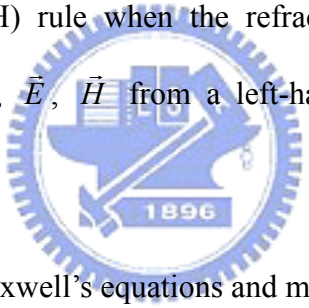
Chapter 2 Theory and Methodology

2-1 Introduction

2-1.1 Origin of the negative refraction

In 1968, V. G. Veselago, published a paper "The electrodynamics of substances with simultaneously negative values of ε and μ", on the Sov. Phys. Usp. [1] He raised firstly a new conception about materials that have a negative index of refraction *n*. These materials have simultaneously negative permittivity ε and permeability μ. We knew that transmitted behavior of electromagnetic wave in common materials obey the right-handed (RH) rule; however it will obey the left-handed (LH) rule when the refractive index in materials is negative. Therefore, these materials, $\vec{k}$, $\vec{E}$, $\vec{H}$ from a left-handed set of vectors, are also called left-handed materials (LHM).



First, we start from the Maxwell's equations and material equation:

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$
$$\nabla \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t} \qquad (2.1)$$

$$\vec{B} = \mu \vec{H}$$
$$\vec{D} = \varepsilon \vec{E} \qquad (2.2)$$

We consider a dielectric material with no free charge or currents (ρ=**J**=0) and apply $e^{i(\vec{k}\bullet\vec{r}-\omega t)}$ to Eq. (2.1) and (2.2), so that we can obtain the following equations:

$$\vec{k} \times \vec{E} = \omega \mu \vec{H}$$
$$\vec{k} \times \vec{H} = -\omega \varepsilon \vec{E} \qquad (2.3)$$

In Eq. (2.3), there are four cases of classification as the following:

(1) $\varepsilon > 0, \mu > 0 \Rightarrow$ **E**, **H**, and **k** construct a right-handed (RH) set, i.e. common materials;

(2) $\varepsilon < 0, \mu < 0 \Rightarrow$ **E**, **H**, and **k** construct a left-handed (LH) set, i.e. LHM;

(3) $\varepsilon > 0, \mu < 0 \Rightarrow$ EM wave cannot propagate in this material;

(4) $\varepsilon < 0, \mu > 0 \Rightarrow$ EM wave cannot propagate in this material.

Here, cases (1) and (2) respectively obey the right-handed rule and the left-handed rule, but cases (3) and (4) are not permitted. Moreover, the direct of Poynting vector $\vec{S}$ doesn't be changed by material properties, it is only relevant to $\vec{E}$ and $\vec{H}$.

$$\vec{S} = \vec{E} \times \vec{H} \tag{2.4}$$

The relations of the vectors $\vec{E}$, $\vec{H}$, $\vec{k}$, and $\vec{S}$ are shown in Fig. 2-1: (a) Poynting vector $\vec{S}$ and $\vec{k}$ have the same directions, i.e. $\vec{S} \bullet \vec{k} > 0$; (b) Poynting vector $\vec{S}$ and $\vec{k}$ have the opposite directions, i.e. $\vec{S} \bullet \vec{k} < 0$.

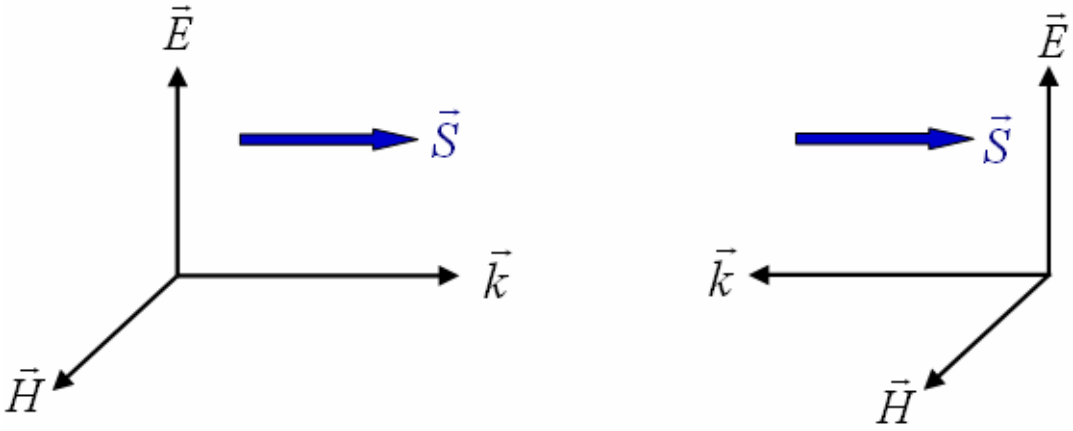


Fig.2-1 Relations of the vectors **E**, **H**, **k**, and **S**. (a) If ε>0 and μ>0, **E**, **H**, and **k** obey the right-handed rule, and **S** and **k** have the same directions. (b) If ε<0 and μ<0, **E**, **H**, and **k** obey the right-handed rule, and **S** and **k** have the same directions.

Eq. (2.5) is the boundary condition of electromagnetism, and the interface is built of two

different media (i.e. incident medium is 1, and refractive medium is 2).

$$\begin{aligned} E_{t1} &= E_{t2}, \\ H_{t1} &= H_{t2}, \\ \varepsilon_1 E_{n1} &= \varepsilon_2 E_{n2}, \\ \mu_1 H_{n1} &= \mu_2 H_{n2}. \end{aligned} \tag{2.5}$$

We discover that the normal components of electric field $\vec{E}$ and magnetic field $\vec{H}$ are affected by the material properties, but the tangential components are not. Therefore, we assume a frame: an electromagnetic wave introduces to medium from the air, and observe the refractive behavior in two sides of the interface [seen in Fig. 2-2]: (A) If $\varepsilon > 0$ and $\mu > 0$, the direction of tangential and normal components of the electric field $\vec{E}$ and magnetic field $\vec{H}$ are invariant, and refractive angle is θ_0; (B) if $\varepsilon < 0$ and $\mu < 0$, the direction of tangential components are invariant, but the direction of normal components are opposite, and the refractive angle is $-\theta_0$.

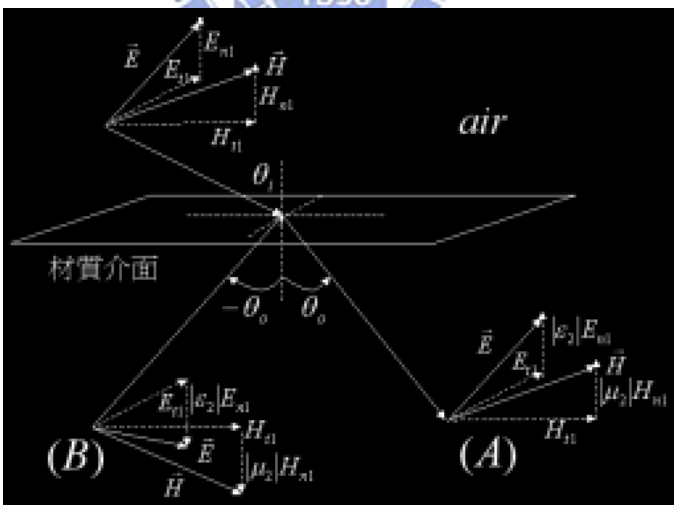


Fig.2-2 An electromagnetic wave introduce to medium from the air. The direction of tangential components of the **E** and **H** are invariant, and the direction of normal components: (A) If ε>0 and μ>0 are invariant, and refractive angle is θ; (B) if ε<0 and μ<0 are opposite, and refractive angle is –θ.

According to the path of electromagnetic wave in Fig. 2-2, we can conclude that: If the refractive medium has simultaneously negative permittivity ε and permeability μ, the incident wave and the refractive wave are at the same side of the normal of the interface. But this phenomenon is apparently inconsistent with the Snell's law, namely Eq. (2.6), so that we must revise it.

$$\frac{\sin\theta_1}{\sin\theta_2} = \frac{n_2}{n_1} = \sqrt{\frac{\varepsilon_2\mu_2}{\varepsilon_1\mu_1}}, \tag{2.6}$$

Here the incident and refractive media are symbolized by 1 and 2 respectively. If medium 1 is air, and medium 2 is a left-handed material, then refractive angle is negative (i.e. $-\theta_2$) due to $\varepsilon_2 < 0$ and $\mu_2 < 0$, hence the function of sine is negative, and the refractive index n_2 of Eq. (2.6) must be revised to negative. In other words, the materials which have simultaneously negative permittivity ε and permeability μ (i.e. LHM) are also named negative materials.

Although naturally occurring materials with simultaneously negative permittivity and permeability are not known; one left-handed material has been artificially realized as a periodic lattice of metallic rods and split-ring resonators. [3,4] Recently, the study of negative refraction has further received much attention both from the theoretical and experimental points of view. [5-8]

2-1.2 Refraction phenomenon in photonic crystals

What is the refraction phenomenon of light in photonic crystals? A photonic crystal is a structure whose refractive index is periodically modulated, and the resultant photonic dispersion demonstrates a band structure analogous to the electronic band structure in a solid,

shown as Fig. 2-3. The one-dimensional version of a photonic crystal has long been known as a multilayer reflector, but two- and three-dimensional photonic crystals have only recently started to attract attention after the appearance of a prediction that photonic insulators can be developed by photonic crystals.

In photonic crystals, light travels as Bloch waves, in a similar way to plane waves in continuous material. Bloch waves travel through crystals with a definite propagation direction despite the presence of scattering, but their propagation is complicated because it is influenced by the band structure. A very detailed photonic band structure was successfully obtained by the measurement, which was published by M. Notomi *et al.* [12]. This experiment directly shows that the light propagation is definitely determined by the photonic band structure (PBS). This means that, if we want to investigate the light propagation in photonic crystals, what we have to do is just to calculate the corresponding photonic band structure.

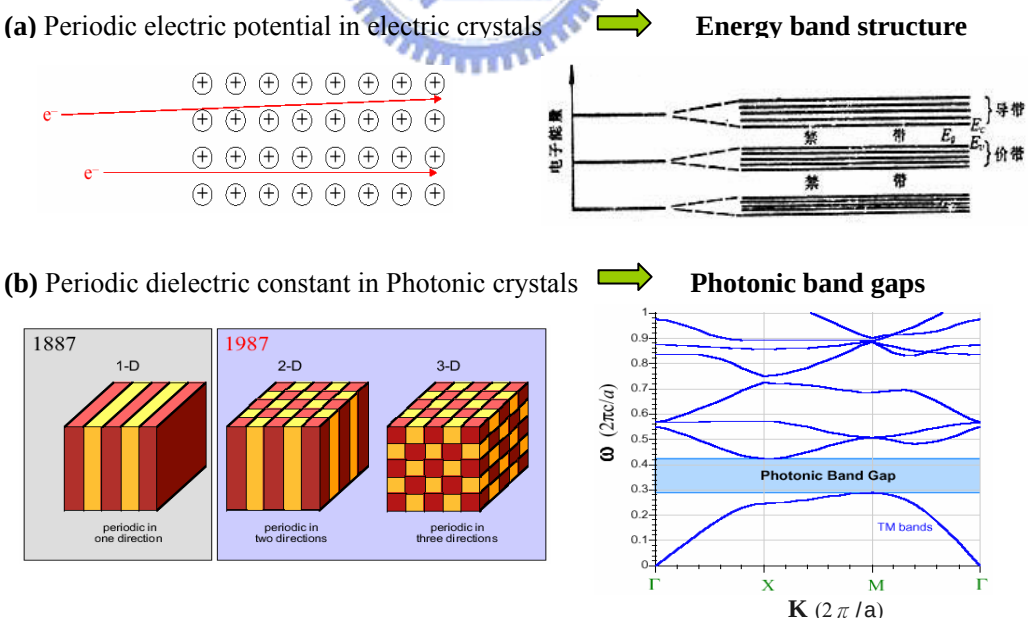


Fig.2-3 (a) electronic energy band structure in a solid with periodic electric potential. (b) Photonic band structures in the photonic crystals with 1D, 2D, and 3D periodic dielectric constant.

In conventional geometrical optics, light propagation in dielectric materials is described by the Snell's law and phase refractive index (n_p). However, the phase velocity (v_p) is defined as the velocity of the propagation of an equal phase surface which cannot be defined rigorously in the photonic crystals, since its eigenfunction is a superposition of plane waves. This means that the phase velocity cannot be defined appropriately in photonic crystal. Recently, the phase refractive index of photonic crystals has been discussed by several authors in the long wavelength limit [13-15]. They have homogenized the periodic structures and deduced an appropriate phase index in the low frequency limit. However, such a result cannot be extended to higher frequencies of which wavelength becomes comparable to, or smaller than, the lattice period. Since most of interesting phenomena, including unusual beam propagation, occur outside the low-frequency limit, we are not satisfied with this homogenization method to understand the light propagation in photonic crystals.

Dowling *et al.* used essentially the some argument, which the phase refraction index equation is n=*ck/w*, to predict an ultra small index for photonic crystals. [16] This effect is due to the reduction of wave vector *k* near the zone center as a result of the band folding. However, this argument leads to an ultra small *n* even for an empty lattice with the same crystal structure. In their photonic crystal model, we know that light propagation in such an empty-lattice photonic crystal (at least when its frequency does not satisfy the Bragg condition) should be normal; however, this model still predicts abnormal phase index. This apparent contradiction shows that the deduced small *n* does not possess real meaning and that the band folding itself does not lead to unusual beam propagation. [9] This contradiction arises mainly because we have only considered *k* in the above analysis. We must also consider the group velocity vector to study beam propagation in photonic crystals.

The group velocity ($\vec{v}_g$), which is the velocity of the propagation of a wave packet, can be defined as usual:

$$\vec{v}_g = \frac{\partial w}{\partial \vec{k}} \tag{2.7}$$

The energy velocity is defined as the velocity of the propagation of the electromagnetic energy. The propagation of the electromagnetic energy is described by Poynting's vector. The time-averaged Poynting's vector is given by

$$\vec{S}_{\vec{k}n}(r) \equiv average < \mathrm{Re}\left[\vec{E}_{\vec{k}n}(\vec{r})e^{-iw_{kn}t}\right] \times \mathrm{Re}\left[\vec{H}_{\vec{k}n}(\vec{r})e^{-iw_{kn}t}\right] > \tag{2.8}$$

$$= \frac{1}{2}\mathrm{Re}\left[\vec{E}_{\vec{k}n}(\vec{r}) \times \vec{H}^{*}_{\vec{k}n}(\vec{r})\right].$$

On the other hand, the time-averaged electromagnetic energy density $U_{\vec{k}n}(\vec{r})$ is given by

$$U_{\vec{k}n}(\vec{r}) \equiv \frac{\varepsilon_0 \varepsilon(\vec{r})}{2} average\left\{\left\{\mathrm{Re}[\vec{E}_{\vec{k}n}(\vec{r})e^{-i\omega_{kn}t}]\right\}^2\right\} + \frac{\mu_0}{2} average\left\{\left\{\mathrm{Re}[\vec{H}_{\vec{k}n}(\vec{r})e^{-i\omega_{kn}t}]\right\}^2\right\} \tag{2.9}$$

$$= \frac{1}{4}\left\{\varepsilon_0 \varepsilon(\vec{r})\left|\vec{E}_{kn}(\vec{r})\right|^2 + \mu_0\left|\vec{H}_{kn}(\vec{r})\right|^2\right\}$$

Thus, the energy velocity $\vec{v}_e$ is defined as

$$\vec{v}_e = \frac{\left\langle \vec{S}_{kn}(\vec{r}) \right\rangle}{\left\langle \vec{U}_{kn}(\vec{r}) \right\rangle} \tag{2.10}$$

Where $\langle \cdots \rangle$ means the spatial average.

Now, the group velocity is equal to the energy velocity even though the dielectric constant is modulated periodically. The proof was given by Yeh [17].

$$\vec{v}_e = \vec{v}_g \tag{2.11}$$

So far we claim that directions for the group velocity, energy velocity and Poynting vector are identical. Furthermore, in order to follow the geometrical approaches for photonic crystals, we still need to study the equal frequency surface (EFS) of the photonic band

structure to discuss the positive and negative refractive phenomenon. More detailed explanation for them will be given at the section 3-1.

2-2 Plane-wave expansion method for band structure calculation [34]

Owing to study the propagation of light in a photonic crystal, we must possess the photonic band structure (dispersion relation) and equal frequency surface (EFS). Therefore, we can apply a calculation method, plane-wave expansion method, to get them.

First, we start from the Maxwell's equations in CGS units:

$$\begin{aligned} \nabla \bullet \vec{B} &= 0, & \nabla \times \vec{\mathrm{E}} + \frac{1}{\mathrm{c}} \frac{\partial \vec{B}}{\partial t} &= 0, \\ \nabla \bullet \vec{D} &= 4\pi\rho, & \nabla \times \vec{\mathrm{H}} - \frac{1}{\mathrm{c}} \frac{\partial \vec{D}}{\partial t} &= \frac{4\pi}{c} \vec{J}, \end{aligned} \tag{2.12}$$

Where ***D*** and ***B*** are the displacement and magnetic induction fields, and ρ and ***J*** are the free charge and current densities. The light propagates within a periodic dielectric medium, a composite of regions of homogeneous dielectric material, with no free charge or currents (ρ=***J***=0).

First we assume the field strengths are small enough so that we are in the linear regime, or the operation frequency region far away from the resonance frequency region of the photonic materials. Second, we ignore any explicit frequency dependence of the dielectric constant and treat $\varepsilon(\mathbf{r})$ as purely real, i.e., the materials which construct the photonic crystals are non-dispersive. Third, we assume the medium is macroscopic and isotropic, so that $\mathbf{E}(\mathbf{r},w)$ and $\mathbf{D}(\mathbf{r},w)$ are related by a scalar dielectric constant $\varepsilon(\mathbf{r},w)$.

$$\vec{D}(\vec{r}) = \varepsilon(\vec{r})\vec{E}(\vec{r}) \tag{2.13}$$

Where the magnetic permeability is very close to unity and we may set $\boldsymbol{B} = \boldsymbol{H}$ for the most interesting dielectric materials. Then, we can assume the fields that happen to vary harmonically with time, so that we have

$$\begin{aligned} \overrightarrow{H}(\vec{r},t) &= \overrightarrow{H}(\vec{r}) \bullet e^{i\omega t} \\ \overrightarrow{E}(\vec{r},t) &= \overrightarrow{E}(\vec{r}) \bullet e^{i\omega t} \end{aligned} \quad . \tag{2.14}$$

The electromagnetic waves are considered to be transverse because there is no free charge or current. If we eliminate Eq. (2.14) in (2.12), we obtain the following equations:

$$\Theta_E \overrightarrow{E}(\vec{r}) \equiv \frac{1}{\varepsilon(\vec{r})} \nabla \times \{\nabla \times \overrightarrow{E}(\vec{r})\} = \frac{\omega^2}{c^2} \overrightarrow{E}(\vec{r}), \tag{2.15}$$

$$\Theta_H \overrightarrow{H}(\vec{r}) \equiv \nabla \times \{\frac{1}{\varepsilon(\vec{r})} \nabla \times \overrightarrow{H}(\vec{r})\} = \frac{\omega^2}{c^2} \overrightarrow{H}(\vec{r}). \tag{2.16}$$

Eq. (2.15) and (2.16) are solved as the eigen-value problems, and the Θ_H is a Hermitian operator. [8] That means the eigen functions $\boldsymbol{H_n}$ of Θ_H form a orthogonal complete set. We can apply the Bloch's theorem to Eq. (2.15) and (2.16), because $\boldsymbol{\varepsilon(r)}$ is a period function. These wave equations can be solved by a plane-wave expansion method.

In photonic crystals, the dielectric constant is periodic, with

$$\varepsilon(\vec{r}) = \varepsilon(\vec{r} + \overrightarrow{a_i}) \qquad (i = 1,2,3) \tag{2.17}$$

where $\boldsymbol{\{a_i\}}$ is the primitive lattice vector of the photonic crystal. Because of this spatial periodicity, we introduce the primitive reciprocal lattice vectors $\{\boldsymbol{b}_i$; i=1,2,3$\}$ and the arbitrary reciprocal lattice vector can be defined as $\{\boldsymbol{G}\}$

$$\begin{aligned} a_i \bullet b_j &= 2\pi\delta_{ij} \\ G &= l_1 b_1 + l_2 b_2 + l_3 b_3 \end{aligned} \quad , \tag{2.18}$$

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

$$\frac{1}{\varepsilon(r)} = \sum_G \varepsilon^{-1}(G)\exp(iG\bullet r) \tag{2.19}$$

we have $\varepsilon^{-1*}(G) = \varepsilon^{-1}(-G)$ due to the dielectric function is real. By applying Bloch's theorem to Eq. (2.15) and (2.16) with a periodic potential $\varepsilon^{-1}(r)$, ***E(r)*** and ***H(r)*** are characterized by a wave vector ***k*** and a index of band *n* in the first Brillouin zone and expressed as

$$\begin{aligned} \vec{E}(r) &= \vec{E}_{kn}(r) = \vec{u}_{kn}(r)e^{ik\bullet r}, \\ \vec{H}(r) &= \vec{H}_{kn}(r) = \vec{v}_{kn}(r)e^{ik\bullet r}, \end{aligned} \tag{2.20}$$

where $\vec{u}_{kn}(r)$ and $\vec{v}_{kn}(r)$ are periodic vectorial functions that satisfy the following relations:

$$\begin{aligned} \vec{u}_{kn}(r + a_i) &= \vec{u}_{kn}(r) \\ \vec{v}_{kn}(r + a_i) &= \vec{v}_{kn}(r) \qquad for\ i = 1,2,3 \end{aligned} . \tag{2.21}$$

By introducing plane-wave basis to expand $\vec{u}_{kn}(r)$ and $\vec{v}_{kn}(r)$, we obtain

$$\begin{aligned} \vec{E}_{kn}(r) &= \sum_G \vec{E}_{kn}(G)\exp\{i(k+G)\bullet r\}, \\ \vec{H}_{kn}(r) &= \sum_G \vec{H}_{kn}(G)\exp\{i(k+G)\bullet r\}. \end{aligned} \tag{2.22}$$

The expansion coefficients in reciprocal lattice space, i.e. $E_{kn}(G)$ and $H_{kn}(G)$ are denoted by the same symbols as the original ones in real space. Substituting Eq. (2.22) and (2.19) into (2.15) and (2.16), we obtain the following eigenvalue equations for the expansion coefficients $\{E_{kn}(G)\}$ and $\{H_{kn}(G)\}$:

$$\begin{aligned} -\sum_{G'} \varepsilon^{-1}(G-G')(k+G')\times\{(k+G')\times E_{kn}(G')\} &= \frac{\omega_{kn}^2}{c^2}E_{kn}(G), \\ -\sum_{G'} \varepsilon^{-1}(G-G')(k+G')\times\{(k+G')\times H_{kn}(G')\} &= \frac{\omega_{kn}^2}{c^2}H_{kn}(G). \end{aligned} \tag{2.23}$$

The vector electromagnetic field in the 2D photonic lattice can be decomposed into two independent polarization components, i.e. an E polarization (TM mode) for which the electric

field is parallel to the rod axis (E_z only), and an H polarization (TE mode) for which the magnetic field is parallel to the rod axis (H_z only). In two-dimensional photonic crystals, Eq. (2.23) reduces to

$$\sum_{G'} |k+G'||k+G|\varepsilon^{-1}(G-G')E_{kn}(G')\} = \frac{\omega_{kn}^2}{c^2}E_{kn}(G), \tag{2.24}$$

where Eq. (2.24) is the master equation of TM mode. Similarly, the master equation of TE mode can be written as

$$\sum_{G'} (k+G')\bullet(k+G)\varepsilon^{-1}(G-G')H_{kn}(G')\} = \frac{\omega_{kn}^2}{c^2}H_{kn}(G). \tag{2.25}$$

For the photonic band calculating, the expansion coefficients $\{\varepsilon^{-1}(G)\}$ in Eq. (2.19) is necessary to be calculated by the plane-wave expansion method. The inverse Fourier transform gives

$$\varepsilon^{-1}(G) = \frac{1}{V}\int_V dr\varepsilon^{-1}(r)\exp(-iG\bullet r), \tag{2.26}$$

where V denotes the volume of the unit cell of the photonic crystal. In general, this integral should be evaluated numerically by FFT method. However, if the shapes of the dielectric components in the unit cell are simple enough, we can calculate it analytically.

2-3 FDTD method for electromagnetic simulation

The FDTD and related space-grid time-domain techniques, techniques introduced by Yee in 1966, are direct solution methods for Maxwell's curl equations. [18] Since 1990, when engineers in the general electromagnetic community became aware of the modeling capabilities afforded by FDTD and related techniques, the interest in this area has expanded well beyond defense technology. Presently these methods have been used to solve numerous

scattering problems on dielectrics, especially in periodic structure.

2-3.1 Free space formulation [19]

The time-dependent Maxwell's curl equations in free space are

$$\begin{aligned}\frac{\partial \boldsymbol{E}}{\partial t} &= \frac{1}{\varepsilon_0}\nabla \times \boldsymbol{H} \\ \frac{\partial \boldsymbol{H}}{\partial t} &= -\frac{1}{\mu_0}\nabla \times \boldsymbol{E}\end{aligned} \tag{2-27}$$

In general, Eq. (2-27) represent three equations each, where the ***E*** and ***H*** are vectors in three dimensions. We will start with a simple one-dimensional case using only E_x and H_y, so Eq. (2-27) become

$$\begin{aligned}\frac{\partial E_x}{\partial t} &= -\frac{1}{\varepsilon_0}\frac{\partial H_y}{\partial z} \\ \frac{\partial H_y}{\partial t} &= -\frac{1}{\mu_0}\frac{\partial E_x}{\partial z}.\end{aligned} \tag{2-28}$$

There are the equations of a plane wave with the electric field oriented in the x direction, magnetic field oriented in the y direction, and traveling in the z direction.

Taking the central difference approximations for both the temporal and spatial derivatives gives

$$\begin{aligned}\frac{E_x^{n+1/2}(k) - E_x^{n-1/2}(k)}{\Delta t} &= -\frac{1}{\varepsilon_0}\frac{H_y^n(k+1/2) - H_y^n(k-1/2)}{\Delta x} \\ \frac{H_y^{n+1}(k+1/2) - H_y^n(k+1/2)}{\Delta t} &= -\frac{1}{\mu_0}\frac{E_x^{n+1/2}(k+1) - E_x^{n+1/2}(k)}{\Delta x}\end{aligned} \tag{2-29}$$

In these two equations, time is specified by the superscripts, i.e., "n" actually means a time $t = \Delta t \cdot n$. Remember, we have to discrete everything for formulation into the computer. The term "$n+1$" means one time step later. The terms in parentheses represent distance, i.e., "k"

actually means the distance $z = \Delta x \cdot k$. (However, Δx is so commonly used for a spatial increment that I will use Δx.) The formulation of Eq. (2-29) assumes that the ***E*** and ***H*** fields are interleaved in both space and time. ***H*** uses the argument k+1/2 and k-1/2 to indicate that the ***H*** field values are assumed to be located between the E field values.

As illustrated in Fig. 2-4, the Yee algorithm also centers its ***E*** and ***H*** components in time in what is termed a leapfrog arrangement. All of the ***E*** components in the modeled space are completed and stored in memory for a particular time point using previously stored ***H*** data. Then all of the ***H*** computations in the space are completed and stored in memory using the ***E*** data just computed. The cycle begins again with the re-computation of the ***E*** components based on the newly obtained ***H***. This process continues until time-stepping is concluded.

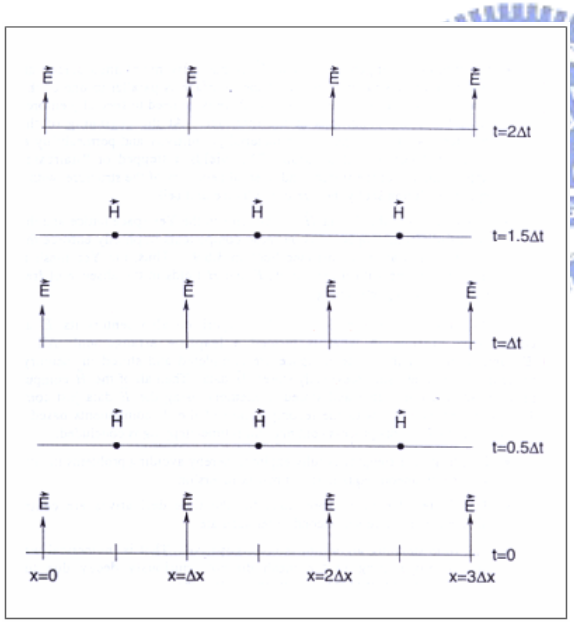


Fig.2-4 Space-time chart of the Yee algorithm for a one-dimensional wave propagation example showing the use of central differences for the space derivatives and leapfrog for the time derivatives. Initial conditions for both electric and magnetic fields are zero everywhere in the grid.

Let us return to the discussion of 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"

$$\Delta t \le \frac{\Delta x}{\sqrt{n}c} \tag{2-30}$$

where n is the dimension of the simulation and c is the speed of light.

Of course we still need to add incident wave source condition and absorbing boundary condition. It is a great subject in talking about the wave source condition.

2-3.2 Simulation in periodic structure

Owing to simulate the wave propagation in a photonic crystal medium which is periodic-dielectric distribution, we have to add the relative dielectric constant ε_r to Maxell's equations:

$$\begin{aligned} \frac{\partial \vec{E}}{\partial t} &= \frac{1}{\varepsilon_r \varepsilon_0} \nabla \times \vec{H} \\ \frac{\partial \vec{H}}{\partial t} &= -\frac{1}{\mu_0} \nabla \times \vec{E} \end{aligned} \tag{2-31}$$

In photonic crystal medium, the dielectric constant ε_r is periodic.

We have been using the form of Maxwell's equations, which use only the ***E*** and ***H*** files. We will begin by normalizing these equations, using

$$\begin{aligned} \tilde{E} &= \sqrt{\frac{\varepsilon_0}{\mu_0}} \cdot E \\ \tilde{D} &= \sqrt{\frac{1}{\varepsilon_0 \cdot \mu_0}} \cdot D, \end{aligned} \tag{2-32}$$

which leads to

$$\begin{aligned} \frac{\partial \tilde{\boldsymbol{D}}}{\partial t} &= \frac{1}{\sqrt{\varepsilon_0 \mu_0}} \nabla \times \boldsymbol{H} \\ \tilde{\boldsymbol{D}}(w) &= \varepsilon_r^*(w) \cdot \tilde{\boldsymbol{E}}(w) \\ \frac{\partial \boldsymbol{H}}{\partial t} &= -\frac{1}{\sqrt{\varepsilon_0 \mu_0}} \nabla \times \tilde{\boldsymbol{E}}, \end{aligned} \tag{2-33}$$

where ***D*** is the electric flux density. Notice that Eq. (2-33) is written in the frequency domain.

We will assume we are dealing with a lossy dielectric medium of the form

$$\varepsilon_r^*(w) = \varepsilon_r + \frac{\sigma}{j\omega\varepsilon_0} \tag{2-34}$$

and substitute Eq.(2-34) into (2-33):

$$D(w) = \varepsilon_r \cdot E(w) + \frac{\sigma}{jw\varepsilon_0} E(w). \tag{2-35}$$

Taking the first term into the time domain is not a problem because it is simple multiplication. In the second term, Fourier theory tells us that $1/jw$ in the frequency domain is integration in the time domain, so Eq. (2-35) becomes

$$D(t) = \varepsilon_r \cdot E(t) + \frac{\sigma}{\varepsilon_0}\int_0^t E(t') \cdot dt' \tag{2-36}$$

we will want to go to the sampled time domain, so the integral will be approximated as a summation over the time steps Δt

$$D^n = \varepsilon_r \cdot E^n + \frac{\sigma \cdot \Delta t}{\varepsilon_0}\sum_{i=0}^{n} E^i = \varepsilon_r \cdot E^n + \frac{\sigma \cdot \Delta t}{\varepsilon_0} E^n + \frac{\sigma \cdot \Delta t}{\varepsilon_0}\sum_{i=0}^{n-1} E^i \tag{2-37}$$

further we can calculate E^n

$$E^n = \frac{D^n - \frac{\sigma \cdot \Delta t}{\varepsilon_0}\sum_{i=0}^{n-1} E^i}{\varepsilon_r + \frac{\sigma \cdot \Delta t}{\varepsilon_0}} \tag{2-38}$$

Assume that we are asked to calculate the E field distribution at every point in a dielectric medium subject to illumination at various frequencies. One approach would be to use a sinusoidal source and iterate the FDTD program until we observe that a steady state has been reached, and determine the resulting amplitude and phase at every point of interest in the

medium.

Suppose we want to calculate the Fourier transform of the E field $E(t)$ at a frequency f_1. This can be done by the equation

$$E(f_1)=\int_0^{t_T} E(t)\cdot e^{-j2\pi f_1 t}dt. \tag{2-39}$$

Notice that the lower limit of the integral is 0 because the FDTD program assumes all causal functions. The upper limit is t_T, the time at which the FDTD iteration is halted. Rewriting Eq. (2-39) in a finite difference form.

$$E(f_1)=\sum_{n=0}^{T} E(n\bullet\Delta t)\bullet e^{-j2\pi f_1(n\bullet\Delta t)} \tag{2-40}$$

Where T is the number of iterations and Δt is the time step, so $t_T = T\cdot\Delta t$. Eq. (2-40) may be divided into its real and imaginary parts

$$E(f_1)=\sum_{n=0}^{T} E(n\cdot\Delta t)\cdot\cos(2\pi f_1\cdot\Delta t\cdot n)-j\sum_{n=0}^{T} E(n\cdot\Delta t)\cdot\sin(2\pi f_1\cdot\Delta t\cdot n). \tag{2-41}$$

Note that there is an amplitude and phase associated with every frequency at each cell.

Although, the absorbing boundary conditions (ABCs) are necessary to keep outgoing ***E*** and ***H*** field form being reflected back into the problem space. Normally, in calculating the ***E*** field, we need to know the surrounding ***H*** values; that is a fundamental assumption of the FDTD method. At the edge of the problem space we will not have the value to one side; however, because we know that there are no sources outside the problem space, we have an advantage what the fields at the edge must be propagating outward. We will use these two facts to estimate the value at the end.

One of the most flexible and efficient ABCs is the perfectly matched layer (PML)

developed by Berenger [20]. In our simulation problem, we use this way to prevent the boundary refraction of the propagation light. Whereas, owing to simulate a plane wave in a 2D FDTD program, the problem space will be divided up into two regions, the total field and the scattered field, as shown in Fig. 2-5. There are two primary reasons for doing this: (1) The propagated 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, i.e., a certain portion of the impinging wave is reflected back into the problem space. By subtraction the incident field, the amount of the radiation field hitting the boundary is minimized, thereby reducing the amount of error.

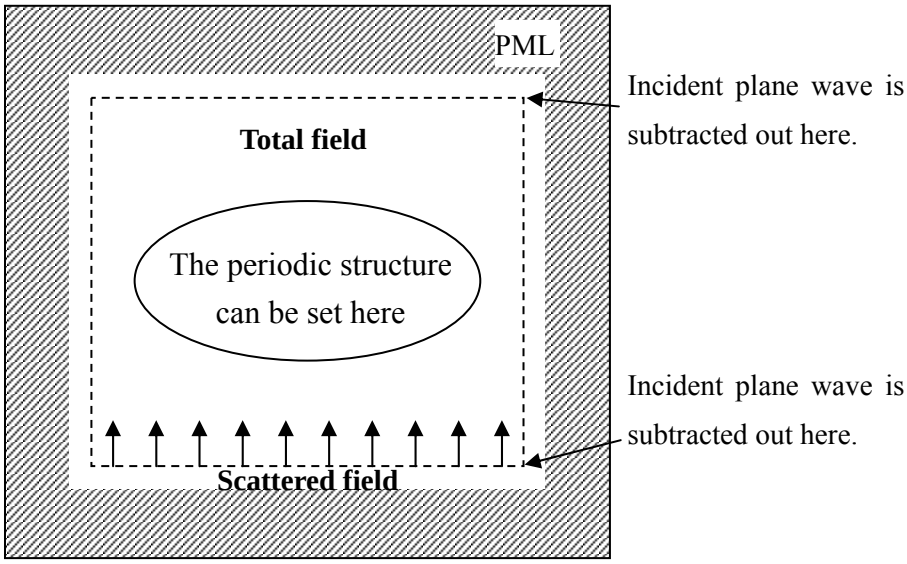


Fig.2-5 Total field/scattered field of the two-dimensional problem space.