Chapter 2 Theory and Methodology

The propagation behavior of light is determined by the four Maxwell's equations [15]. We consider the light propagation within a periodic dielectric medium, a composite of regions of homogeneous dielectric material, with no free charge or currents (ρ=**J**=0). Therefore, the four Maxwell's equations given in MKS units are as follows.

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

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

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

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

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

2-1 Introduction

In order to solve the wave equations derived from Maxwell's equations, we need the so-called constitutive equations related **D** to **E** and **B** to **H**. Since we do not deal with magnetic material, we assume the magnetic permeability of the photonic crystal is equal to that in free space with μ_0 being the permeability in vacuum:

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

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

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

For simplifying the problem, we make three 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 and non-absorptive, so the ε(**r**,ω) is treated as a real. According to the last three assumptions, the relation between **D** and **E** can be rewritten as this form:

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

For most dielectric materials of interest, the magnetic permeability is very close to unity so we may set $B = \mu_0 H$. If a monochromatic electromagnetic wave is incident, all components of the electric and magnetic fields are harmonic functions of time and the same frequency.

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

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 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). By the so-called *plane-wave expansion method*, these eigen equations can be solved, and then we can obtain the dispersion relation of the eigenmodes, or the *photonic band structure* [16] [17].

2-2 Omnidirectional one-dimensional photonic crystal and band structure

2-2.1 One-dimensional photonic crystal and typical band structure

A one-dimensional (1-D) photonic crystal (PC) has an index of refraction that is periodic in one direction and consists of endlessly repeating stacks of dielectric slabs, which alternate in thickness from d_1 to d_2 and in index of refraction from n_1 to n_2. In our research, we choose TiO_2 (n_1=2.36) and SiO_2 (n_2=1.47) as the two slabs. *Lattice constant* D is defined as d_1+d_2. The general photonic band structure calculated form 1-D PC is shown in Fig 2-1.

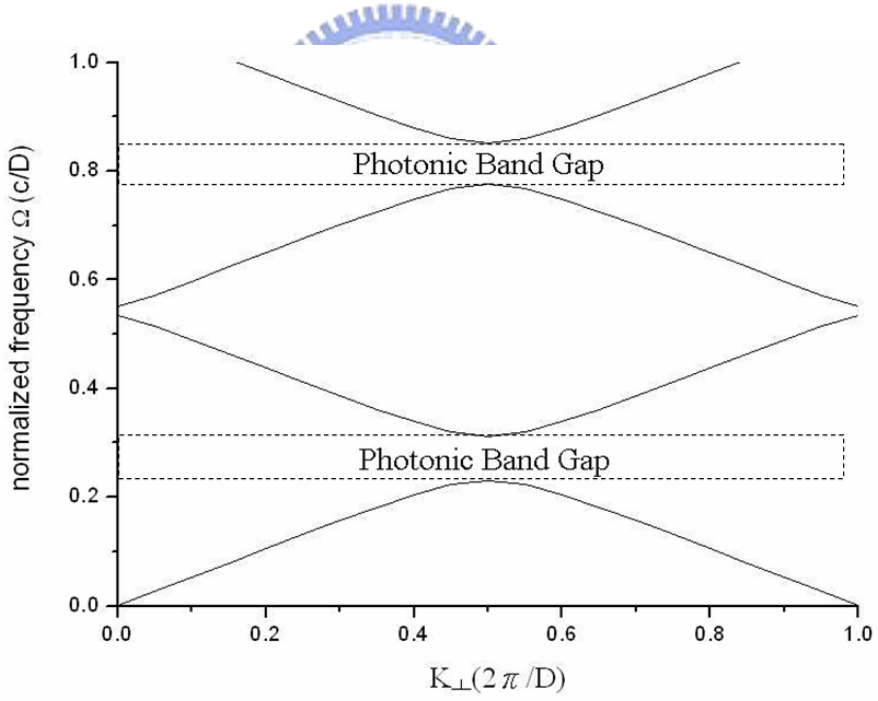

Fig. 2-1 Band structure (the relation of ω to k) of 1-D PC.

The vertical coordinate describes the normalized frequency Ω in unit c/D, i.e. $\Omega=\omega D/2\pi c$. Where ω is angular frequency and c is speed of light. The horizontal coordinate describes the normalized wave vector, whose direction is perpendicular to the interface of

slabs, in unit $2\pi/D$. We can see there are four allowed photonic bands which are the eigen modes of the eigen equations in Fig 2-1, and all photonic bands are symmetrical at $K_{\perp}=\pi/D$. There are no photonic bands inside the square surrounded by dash lines, i.e., there are no electromagnetic modes available within these frequency ranges in the photonic crystal. Therefore, the frequency ranges are the so-called photonic band gaps; the incident wave within the frequency ranges cannot pass through this photonic crystal.

2-2.2 Omnidirectional band structure

In previous section, we only consider that the incident light is normally incident to the PC. Besides normal incidence, the incident light can be either *TE-polarized* (**E** is perpendicular to the plane of incidence) or *TM-polarized* (**H** is perpendicular to the plane of incidence). In order to analyze and realize these conditions, we calculate the distinguishing band structure which is shown in Fig 2-2.

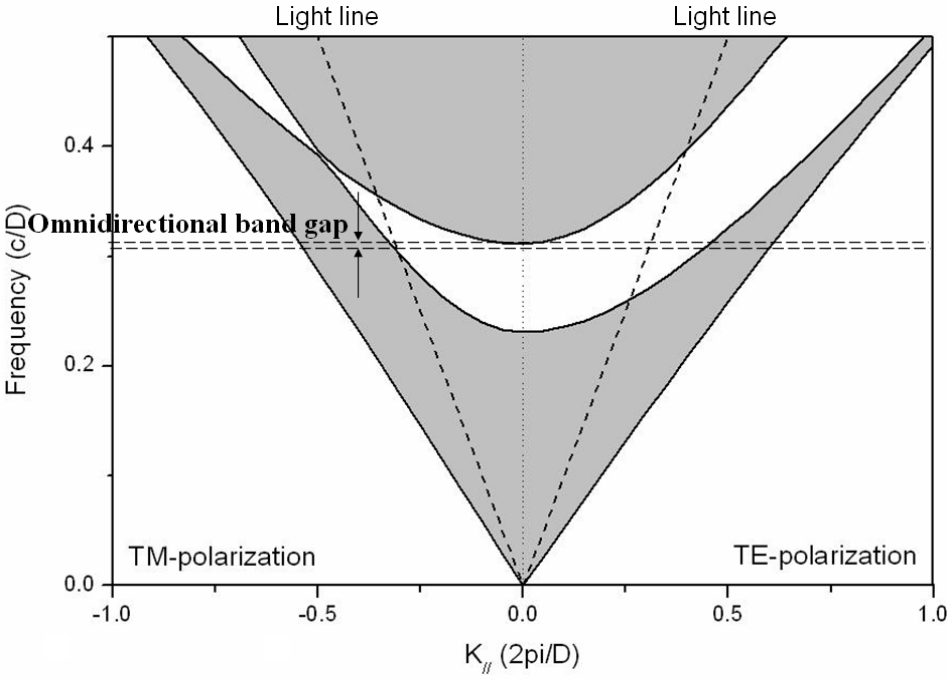

Fig. 2-2 Omnidirectional band structure of 1-D PC. The frequency range within two horizontal dash line is the so-call omnidirectional bandgap.

The critical difference between these two band structures is the horizontal coordinate. $K_{//}$ means that the normalized wave vector is parallel to the interface of slabs. Because the photonic crystal is periodic in $K\perp$ direction and homogeneous in $K_{//}$ direction, the electromagnetic modes can be characterized by a wave vector k, with $K\perp$ restricted to $0 \le K\perp \le \pi/D$ and $K_{//}$ regarded as $K_{//} \ge 0$. The allowed mode frequencies Ω_n for each possible choice of k constitute the band structure of the crystal. The functions Ω_n ($K_{//}$, $K\perp$), for each n, are the photonic bands mentioned above.

For each value of $K_{//}$, the mode frequencies Ω_n for all possible values of $K\perp$ were plotted in Fig. 2-2. That's why the photonic bands in Fig. 2-1 and in Fig. 2-2 are "thin lines" and "broad regions" respectively. In the gray region there are electromagnetic modes for some value of $K\perp$, whereas in the white regions there are no electromagnetic modes, regardless of $K\perp$. The *TE-polarized* modes are plotted to the right side of the band structure, and the *TM-polarized* modes to the left. Thus incident light from any direction with any polarizations is shown in this band structure, which we defined as *omnidirectional band structure*. The word "omnidirection" means "all-direction". [5]

2-2.3 Omnidirectional bandgap and reflection

We notice that there is no complete bandgap in Fig. 2-2 because each frequency has corresponding allowed modes. However, the absence of bandgap doesn't prohibit *omnidirectional reflection*, the leading capability of photonic crystal.

We have to know what is the connection between the incident propagation wave and the allowed modes in photonic crystal. So we give a simple demonstration below. From $c = f \cdot \lambda$, we get

$$\omega = \frac{c}{n} \cdot k = \frac{c \cdot k_{//}}{n \cdot \sin\theta}, \tag{2.11}$$

where n is the refractive index of ambient medium. And then, the normalized parameters are

$$\Omega = \frac{\omega \cdot D}{2\pi c}, \qquad K_{//} = k_{//} \cdot (\frac{D}{2\pi}). \tag{2.12}$$

After substituting (2.12) into (2.11), we obtain the following result

$$\Omega = (\frac{1}{n \cdot \sin\theta}) \cdot K_{//}, \tag{2.13}$$

where θ is the incidence angle. Therefore, the EM wave incident from outside medium, whose refractive index is n, can couple into the modes lying on the oblique straight line whose slope is $\frac{1}{n \cdot \sin\theta}$ in band structure. In our whole research, we suppose the ambient medium is air, so we always take n=1. When θ =90°, the equation $\Omega = K_{//}$ is defined as ***light line***, which is the two oblique dash lines in Fig. 2-2. Thus, any incident wave laughed from outside medium can only excite the modes inside the "line cone". There are no allowed bands within the two horizontal dash lines inside the line cone, so we define this frequency range as ***omnidirectional bandgap***. Consequently, the 1-D photonic crystal is able to exhibit omnidirectional reflection for incident light from any direction with any polarization within omnidirectional bandgap.

2-3 Transfer matrix method

We consider the problem of the reflection and transmission of electromagnetic radiation through a thin film using the 2 × 2 matrix. The dielectric structure is described by

$$n(x) = \begin{cases} n_1, & x < 0, \\ n_2, & 0 < x < d, \\ n_3, & x > d, \end{cases} \qquad \text{(see Fig. 2-3)}$$

where d is the thickness of the film. We assume the wave propagates on the xz plane, and the

electric field is either a TE wave (E//y) or a TM wave (H//y).

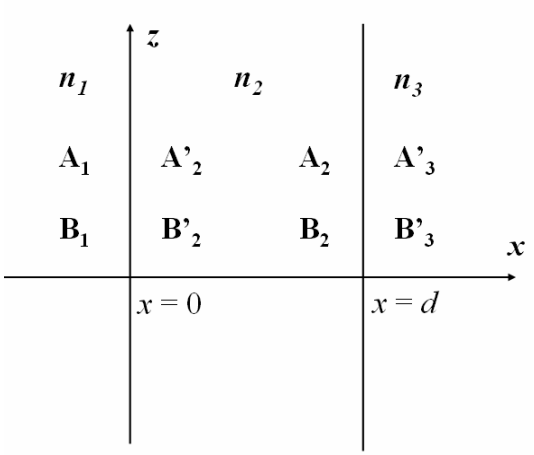

Fig. 2-3 A thin film of dielectric medium.

The electric field *E(x)* consists of a right-traveling wave and a left-traveling wave, can be written as $E(x) = Re^{-ik_x x} + Le^{ik_x x} \equiv A(x) + B(x)$, where $\pm k_x$ are the *x* components of the wave vector and *R* and *L* are constants in each homogeneous layer. We define *A(x)* as the amplitude of the right-traveling wave and *B(x)* as that of left-traveling wave. To illustrate the matrix method, we define

$$A_1 = A(0^-), A'_2 = A(0^+), A_2 = A(d^-), A'_3 = A(d^+),$$
$$B_1 = B(0^-), B'_2 = B(0^+), B_2 = B(d^-), B'_3 = B(d^+),$$

respectively, where 0^- represents the left side of the interface, $x = 0$, and 0^+ represents the right side of the same interface. d^- and d^+ are similarly defined. *E(x)* for TE wave is a continuous function of *x*. If we represent the two amplitudes of E(x) as column vectors, they are related by (see Fig. 2-3)

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = D_1^{-1} D_2 \begin{pmatrix} A'_2 \\ B'_2 \end{pmatrix} \equiv D_{12} \begin{pmatrix} A'_2 \\ B'_2 \end{pmatrix}, \tag{2.14}$$

$$\begin{pmatrix} A'_2 \\ B'_2 \end{pmatrix} = P_2 \begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \begin{pmatrix} e^{i\phi_2} & 0 \\ 0 & e^{-i\phi_2} \end{pmatrix} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}, \tag{2.15}$$

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = D_2^{-1} D_3 \begin{pmatrix} A_3' \\ B_3' \end{pmatrix} \equiv D_{23} \begin{pmatrix} A_3' \\ B_3' \end{pmatrix}, \tag{2.16}$$

where D_1, D_2, and D_3 are the *dynamical matrices*, which can be obtained by matching the boundary conditions at the interface. They are

$$D_\alpha = \begin{cases} \begin{pmatrix} 1 & 1 \\ n_\alpha \cos\theta_\alpha & -n_\alpha \cos\theta_\alpha \end{pmatrix} & \text{for } TE \text{ wave,} \\ \begin{pmatrix} \cos\theta_\alpha & \cos\theta_\alpha \\ n_\alpha & -n_\alpha \end{pmatrix} & \text{for } TM \text{ wave,} \end{cases} \tag{2.17}$$

where α=1, 2, 3 and θ_α is the ray angle in each layer. P_2 is the so-called *propagation matrix*, which accounts for propagation through the bulk of the layer. The phase φ_2 is given by $\phi_2 = k_{2x} d$.

From Eqs. (2.14)—(2.16), the amplitudes A_1, B_1 and A_3', B_3' are related by

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = D_1^{-1} D_2 P_2 D_2^{-1} D_3 \begin{pmatrix} A_3' \\ B_3' \end{pmatrix}, \tag{2.18}$$

The Snell's Law $n_\alpha \sin\theta_\alpha = const.$ can connect the ray angle in each layer. Note that the column vectors representing the plane-wave amplitudes in each layer are related by a product of 2 × 2 matrices in sequence. Each side of an interface is represented by a dynamical matrix, and the bulk of each layer is represented by a propagation matrix. Such a recipe can be extended to the case of multilayer structures.

Now we consider the case of multilayer. Similarly to Eq. (2.18), the relation between the amplitudes of the first medium (0) and final medium (s) can be written as

$$\begin{pmatrix} A_0 \\ B_0 \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} A_s' \\ B_s' \end{pmatrix}, \tag{2.19}$$

with the matrix given by

$$\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = D_0^{-1} \left[\prod_{\alpha=1}^{N} D_\alpha P_\alpha D_\alpha^{-1} \right] D_s \tag{2.20}$$

N is the number of layers.

Now we discuss the reflectance and transmittance. When the light is incident from medium 0, the reflection and transmission coefficients are defined as

$$r = \left(\frac{B_0}{A_0} \right)_{B_s'=0}, \tag{2.21-1}$$

$$t = \left(\frac{A_s'}{A_0} \right)_{B_s'=0}, \tag{2.21-2}$$

Using the matrix equation (2.19) and definitions (2.21), we obtain

$$r = \frac{M_{21}}{M_{11}} \tag{2.22-1}$$

$$t = \frac{1}{M_{11}}. \tag{2.22-2}$$

Reflectance is given by

$$R = |r|^2 = \left| \frac{M_{21}}{M_{11}} \right|^2, \tag{2.23-1}$$

provided medium 0 is lossless.

If the bounding media (0, s) are both pure dielectric with real n_s and n_0, transmittance T is given by

$$T = \frac{n_s \cos\theta_s}{n_0 \cos\theta_0} |t|^2 = \frac{n_s \cos\theta_s}{n_0 \cos\theta_0} \left| \frac{1}{M_{11}} \right|^2. \tag{2.23-2}$$

Consequently, by using transfer matrix method we can simulate the transmission of a wave incident to a multilayer consisting of finite layers. [18]

Now, we calculate the band structure of a 1-D PC by plane wave expansion method, and taking the incidence angle $\theta_0 = 0^o$ to calculate the transmission spectra through this 1-D PC with ten periods by using transfer matrix method. The results are shown in Fig. 2-4.

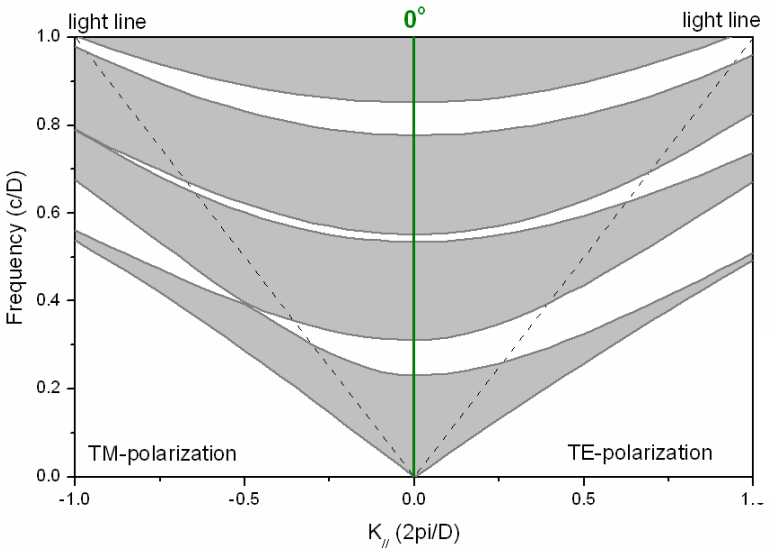

Fig. 2-4(a) The band structure of 1-D PC. Whose n_1=2.36, n_2=1.47, and d_1/d_2=0.7.

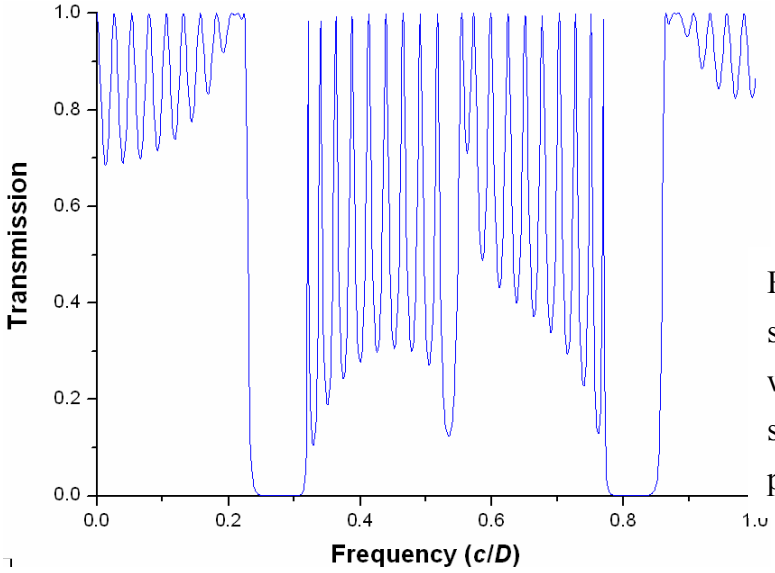

Fig. 2-4(b) The transmission spectra of normal incident wave passing through the same structure of 1-D PC with 10 periods.

In Fig. 2-4(b), we can see that there are three bandgaps, and the second bandgap is the narrowest. This result matches the band structure in Fig. 2-4(a), where the thick line at center describes the behavior of normal incident wave. However, on the four allowed bands, the transmission cannot always keep 100% at each normalized frequency (see Fig. 2-4(b)). The transmission curve dips at some frequencies. They are so-called *ripples*. The ripple effect always appears at optical coated thin films. This phenomenon is caused by the interference of light wave from the finite multilayers. The number of ripples increases as the number of

coating layers is increased. In this case, the transmission spectra calculated from ten periods have nine or ten ripple peaks at each allowed band.

In 1-D case, transfer matrix method (TMM) is an exact solution, so it can simulate more correct results of finite 1-D PC than the plane wave expansion method that treats infinite PC. The band structure is calculated by solving the eigen equation of a unit cell of 1-D PC that doesn't consider the finite periods and the interference of wave. Therefore, after designing a device by using plane wave expansion method, we have to check the transmittance by TMM.