwell's equations should satisfy the next eigenvalue equations.

$$\Theta\vec{E}(\vec{r}) \equiv \frac{1}{\varepsilon(\vec{r})}\nabla \times \{\nabla \times \vec{E}(\vec{r})\} = \frac{\omega^2}{c^2}\vec{E}(\vec{r}) \tag{2.11}$$

$$\Theta\vec{H}(\vec{r}) \equiv \nabla \times \{\frac{1}{\varepsilon(\vec{r})}\nabla \times \vec{H}(\vec{r})\} = \frac{\omega^2}{c^2}\vec{H}(\vec{r}) \tag{2.12}$$

Because ε is a periodic function of the spatial coordinate r, we can apply Bloch's theorem to Eqs. (2.11) and (2.12). $E(r)$ and $H(r)$ are thus characterized by a wave vector *k* in the first Brillouin zone and a band index *n* and expressed as

$$E(r) = E_{kn}(r) = u_{kn}(r)e^{ik\cdot r} \tag{2.13}$$

$$H(r) = H_{kn}(r) = v_{kn}(r)e^{ik\cdot r}, \tag{2.14}$$

where $u_{kn}(r)$ and $v_{kn}(r)$ are periodic vectorial functions:

$$u_{kn}(r+a_i)=u_{kn}(r) \tag{2.15}$$

$$v_{kn}(r+a_i)=v_{kn}(r), \quad \text{for } i=1,2,3. \tag{2.16}$$

These periodic functions can be expanded in Fourier series like $\varepsilon^{-1}(r)$ in Eq. (2.10). This Fourier expansion leads to the following form of the eigenfunctions:

$$E_{kn}(r)=\sum_G E_{kn}(G)\exp\{i(k+G)\cdot r\} \tag{2.17}$$

$$H_{kn}(r)=\sum_G H_{kn}(G)\exp\{i(k+G)\cdot r\}. \tag{2.18}$$

Substituting Eqs. (2.10), (2.17) and (2.18) into Eqs. (2.11) and (2.12), we obtain the following eigenvalue equations for the expansion coefficients $\{E_{kn}(G)\}$ and $\{H_{kn}(G)\}$:

$$-\sum_{G'}\kappa(G-G')\{(k+G')\times(k+G')\times E_{kn}(G')\}=\frac{\omega_{kn}^2}{c^2}E_{kn}(G) \tag{2.19}$$

$$-\sum_{G'}\kappa(G-G')(k+G)\times\{(k+G')\times H_{kn}(G')\}=\frac{\omega_{kn}^2}{c^2}H_{kn}(G), \tag{2.20}$$

where ω_{kn} denotes the eigen-angular frequency of $E_{kn}(r)$ and $H_{kn}(r)$. By solving one of these two sets of equation numerically, we can obtain the dispersion relation of the eigenmodes, or the photonic band structure. This numerical method, which is based on the Fourier expansion of the electromagnetic field and the dielectric function, is called the plane-wave expansion method.

2-3 Finite-difference time domain method (FDTD) [28]

In 1966 Yee [27] proposed a technique to solve Maxwell's curl equations using the finite-difference time-domain (FDTD) technique. The FDTD method belongs to the general class of differential time domain numerical modeling methods. Since it is a time-domain technique it can cover a wide frequency range with a single simulation run. That's why the Finite-Difference Time-Domain (FDTD) is one of the most popular electromagnetic modeling techniques.

When the differential form of Maxwell's equations is examined, it can be seen that the time derivative of the E field is related to the Curl of the H field ($\nabla \times H$). This can be simplified to state that the rate of the change in the E field (the time derivative) is dependent on the change in the H field across space (the Curl). This results in the basic FDTD equation that the new value of the E field is related to the old value of the E field (hence the difference in time) and the difference in the old value of the H field on either side of the E field point in space. Naturally this is a simplified description, as illustrated in Fig. 2-1.

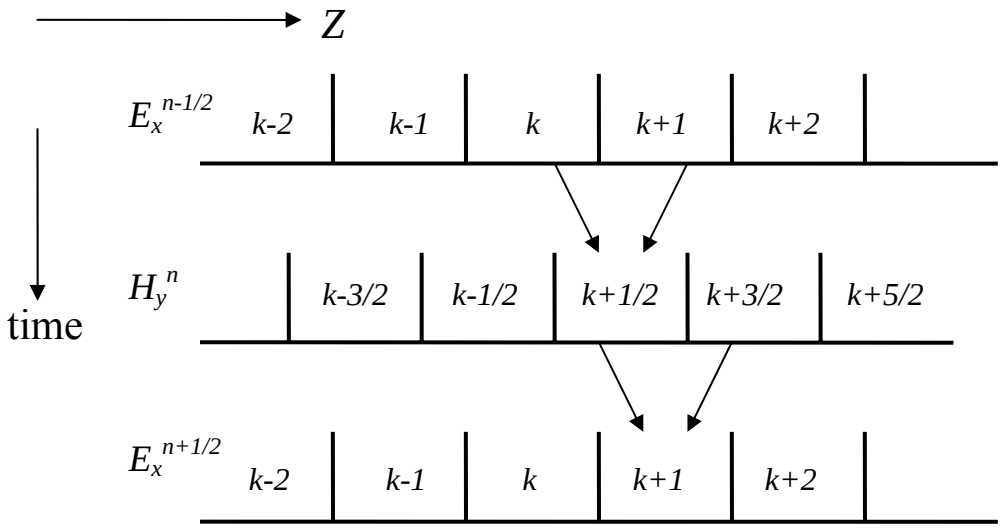

Fig. 2-1. Interleaving of the ***E*** and ***H*** fields in space and time in the FDTD formulation.

2-3.1 One-dimensional simulation with the FDTD method

Now we will start with simple one-dimensional differential equations. The time-dependent Maxwell's curl equations in free space are

$$\frac{\partial E}{\partial t} = \frac{1}{\varepsilon_0} \nabla \times H \tag{2.21a}$$

$$\frac{\partial H}{\partial t} = -\frac{1}{\mu_0} \nabla \times E. \tag{2.21b}$$

E and ***H*** are vectors in three dimensions. When we consider only in one dimension case, the ***E*** and ***H*** simply to $\boldsymbol{E_x}$ and $\boldsymbol{H_y}$, so the Eq. (2.21a) and (2.21b) becomes

$$\frac{\partial E_x}{\partial t} = -\frac{1}{\varepsilon_0} \frac{\partial H_y}{\partial z} \tag{2.22a}$$

$$\frac{\partial H_y}{\partial t} = -\frac{1}{\mu_0} \frac{\partial E_x}{\partial z}. \tag{2.22b}$$

Above equations mean the electric field oriented in the *x* direction, the magnetic field oriented in the *y* direction, and traveling in the *z* direction. Taking the central difference approximation for both the temporal and spatial derivatives gives

$$\frac{E_x^{n+1/2}(k) - E_x^{n-1/2}(k)}{\Delta t} = -\frac{1}{\varepsilon_0} \frac{H_y^n(k+1/2) - H_y^n(k-1/2)}{\Delta z} \tag{2.23a}$$

$$\frac{H_y^{n+1}(k+1/2) - H_y^n(k+1/2)}{\Delta t} = -\frac{1}{\mu_0} \frac{E_x^{n+1/2}(k+1) - E_x^{n+1/2}(k)}{\Delta z}. \tag{2.23b}$$

In these two equations, "*n*" actually means a time $t = \Delta t \cdot n$. The term "*n+1*" means one time

step later. "*k*" actually means the distance $z = \Delta z \cdot k$. The formula of Eqs. (2.23a) and (2.23b) assumes that the ***E*** and ***H*** fields are interleaved in both space and time. ***H*** uses the arguments $k+1/2$ and $k-1/2$ to indicate that the ***H*** field values are assumed to be located between the ***E*** field values. Similarly, the $n+1/2$ or $n-1/2$ superscript indicates that it occurs slightly after or before *n*, respectively.

Eq. (2.23a) and (2.23b) can be rearranged to

$$E_x^{n+1/2}(k) = E_x^{n-1/2}(k) - \frac{\Delta t}{\varepsilon_0 \cdot \Delta z}[H_y^n(k+1/2) - H_y^n(k-1/2)] \tag{2.24a}$$

$$H_y^{n+1}(k+1/2) = H_y^n(k+1/2) - \frac{\Delta t}{\mu_0 \cdot \Delta z}[E_x^{n+1/2}(k+1) - E_x^{n+1/2}(k)]. \tag{2.24b}$$

Notice that the calculations are interleaved in both space and time. This is the fundamental paradigm of the finite-difference time-domain (FDTD) method. (2.24a) and (2.24b) 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:

$$\widetilde{E} = \sqrt{\frac{\varepsilon_0}{\mu_0}} E. \tag{2.25}$$

Substituting (2.25) to Eqs. (2.24a) and (2.24b) gives

$$\widetilde{E}_x^{n+1/2}(k) = \widetilde{E}_x^{n-1/2}(k) - \frac{1}{\sqrt{\varepsilon_0 \mu_0}} \frac{\Delta t}{\Delta z}[H_y^n(k+1/2) - H_y^n(k-1/2)] \tag{2.26a}$$

$$H_y^{n+1}(k+1/2) = H_y^n(k+1/2) - \frac{1}{\sqrt{\varepsilon_0 \mu_0}} \frac{\Delta t}{\Delta z}[\widetilde{E}_x^{n+1/2}(k+1) - \widetilde{E}_x^{n+1/2}(k)]. \tag{2.26b}$$

If the cell size Δz is chosen, the time step Δt can be determined by

$$\Delta t = \frac{\Delta x}{2 \cdot c_0} \tag{2.27}$$

where c_0 is the light speed in free space. The reason why we determined the time step Δt to Eq. (2.27) related to the stability of the FDTD method. An electromagnetic wave propagating in free space cannot go faster than the speed of light. To propagate a distance of one cell Δz needs a minimum time of $\Delta t = \frac{\Delta z}{c_0}$. When we get to two-dimensional simulation, we have to allow for the propagation in the diagonal direction, which brings the time requirement to $\Delta t = \frac{\Delta z}{\sqrt{2} c_0}$. Obviously, three-dimensional simulation requires $\Delta t = \frac{\Delta z}{\sqrt{3} c_0}$. This is summarized by the well-known "Courant Condition" [29-30]:

$$\Delta t \le \frac{\Delta z}{\sqrt{n} \cdot c_0}, \tag{2.28}$$

where n is the dimension of the simulation. Hence we will determine Δt in Eq. (2.29). This is not necessarily the best formula! Therefore,

$$\frac{1}{\sqrt{\varepsilon_0 \mu_0}} \frac{\Delta t}{\Delta z} = c_0 \cdot \frac{\Delta z / 2 \cdot c_0}{\Delta z} = \frac{1}{2} \tag{2.29}$$

Rewriting Eq. (2.26a) and (2.26b) in **C** computer code we have

```
ex[k] = ex[k] + 0.5*( hy[k-1] – hy[k] )        (2.30a)
hy[k] = hy[k] + 0.5*( ex[k] – ex[k+1] ).       (2.30b)
```

To switch the source to a sinusoidal source, it is easy to obtain by replacing the parameter *pulse* with the following:

$$\begin{aligned} pulse &= \sin[2 * pi * freq\_in * dt * T] \\ ex[0] &= ex[0] + pulse. \end{aligned} \tag{2.31}$$

2-3.2 The absorbing boundary condition in one dimension

To keep outgoing ***E*** and ***H*** fields from being reflected by the calculation boundary then back into the problem space, the absorbing boundary conditions (ABC) are necessary. The fields at the edge must be propagating outward. In one time step of the FDTD algorithm it travels

$$distance = c_0 \cdot \Delta t = c_0 \cdot \frac{\Delta x}{2 \cdot c_0} = \frac{\Delta x}{2}. \tag{2.32}$$

This equation basically explains that it takes two time steps for a wave front to cross one cell. So a common sense approach tells us that an ABC might be

$$\begin{aligned} E_x^n(0) &= E_x^{n-2}(1) \\ E_x^n(k) &= E_x^{n-2}(k-1). \end{aligned} \tag{2.33}$$

Simply store a value of $E_x(1)$ two time steps before in $E_x(0)$. Boundary conditions such as these have been implemented at both ends of the E_x array. Below are the examples of C computer code in one-dimensional absorbing boundary conditions. Additional parameters are used to store the boundary value for two time steps during the calculation loop.

```
ex[0] = ex_low_m2;
ex_low_m2 = ex_low_m1;
ex_low_m1 = ex[1];
```

(2.34)

```
ex[KE-1] = ex_high_m2;
ex_high_m2 = ex_high_m1;
ex_high_m1 = ex[KE-2];
```

2-3.3 Two-dimensional formulation and perfectly matched layer (PML) boundary condition

We start again with the normalized Maxwell's equations:

$$\frac{\partial \widetilde{D}}{\partial t} = \frac{1}{\sqrt{\varepsilon_0 \mu_0}} \nabla \times H \tag{2.35a}$$

$$\widetilde{D}(\omega) = \varepsilon_r^*(\omega) \cdot \widetilde{E}(\omega) \tag{2.35b}$$

$$\frac{\partial H}{\partial t} = -\frac{1}{\sqrt{\varepsilon_0 \mu_0}} \nabla \times \widetilde{E}. \tag{2.35c}$$

where $\widetilde{E} = \sqrt{\frac{\varepsilon_0}{\mu_0}} \vec{E}$ and $\widetilde{D} = \frac{1}{\sqrt{\varepsilon_0 \mu_0}} \vec{D}$. In two dimension cases, there exists two groups of three vectors. One is the transverse magnetic (TM) mode, which is composed of $\widetilde{E}_z$, H_x, and H_y. Another is the transverse electric (TE) mode, which is composed of $\widetilde{E}_x$, $\widetilde{E}_y$, and H_z. Here we work with the TM mode for example. Therefore, Eq. (2.35) are now reduced to

$$\frac{\partial D_z}{\partial t} = \frac{1}{\sqrt{\varepsilon_0 \mu_0}} \left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right) \tag{2.36a}$$

$$D_z(\omega) = \varepsilon_r^*(\omega) \cdot E_z(\omega) \tag{2.36b}$$

$$\frac{\partial H_x}{\partial t} = -\frac{1}{\sqrt{\varepsilon_0 \mu_0}} \frac{\partial E_z}{\partial y} \tag{2.36c}$$

$$\frac{\partial H_y}{\partial t} = \frac{1}{\sqrt{\varepsilon_0 \mu_0}} \frac{\partial E_z}{\partial x}. \tag{2.36d}$$

The two-dimensional systemic interleaving of the calculated fields is more complex than one dimension. That is illustrated in Fig. 2-2 below.

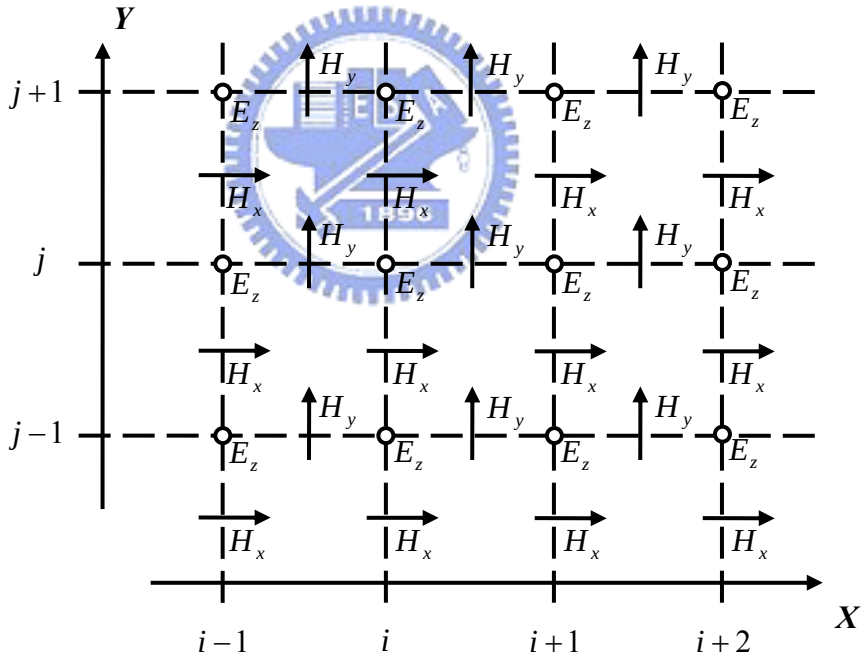

Fig. 2-2. Interleaving of the *E* and *H* fields for the two-dimensional TM formulation.

Putting Eqs. (2.36a), (2.36c) and (2.36d) into the difference scheme results in the following difference equations:

$$\frac{D_z^{n+1/2}(i,j)-D_z^{n-1/2}(i,j)}{\Delta t}=\frac{1}{\sqrt{\varepsilon_0\mu_0}}\left(\frac{H_y^n(i+1/2,j)-H_y^n(i-1/2,j)}{\Delta x}\right)$$

$$-\frac{1}{\sqrt{\varepsilon_0\mu_0}}\left(\frac{H_x^n(i,j+1/2)-H_x^n(i,j-1/2)}{\Delta x}\right) \tag{2.37a}$$

$$\frac{H_x^{n+1}(i,j+1/2)-H_x^n(i,j+1/2)}{\Delta t}=-\frac{1}{\sqrt{\varepsilon_0\mu_0}}\frac{E_z^{n+1/2}(i,j+1)-E_z^{n+1/2}(i,j)}{\Delta x}) \tag{2.37b}$$

$$\frac{H_y^{n+1}(i+1/2,j)-H_y^n(i+1/2,j)}{\Delta t}=\frac{1}{\sqrt{\varepsilon_0\mu_0}}\frac{E_z^{n+1/2}(i+1,j)-E_z^{n+1/2}(i,j)}{\Delta x}). \tag{2.37c}$$

We have briefly mentioned the issue of absorbing boundary conditions (ABCs) in discussion of one dimension. In the two-dimensional simulations, the program contains two-dimensional matrices for the values of all the fields (i.e. dz, ez, hx and hy). Suppose we are simulating a wave generated from a point source (in the center of the calculation field) propagating in the free space. As the wave propagates outward, it will eventually come to the edge of the allowable space, which is dictated by how the matrices have been dimensioned in the program. If we had done nothing about this, reflections would have been generated that would go back inward. Then we will have no way to tell the real wave and the reflected wave. This is the reason for the existence of ABCs. The most flexible and efficient ABCs is the perfectly matched layer (PML) developed by Berenger [30]. The basic idea of how PML works can be easily understood by the following description. If a wave propagating in medium A and it impinges upon medium B, the amount of reflection can be determined by the intrinsic impedances of two media

$$\Gamma=\frac{\eta_A-\eta_B}{\eta_A+\eta_B}, \tag{2.38}$$

where the impedance is

$$\eta = \sqrt{\frac{\mu}{\varepsilon}}. \tag{2.39}$$

If μ changed with ε so η still remained a constant, Γ would be zero and no reflection will occur. But this is still helpless to our problem, because waves will continue propagating in the new medium. We really want is a medium that is also lossy so the wave will die out before it hits the boundary. Hence we mark both ε and μ of complex due to their imaginary parts cause decay.

In order to simulate a plane wave propagation in a 2D FDTD program, the space of problem will be divided up into two regions, the *total field* and the *scattered field* (Fig. 2-3). There are two reasons for doing this: (1) The propagating plane wave should not interact with the absorbing boundary conditions; (2) the load on the absorbing boundary conditions should be minimized. These boundary conditions are not perfect. By subtracting the incident field, the amount of the radiating field hitting the boundary is minimized, thereby reducing the calculation error.

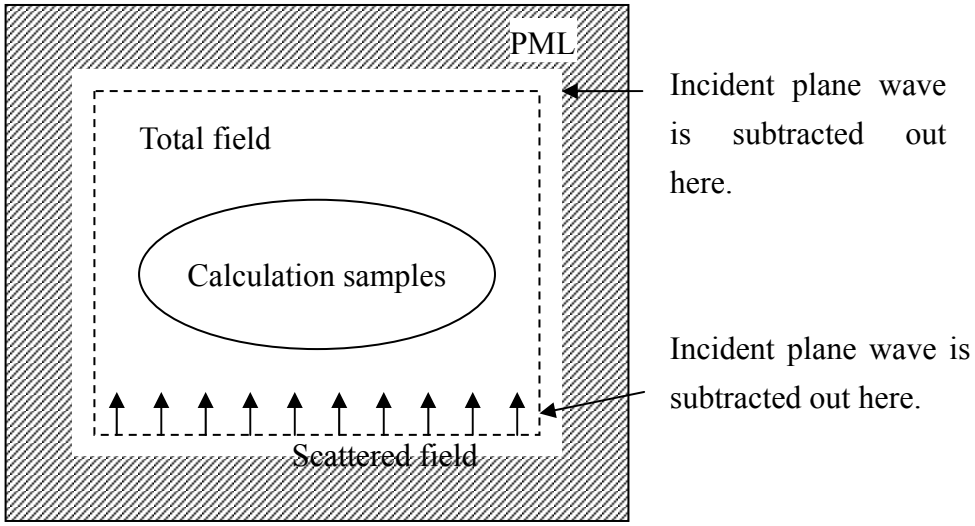

Fig. 2-3. Total field/scattered field of the two-dimensional problem space.

2-4 Tight binding method in solid state physics

In the later discussion of energy transport in the photonic crystal waveguides we will apply the tight binding approximation to support our argument. Hence we here do a simple introduction of what is the tight binding method and its meaning in solid state physics [31].

When many atoms stay closely to become the crystal, their wave functions will overlap each other. If we consider only two atoms, their combined wave functions are $\psi_A \pm \psi_B$. The electron energy of state $\psi_A + \psi_B$ is lower than one of state $\psi_A - \psi_B$. After they approach to each other, the Coulomb force between nucleuses and electrons can cause the energy level division and becomes energy band. The approximation method to obtain the energy band structure by calculating the free atomic wave functions is called tight binding approximation (TB) or linear combination of atomic orbitals (LCAD). Assume that an electron with ground state $\varphi(r)$ exercises within a single atom's potential $U(r)$, where the $\varphi(r)$ denoted as *s* state. It is too complex if we solve the energy band problem by using degenerated atomic

energy levels. Therefore, we assume that the influence between two atoms is quite small, and then we can have an approximative wave function of the entire crystal:

$$\psi_k(r) = \sum_j C_{kj}\varphi(r - r_j)\,. \tag{2.40}$$

If $C_{k,j} = N^{-1/2}e^{ik\cdot r_j}$ in Eq. (2.40) is for a crystal with N atoms, the Bloch form of the above equation can be expressed as

$$\psi_k(r) = N^{-1/2}\sum_j \exp(ik\cdot r)\varphi(r - r_j)\,,\ \ \psi_k(r+T) = \exp(ik\cdot T)\psi_k(r)\,, \tag{2.41}$$

where T is the primitive vector of connecting two lattice points. To calculate the 1st level energy by doing the Hamiltonian matrix diagonalization as follow:

$$\langle k|H|k\rangle = N^{-1}\sum_j\sum_m \exp[ik\cdot(r_j - r_m)]\langle\varphi_m|H|\varphi_j\rangle, \tag{2.42}$$

where $\varphi_m \equiv \varphi(r - r_m)$. Let $\rho_m = r_m - r_j$, then

$$\langle k|H|k\rangle = \sum_m \exp(ik\cdot\rho_m)\int dV\varphi^*(r-\rho_m)H\varphi(r)\,. \tag{2.43}$$

In Eq. (2.43), we do the integration to only an atom and other atoms nearby which are tied up by ρ. We can rewrite it as:

$$\int dV\varphi^*(r)H\varphi(r) = -a\,;\ \ \int dV\varphi^*(r-\rho)H\varphi(r) = -\gamma \tag{2.44}$$

To set $\langle k|k\rangle = 1$, the 1st level energy is

$$\langle k|H|k\rangle = -a - \gamma \sum_m \exp(ik \cdot \rho_m) = \varepsilon_k \,. \tag{2.45}$$

The relation between overlapping energy γ and atomic spacing ρ in two hydrogen atoms which are both in 1s state can be clearly calculated. Using the Rydberg-energy unit, $Ry = me^4 / 2\hbar^2$, we have

$$\gamma(Ry) = 2(1 + \rho / a_0)\exp(-\rho / a_0)\,. \tag{2.46}$$

Considering to a simple cubic structure, the positions of the closest atoms are

$$\rho_m = (\pm a,0,0);\quad (0,\pm a,0);\quad (0,0,\pm a)\,. \tag{2.47}$$

So the equation (2.45) becomes

$$\varepsilon_k = -a - 2\gamma(\cos k_x a + \cos k_y a + k_z a)\,. \tag{2.48}$$

Other example likes the **fcc** structure which has twelve closest atoms and its band structure can be described as

$$\varepsilon_k = -a - 4\gamma(\cos\frac{1}{2}k_y a \cos\frac{1}{2}k_z a + \cos\frac{1}{2}k_z a \cos\frac{1}{2}k_x a + \cos\frac{1}{2}k_x a \cos\frac{1}{2}k_y a)\,. \tag{2.49}$$

Hence the tight-binding approximation method provides a very simple way to do the atomic

energy band structure analysis. This way can also be applied to the discussion of the small coupling effect inside a photonic crystal coupled-cavities waveguides (CCWs).

2-5. Mode coupling between PCWs

A straightforward approach to the evaluation of the coupling length can be based on the FDTD. This method allows tracing the evolution of the EM field in real time. Launching an initialization field at the beginning of the first waveguide, we can observe the distance at which the EM field leaves the first waveguide and arrives at the second one. An example of such a calculation is given in Fig. 2-4.

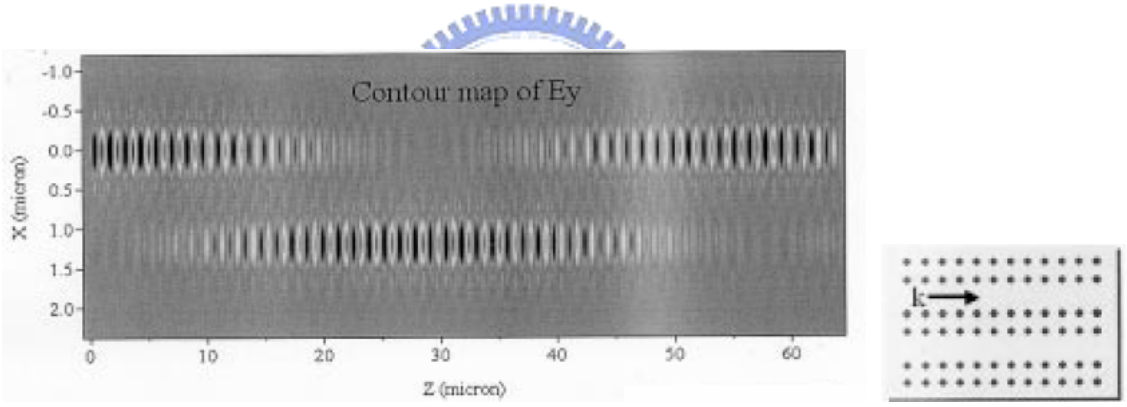

Fig. 2-4. Typical field map in planar PhC with two parallel channel waveguides calculated using "FullWave" software.

As was shown in [32], in the absence of the interaction between the two waveguides, a normal mode of one isolated waveguide is also a normal mode of the system of the two waveguides. Let us denote the mode localized in the first waveguide as $|\psi_1\rangle$ and that in the second one as $|\psi_2\rangle$. These two modes have the same frequency ω. They are degenerate states. Once a perturbation is switched on, this frequency splits into two frequencies ω_1 and ω_2, where $\Delta\omega = \omega_1 - \omega_2 << \omega$. Suppose we know exactly the normal modes $|\psi_1'\rangle$ and $|\psi_2'\rangle$ of

the perturbed system corresponding to these frequencies. Using perturbation theory, we can write

$$|\psi_1\rangle = C_1|\psi_1'\rangle + C_2|\psi_2'\rangle. \tag{2.50}$$

Suppose that, at time t = 0, mode $|\psi_1\rangle$ is launched into first waveguide. Time evaluation of the EM field in this case can be written as

$$|\psi_1(t)\rangle = C_1|\psi_1'\rangle \cdot e^{i\omega_1 t} + C_2|\psi_2'\rangle \cdot e^{i\omega_2 t}. \tag{2.51}$$

In the case of identical waveguides, $|C_1| = |C_2|$. Using this equation and (2.50), one can obtain

$$|\psi_1(t)\rangle = \phi(r) \cdot \sin(\frac{\Delta\omega \cdot t}{2}) \cdot \sin(\omega \cdot t). \tag{2.52}$$

From Eq. (2.52), we can see that the time *T* of the transformation of state $|\psi_1\rangle$ to state $|\psi_2\rangle$ is $0.5 \cdot (\omega / \Delta\omega) \cdot T_0$, where T_0 is the period of the EM field oscillations. The value of the frequency splitting Δω due to the interaction between waveguides can be evaluated from MIT photonic-bands (MPB) calculation using the supercell approach, the supercell includes both interacting waveguides. We can then obtain time *T* by only evaluating the desired coupled length, group velocity $v_g = d\omega / dk$, in the waveguide. This can be easily obtained from the MPB band structure calculation for a single waveguide. Finally, we have the coupling length *L*, is given by

$$L = T \cdot v_g \,. \tag{2.53}$$

Substituting the following Eq. (2.54) and $v_g = d\omega / dk$ into (2.53)

$$T = 0.5 \cdot (\frac{\omega}{\Delta\omega}) \cdot \lambda_0 , \tag{2.54}$$

we can finally determine the desired coupling length which takes the form

$$L = 0.5 \frac{\omega}{\Delta\omega} v_g \lambda_0 . \tag{2.55}$$

Hence, if we replace the v_g by $d\omega / dk$ and λ_0 by $\frac{1}{f}$ (where λ_0 and f are normalized wavelength and frequency) in Eq. (2.55). The desired coupling length can be expressed by using split normalized wave-vector (Δk) as following Eq. (2.56)

$$L = 0.5 \frac{\omega}{\Delta\omega} \cdot \frac{d\omega}{dk} \cdot \frac{\Lambda}{2\pi} \cdot \frac{1}{f} = \frac{\Lambda}{2\Delta k} . \tag{2.56}$$

The Λ in Eq. (2.56) represents lattice constant of the PCW. In the later discussion of chapter 3, Eq. (2.56) will be used quite often to forecast the desired coupling length.