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ANALYTICAL STUDY OF LIGHT AND LIQUID CRYSTALS REORIENTATION IN ANISOTROPIC PHOTONIC CRYSTALS USING ONE-DIMENSION FINITE DIFFERENCE TIME DOMAIN (FDTD) METHOD

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ABSTRACT

ANALYTICAL STUDY OF LIGHT AND LIQUID CRYSTALS REORIENTATION IN ANISOTROPIC PHOTONIC CRYSTALS USING ONE-DIMENSION FINITE DIFFERENCE TIME DOMAIN (FDTD) METHOD

(Keywords: Diffraction; Nematic liquid crystals; Birefringence; Anistropic Photonic Crystals; Finite Domain Time Difference; Holography)

This study demonstrate diffractive light from an anisotropic photonic crystal (PCs) based on holographic polymer-dispersed liquid crystals (HPDLCs) that are fabricated using two-beam interference with various pitch and exposure energy. One of the most powerful approaches for the analysis of PCs structure is 2×2 Jones method, which is widely used for most simple cases. But, in case of anisotropic structures which more microscopically or complex, it cannot analyze with accuracy in this method. In this research, we have studied and analyzed the modulation of light and liquid crystal reorientation in one-dimension anisotropic PCs from HPDLCs using FDTD method. HPDLCs is modeling as a mixture of polymer and liquid crystals (LCs) that categorized as an anisotropic medium. FDTD method is directly solve Maxwell's equation with less approximation, so this method can analyze more flexible and general approach for the arbitrary anisotropic media. As the results from FDTD simulation, Bragg diffraction is occurred when Q>10 and highest diffraction efficiency occurred at ± 19 degrees (Bragg angle) when incident beam is *p* polarization. Therefore, we can assumed the liquid crystal is aligned parallel to the grating constant vector $(\mathbf{n} // \mathbf{k})$ from perpendicular alignment $(\mathbf{n} \perp \mathbf{k})$ at low exposure energy or wider pitch grating. Furthermore, by using FDTD method, PCs model with no alignment of different sizes liquid crystal droplets that become smaller to the thickness direction or assumed as polymer are agreed with experimental results. Moreover, we can understand that the trend of diffraction efficiency become wider if the thickness of liquid crystal droplet is shorter.

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CHAPTER I

INTRODUCTION

1.1 Introduction

Photonic crystals (PCs) are highly ordered structures with a periodically modulated refractive index, with periods typically on the length scale of optical wavelengths (380-750nm). The periodicity may exist in one, two or multi-dimensional and the propagation of electromagnetic waves in PCs are based on Bragg diffraction on lattice planes. Furthermore, there is a band of frequencies which light propagation in the PCs is forbidden. It is called photonic band gap (PBG or stop band). A complete PBG occurs when a range of frequencies is forbidden for every state of polarization and propagation direction. Because of their ability to confine, control and manipulate photon in up to 3D, a wide variety of applications are interested such as displays, optical wave-guides, optical data storage, switches, lasers, and sensors [1-2]. Moreover, PCs is also offers opportunities for the miniaturize form and superprism effect which may be exploited in the future to fabricate high-density optical integration circuits [2-3]. Examples of natural photonic crystals structures are exist in hard minerals (opal) and as well as in living creatures (Butterfly wings and fur of the sea mouse). Nevertheless, there is a lot of problems of PCs fabrication depend to the methods themselves such as electron-beam lithography, self-multiphoton polymerization, semiconductor micromatching, nanoprinting, holographic lithography, self assembling of microparticles and cross grating which expensive equipments and materials are necessary [3-4].

1.2 Problem Statement

These days there are a lot of interest in the simulation and analysis of the properties of photonic and optical devices such as PCs. Due to their complex structures that will not allow traditional calculation for light pass through them, FDTD has apparently is the solution to overcome the problem. FDTD method is a very general method to calculate the electromagnetic fields in a structure or arbiratary geometry. Furthermore, no mathematical approximation, high reliability and versatility calculation to explain the liquid crystal reorientation in PCs based on HPDLCs.

However, the calculation is a very challenging task and can effectively be performed by super computer. In addition, the commercial software for FDTD is expensive and we need to derive mathematical equation and run the programming using Fotran90 and Matlab. Therefore, the load to the computing time is long and large memory capacity is needed for accumulating cell size from nano to micro range although in one dimensional calculation. However, the calculation is very accurate since the FDTD method is direct discreatization of Maxwell's equation for wave propagation such as light flow in isotropic or anistropic material. Typically, this method has been used widely in antenna and electromagnetic theory. It is not generally used in photonic because the target structural size or object is too large than the electromagnetic wavelength. Therefore, the load to the computing time is long and large memory capacity is needed. In recent years, improvement in the computer performance has encouraged FDTD method application in photonic.

1.3 Scopes of the Research

The scopes of this research are as the following:

1. The FDTD method were calculated on anisotropic PCs based on HPDLC structure as comparison to conventional method which is Coupled Wave Theory.

2. The research were focused on high reliability and versatility calculation without mathematical approximation to explain the liquid crystal reorientation.

3. This research analyzed detailed structure for high diffraction efficiency depend to liquid crystal reorientation using the relationship between polarization and modulation of light in anisotropic PCs.

1.4 Objectives of the Research

The objectives of this research are:

1. To create one-dimensional FDTD method for high efficiency anistropic PCs.

2. To investigate the modulation of light in anisotopic PCs based on HPDLCs.

3. To explain and clarify how to control and manipulate the modulation of light depends on the reorientation and migration of the LCs.

1.5 Research Methodology

The FDTD method is based on the Yee algorithm and directly solves the Maxwell equation. It is divided into TE FDTD method and TM FDTD method that can be calculated independently and not influence to each other in an isotropic medium. In other words, polarized light is kept the same in an isotropic medium. When there is no change in a direction of wave sources and targeted object, FDTD method is possible to analyze in two dimension problem. In this research, polarized light is change when incident to LCs and both method are mutually influence to each other. To calculate these mutually influences, the permittivity which represent a tensor quantity is used to consider anisotropic medium in FDTD method.

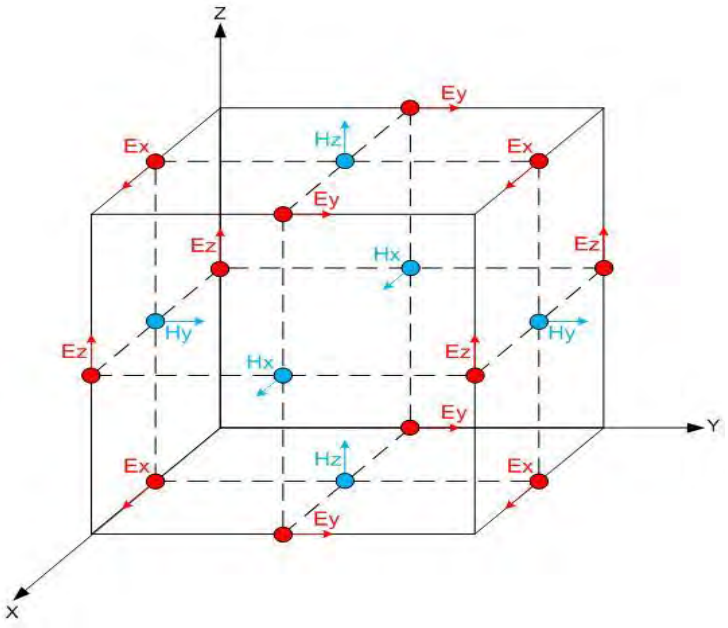


Figure 1.1 : Illustration of a standard Cartesian Yee cell used for FDTD

Nematic liquid crystal (NLCs) is assumed as the material which has uniaxial anisotropy medium consist of extraordinary refractive index n_e and ordinary refractive index n_o respectively. The director N of NLC can be defined in laboratory coordinate and the dielectric tensor can be calculated by coordinate conversion of director direction. In electromagnetic field arrangement, the electric field, ***E*** and electric displacement, ***D*** is assumed to be on the same arrangement.

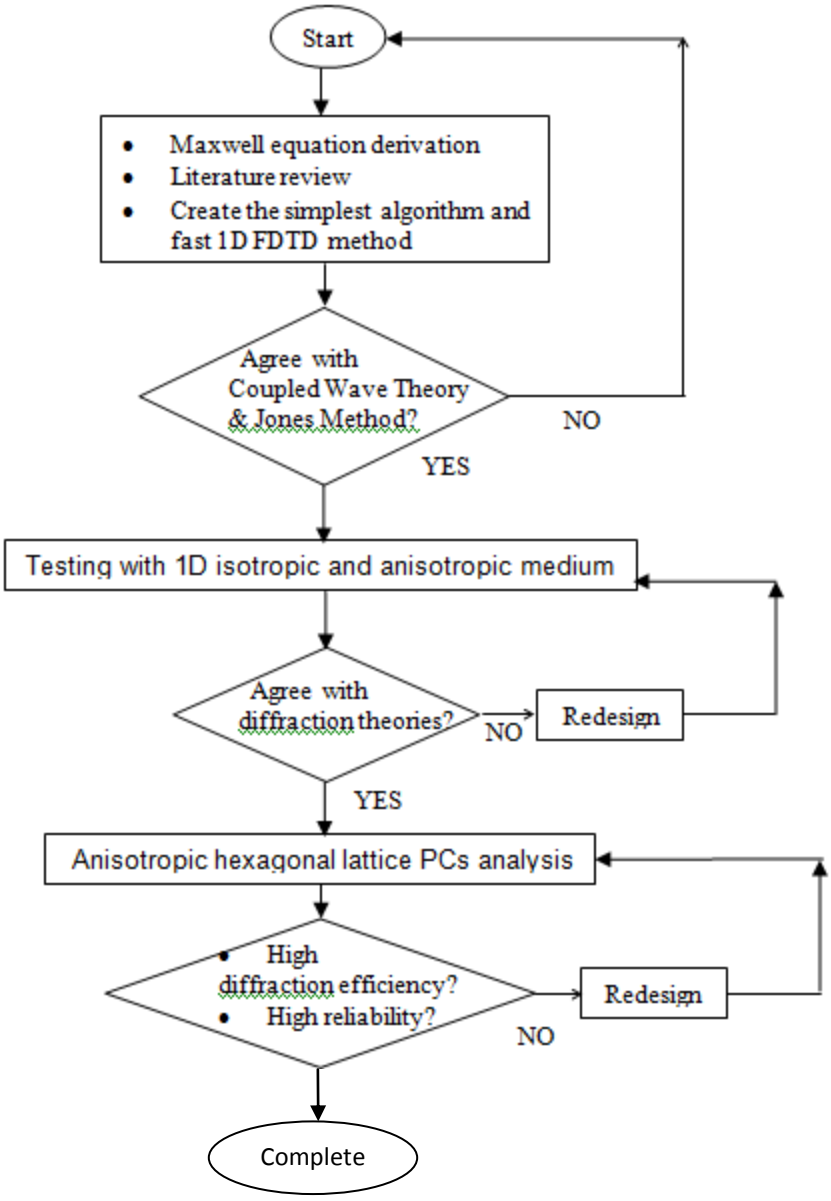


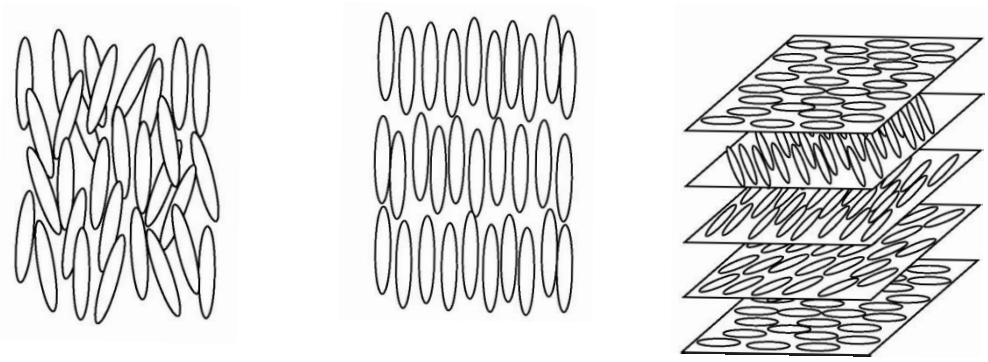
Figure 1.2 Flow Chart of the programming for FDTD Method

CHAPTER II

LITERATURE REVIEW

2.1 Liquid Crystals

We usually thought that matter only exist in three states: solid, liquid, and gas. However, there is a substance at intermediate state between solid and liquid which called as liquid crystal. The proper name of liquid crystal is 'mesomorphic phase' (mesomorphic: of intermediate form). Liquid crystal may flow like a liquid, but have optical anisotropy like the crystal at specific temperature range. Not all substances become liquid crystal at this intermediate state and generally the solid will melt as isotropic liquid. Liquid crystal also viewed as liquid in ordered arrangement of molecules exist. Liquid crystal arises under certain conditions in organic substance having sharply anisotropic molecules that is highly elongated (rodlike) molecules or flat (dislike) molecules. By the interaction of the intermolecular, liquid crystal can be classified into nematic liquid crystal, smectic liquid crystal, and cholesteric liquid crystal as shown in Figure 2.1.



a) nematic liquid crystal b) smectic liquid crystal c) cholesteric liquid crystal

Figure 2.1 Classification of liquid crystal

In this research we used nematic liquid crystal. The molecules are rodlike with their long axes aligned approximately parallel to one another but random at molecules position relation. Microscopically, each molecule of liquid crystal is aligned in various direction and not completely parallel as shown in Figure 2.2. However, macroscopically the molecules are overall suitable for a certain direction which called director. Thus at any point of the molecules, we can define a vector **n** to represent the preferred director in the immediate neighbourhood of the point. In a homogeneous nematic liquid crystal, the director is constant throughout the medium. In an inhomogeneous nematic liquid crystal, the director **n** can change from point to point and in general, a function of space(x,y,z). To determine the overall distribution of the molecules direction, it can be defined using order parameter as

$$S = \frac{1}{2}\left(3\left\langle \cos^2 \theta_i \right\rangle - 1\right) \tag{2.1}$$

θ_i is represent the angle between long axis of individual molecule and the director **n**, $\langle\rangle$ or angular brackets is represent the mean value in macroscopically view. For perfectly parallel alignment, S=1, while for totally random orientations, S=0. Moreover, nematic liquid crystal has an intermediate value of order parameter S which is strongly temperature dependent. At the clearing point, its order parameter S becomes zero and depends on the structure of the molecules in several cases. Typical values of the order parameter S are in the range between 0.6-0.4 at low temperatures.

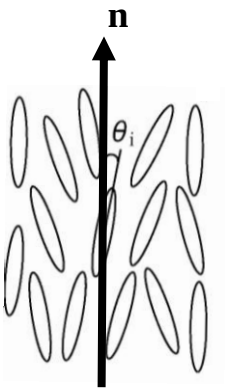


Figure 2.2 Director of liquid crystal

2.2 Birefringence (Optical anisotropy)

The main characteristic of liquid crystal is its anisotropic refractive index similar to uniaxial anisotropic crystal. Liquid crystal and uniaxial anisotropic crystal possesses two difference refractive indexes which consist of ordinary refractive index of n_o and extraordinary refractive index of n_e respectively. The ordinary refractive index is for light with electric field polarization perpendicular to the director (long axis) $n_o = n_\perp$, and the extraordinary refractive index is for light with electric field polarization parallel to the director (long axis) $n_e = n$. Birefringence is defined as

$$\Delta n = n_e - n_o \tag{2.2-1}$$

For liquid crystal, it is convenient to illustrate the light wave propagation in indicatrix as shown in Figure 2.3. Therefore, it can be defined in equation as

$$\left(\frac{x}{n_x}\right)^2 + \left(\frac{y}{n_y}\right)^2 + \left(\frac{z}{n_z}\right)^2 = 1 \tag{2.2-2}$$

where n_x, n_y, and n_z are main refractive indexes, $n_x=n_y\equiv n_o$ are represent the ordinary refractive index and $n_z\equiv n_e$ are represent the extraordinary refractive index. For example, refractive index becomes equal in all direction when the light propagates in z direction which is well known as optical axis. In other direction, electric field vector of the light wave will passes point O and refractive indices are divided into different two value.

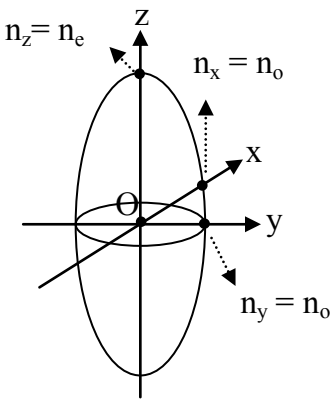
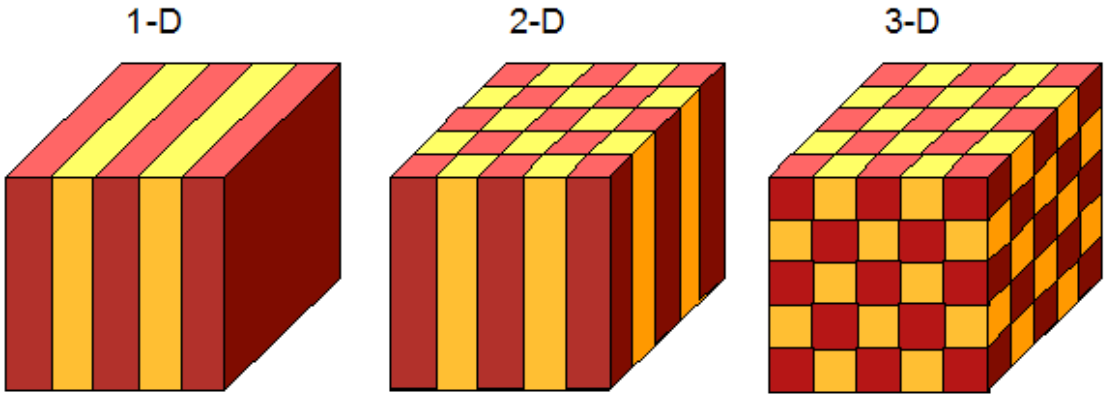


Figure 2.3 Indicatrix of uniaxial crystal

2.3 Photonic Crystals



a) b) c)

Figure 2.3 Photonic crystals dimensional a) periodic in one dimension which is discovered by Lord Rayleigh; b) periodic in two dimension that demonstrated by Thomas Krauss and c) periodic crystals periodic in three dimension.

The periodicity in one, two or multi-dimensional are able to confine, control and manipulate the propagation of light in PCs based on Bragg diffraction on lattice planes. There is a band of frequencies which light propagation in the PCs is forbidden. It is called photonic band gap (PBG or stop band). A complete PBG occurs when a range of frequencies is forbidden for every state of polarization and propagation direction. Because of these properties, a wide variety of applications are interested such as displays, optical wave-guides, optical data storage, switches, lasers, and sensors [1-2].

After the proposal by Yablonovitch in 1993, fabrication of PCs has been investigated intensively [5]. Various techniques to fabricate PCs such as electron-beam lithography, self-multiphoton polymerization, semiconductor micromatching, nanoprinting, holographic lithography, self assembling of microparticles and cross grating have been demonstrated with different levels of success[3-4]. In 1995, Russel *et. al* has successfully constructed hexagonal lattice of air holes in silica glass. This discovery showed PCs possessed two dimension photonic band structures which is the starting point of Photonic Crystal Fiber (PCF) research development. It is quite different from those of conventional fiber optics but still using Total internal reflection (TIR). Using PBG as a new theory of PCF, there are two advantages. There are a big change of effective refractive index of clad depend to the wavelength and the difference refractive indices of core and clad are bigger than conventional fiber optics. Nevertheless, there is a lot of problems of PCF fabrication before realize it as application.

There are several problems of PCs fabrication depend to the methods themselves. For examples, by using lithography method, it requires large and expensive apparatus and not suitable for three dimension geometries. Furthermore, for cross grating method, there are problems such as incoherent exposure by two-beam exposure, lack of phase relationship, and saddle point which combined results of the nonlinearity of the recording material. In addition, it is lack to control lattice parameter of PCs using self assembling of microparticles method. It is also difficult and time consuming for semiconductor micromatching method. Therefore, regarding to above reasons, we decided to used FDTD simulation order to analysis the PCs before fabrication to reduce cost and time.

Analysis of various but coupled (non-tapered) waveguide has also been done and the improvement in the transmission characteristic while moving from butt-coupled to the taper configuration has also been studied by Vijay et. al. they investigated the properties of nonlinear switches and also tapers based on PCs [6]. A plane wave expansion method (PWE) along with the FDTD scheme has been used for the simulations [7-8]. The propagation of electromagnetic signals inside the PBG structures and the penetration depth of the field modes can be conveniently and efficiently studied using the FDTD method [8]. FDTD is a time domain numerical method which acts by discretisation of Maxwell's equations. Time domain methods has been the most accurate computational tools for modeling and simulating the classical electromagnetic problems, including periodic media such as PCs [8-12]. This method allows the user to specify the material at all points in computational domain resulting in natural modeling of various materials and defect therein.

CHAPTER III

METHODOLOGY

3.1 Coupled Wave Theory

A coupled wave analysis is given of the Bragg diffraction of light by thick hologram gratings, which is analogous to Phariseau's treatment of acoustic gratings and to the dynamical theory of X-ray diffraction. The theory remains valid for large diffraction efficiencies where the incident wave is strongly depleted when Q>10. It can be applied to transmission holograms and to reflection holograms.

This theory assumes monochromatic light incident on the hologram grating at or near the Bragg angle and polarized perpendicular to the plane of incidence. Only two significant light waves are assumed to be present in the grating, the incoming "reference" wave *R* and outgoing "signal" wave *S*. Only these two waves obey the Bragg condition at least approximately, the other diffraction order violate the Bragg condition strongly and are neglected. They should be of little influence on the energy interchange between *S* and *R*.

Figure 3.1 shows the model of a hologram grating which is used for this research. The z-axis is chosen perpendicular to the surfaces of the medium, the x-axis in the plane of incident and parallel to the medium boundaries and the y-axis perpendicular to the paper. The fringes planes are oriented perpendicular to the plane incidence and slanted with respect to the medium boundaries at an angle . The grating vector **K** is oriented perpendicular to the fringe planes and is length $K\phi = \frac{2\pi}{\Lambda}$, where Λ is the period of

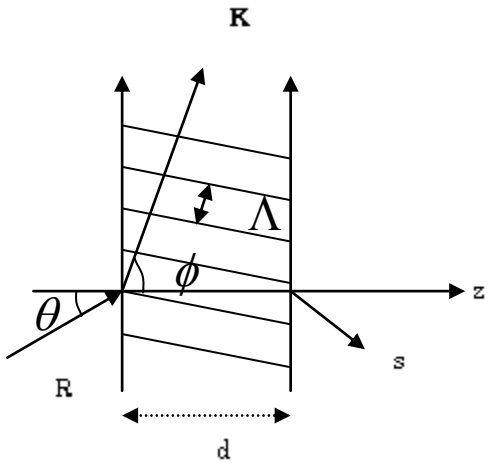


Figure 3.1 Calculation model Coupled Wave Theory

the grating. The same average dielectric constant is assumed for the region inside and outside the grating boundaries. The angle of incidence measured in the medium is θ.

In case of no slant $\phi = \frac{\pi}{2}$ and Bragg condition is obeyed, diffraction efficiency can be calculated by well known equation as below [26].

$$\eta = \frac{\sin(\nu^2 + \varepsilon^2)^{1/2}}{\left(1 + \frac{\varepsilon^2}{\nu^2}\right)} \tag{3.1-1}$$

where

$$\nu = \frac{\pi n_1 d}{\lambda \cos\theta} \tag{3.1-2}$$

and

$$\varepsilon = \frac{\pi n d \Delta\theta \sin(2\theta_B)}{\lambda \cos\theta} \tag{3.1-3}$$

λ is the wavelength of incident beam, *n* is amplitude of index modulation,

d is the sample thickness, θ is the angle of incident in a sample, θ_B is the Bragg angle, and $\Delta\theta = \theta - \theta_B$ is the deviation from the Bragg angle.

3.2 Finite Domain Time Different (FDTD) method [12]

3.2.1 Introduction

In 1966, Kane Yee originated a set of finite-difference equations for the time-dependent Maxwell's curl equations to calculate the electromagnetic fields in discrete space and time directly. This numerical electromagnetic analytical method is well known as FDTD method. Using both electric field, ***E*** and magnetic field, ***H*** information, the solution is more robust than using either electric field or the magnetic field alone with a wave equation. Moreover, there is no mathematical approximation and high versatility that various calculation models can be calculated. Typically, this method has been used widely in antenna and electromagnetic theory. However, it is not generally used in optic because the target structural size or object is too large than the electromagnetic wavelength. Therefore, the load to the computing time is long and large memory capacity is needed. In recent years, improvement in the computer performance has encouraged FDTD method application in optics.

Here, the basic Maxwell's curl equations of FDTD method are given by differential form of

Faraday's Law:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{3.2-1}$$

Ampere's Law:

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + J \tag{3.2-2}$$

Gauss' Law of Electric Field:

$$\nabla \cdot \mathbf{D} = \rho \tag{3.2-3}$$

Gauss' Law of Electric Field:

$$\nabla \cdot \mathbf{B} = 0 \tag{3.2-4}$$

where **E** is electric field, **B** is magnetic flux density, **H** is magnetic field, **D** is electric flux density, J is electric current density and ρ is charge density.

3.2.2 Basic concept

In FDTD method, calculation area is taken to enclose wave source and scattering substance. The calculation area is divided into unit cell as shown in Figure 1.1. Next, by applying Yee algorithm, formulated Maxwell equation is calculated to all cells. A key to Yee algorithm is the components of ***E*** and ***H*** (E_x,E_y,E_z,H_x,H_y,H_z) are staggered and spatially offset from one another. Therefore, Maxwell equation can be solved in the numerical value using first central-difference.

In Yee Algorithm, E and H are offset in time by 1/2 time step using a leapfrog time-stepping technique. The leapfrog time-stepping algorithm is explicit and simultaneous equations can be avoided. In Figure 3.2, Δt is a time step and x is assumed to be a paragraph where time is shown. The electric field is assumed to allocate at integer order of time t=(n-1)Δt、nΔt、(n+1)Δt…, while magnetic field is t=(n-1/2)Δt、(n+1/2)Δt… In an actual calculation, the electric field $\mathbf{E}^n$ is calculated from electric field En^{-1} and t=(n-1) Δt of magnetic field $\mathbf{H}^{n-1/2}$, then $H^{n-1/2}$ and $\mathbf{E}^n$ to calculate $\mathbf{H}^{n+1/2}$. Next the electromagnetic field is calculated sequentially one by one. The liquid crystal director and all six field-components are assumed to vary with two spatial directions *x* and *z*.