Chapter 2

Principle

2.1 Introduction

The great interest of this thesis is to make a dielectric grating with its period smaller than wavelength of incident light which can be treated as an effectively birefringence material. A general dielectric grating is shown in Fig. 2.1. Region O is a homogeneous dielectric with refractive index n_O; and further, region S is a homogeneous dielectric with refractive index n_S. Besides, the grating region is composed of a periodic distribution of two dielectric media with refractive indices n_1 and n_2, respectively. In the case of surface-relief grating, $n_1 = n_O$, $n_2 = n_S$. For simplicity, both dielectric media are supposed to be lossless media. Actually, the grating profile can be arbitrary. However, since any arbitrary grating profile can be approximated by separating the grating region into slabs of rectangular one, the theory of sub-wavelength grating is developed for rectangular profile only in the following sections.

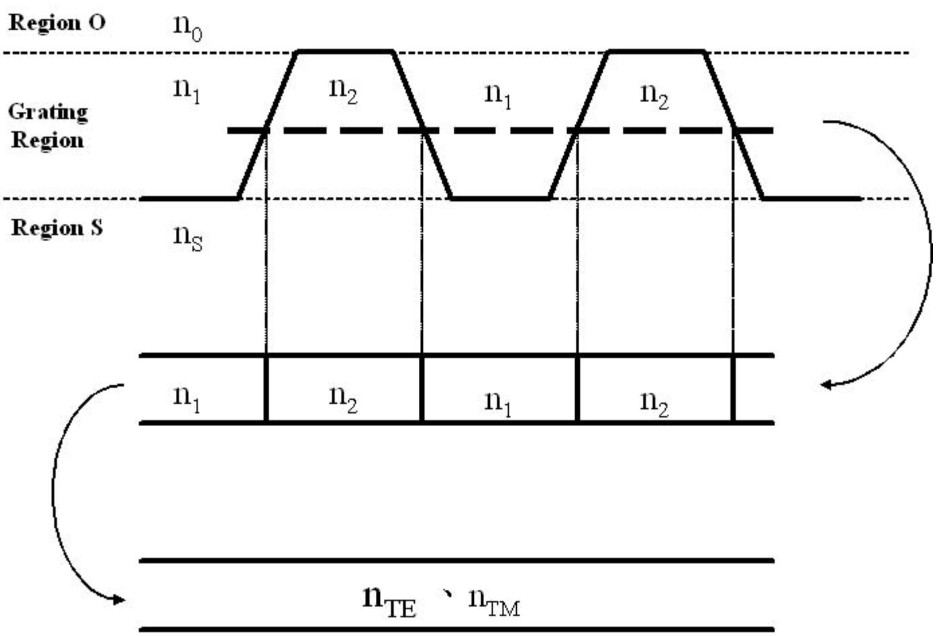

Fig. 2.1 A general dielectric grating.

Therefore, the principle of dielectric grating shall be defined later by considering the simplified grating shown in Fig. 2.2. The grating region is composed of dielectric 1 and dielectric 2 with widths t_1 and t_2, respectively. A rectangular profile can be defined by three parameters: grating period, *p*; grating depth, *d*; and fill factor, *f*, which is defined as $\frac{t_2}{p}$ [15][16].

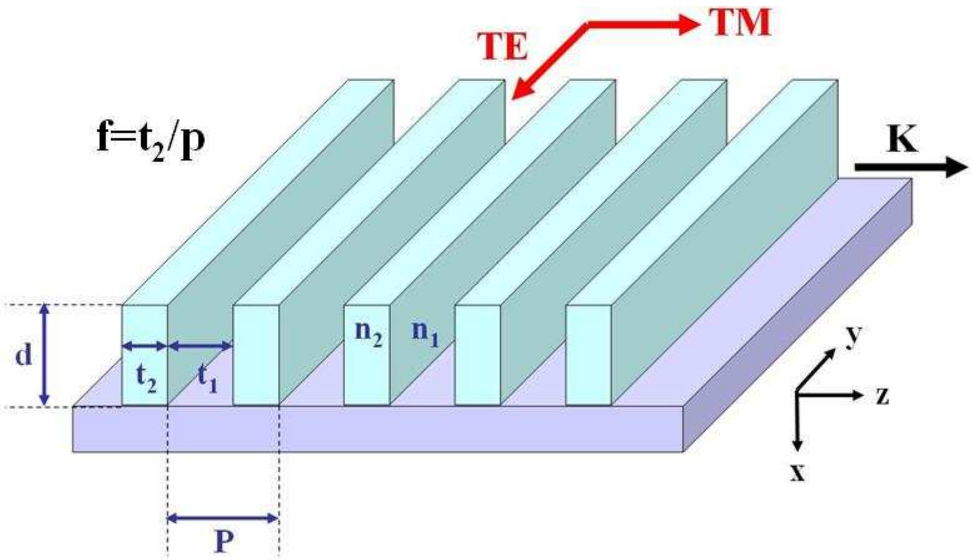

Fig. 2.2 Schematic of a zero-order grating ($p << \lambda$) with the polarized orientations of the incident electric field and definitions of rectangular grating parameters. The fill factor *f* is defined as $\frac{t_2}{p}$.

The optical properties of sub-wavelength grating are usually calculated by *Effective Medium Theory* (EMT). EMT regards the grating region as a uniaxial film between region 1 and region 2 and can derive the values of effective refractive indices: n_{TE} and n_{TM}. Then the reflectance and the transmittance of optical wave with its electric vector parallel and perpendicular to the grating bar are calculated by thin film theory with n_{TE} and n_{TM}. The principle is discussed in detail in the following.

2.2 EMT by Average Weighting Method

Suppose that the grating period *p* is much smaller than the wavelength of incident light λ, the field in the grating region may be regarded as uniform in dielectric 1 and dielectric 2, and the relation of mean field $\vec{E}$ and $\vec{D}$ can be carried out by averaging weighting method with weighting factor $1-f$ and *f*, respectively. The equations of n_{TE} and n_{TM} under normal incidence are derived in sections 2.2.1 and 2.2.2 [16].

The definitions of TE mode and TM mode of the rectangular grating are shown in Fig. 2.2. Under normally incidence, when electric vector $\vec{E}$ is perpendicular to grating vector $\vec{K}$, the incidence is defined as TE wave. On the other hand, when electric vector $\vec{E}$ lies in the incident plane, the incidence is defined as TM wave.

2.2.1 Effective Refractive Index n_{TE}

According to the boundary conditions of Maxwell's equations, the tangential component of the electric vector $\vec{E}$ is continuous across the border [17], so that the electric vector $\vec{E}$ will have the same value in each dielectric layer, and the electric displacements $\vec{D}$ in the two dielectric regions are

$$\vec{D}_1 = \varepsilon_1 \vec{E} \qquad 2.2.1$$

$$\vec{D}_2 = \varepsilon_2 \vec{E} \qquad 2.2.2$$

Here ε_1 and ε_2 are the dielectric constants of dielectric 1 and dielectric 2 respectively. Therefore, the average weighting of electric displacement $\vec{D}$ is

$$\vec{D} = \frac{t_1\varepsilon_1\vec{E} + t_2\varepsilon_2\vec{E}}{t_1 + t_2} \qquad 2.2.3$$

Hence the effective dielectric constant ε_{TE} is given by $\vec{D}$ over $\vec{E}$, therefore,

$$\varepsilon_{//} = \frac{\vec{D}}{\vec{E}}$$

$$= \frac{t_1\varepsilon_1 + t_2\varepsilon_2}{t_1 + t_2}$$

$$= (1-f)\varepsilon_1 + f\varepsilon_2 \qquad 2.2.4$$

With the refractive index $n = \sqrt{\varepsilon}$, the effective refractive index n_{TE} is given as

$$n_{TE} = \sqrt{(1-f)n_1^2 + fn_2^2} \qquad 2.2.5$$

2.2.2 Effective Refractive Index n_{TM}

In the case of TM mode, the electric displacement $\vec{D}$ is parallel to the grating vector $\vec{K}$. According to boundary conditions of Maxwell's equations, the normal component of electric displacement $\vec{D}$ must be continuous across the border. Hence, vectors $\vec{D}$ are the same in both dielectric regions. The corresponding electric field $\vec{E}$ in each dielectric region is

$$\vec{E}_1 = \frac{\vec{D}}{\varepsilon_1} \qquad 2.2.6$$

$$\vec{E}_2 = \frac{\vec{D}}{\varepsilon_2} \qquad 2.2.7$$

The average weighting of electric field $\vec{E}$ is

$$\vec{E} = \frac{t_1 \frac{\vec{D}}{\varepsilon_1} + t_2 \frac{\vec{D}}{\varepsilon_2}}{t_1 + t_2} \qquad 2.2.8$$

Hence, the effective dielectric constant ε_{TM} is given by

$$\varepsilon_{TM} = \frac{\vec{D}}{\vec{E}}$$

$$= \frac{(t_1 + t_2)\varepsilon_1\varepsilon_2}{t_1\varepsilon_2 + t_2\varepsilon_1}$$

$$= \frac{\varepsilon_1\varepsilon_2}{f\varepsilon_1 + (1-f)\varepsilon_2} \qquad 2.2.9$$

Similarly, the effective refractive index n_{TM} is given as

$$n_{TM} = \sqrt{\frac{n_1^2 n_2^2}{f n_1^2 + (1-f) n_2^2}} \qquad 2.2.10$$

Therefore, for different polarization of the incident light, the sub-wavelength grating has different refractive indices, n_{TE} and n_{TM}. Since the amount of birefringence, defined by $\Delta n = \sqrt{\varepsilon_{TM}} - \sqrt{\varepsilon_{TE}}$ depends on the grating profile, this phenomenon is so-called *form birefringence*.

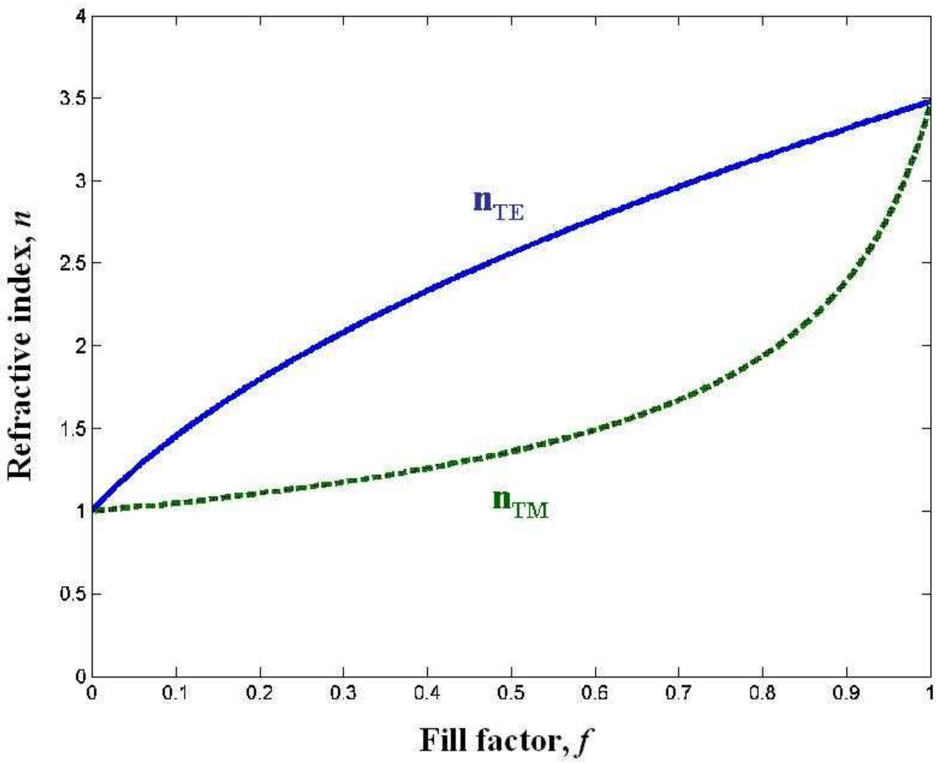

Fig. 2.3 Effective refractive indices, n_{TE} and n_{TM}, versus fill factor *f*. n_1 is equal to 1, and n_2 is equal to 3.48.

2.2.3 Properties of n_{TE} and n_{TM}

The validity of Eq. 2.2.5 and Eq. 2.2.10 can be verified by setting fill factor *f* equals to 0 or 1. For these two special cases, the grating region is made of either dielectric 1 or dielectric 2. Consequently, n_{TE} and n_{TM} are of the same value and reduce to n_1 or n_2. The relation of n_{TE} and n_{TM} versus fill factor *f* is plotted in Fig. 2.3, and several interesting properties of sub-wavelength gratings are observed. First, the values of n_{TE} and n_{TM} are changed with fill factor *f* and are between n_1 and n_2. In other words, sub-wavelength grating can be utilized as artificial materials of variable index of refraction. This property is useful in antireflection (AR) coating, whose condition can be fulfilled by such artificial materials. Second, n_{TE} is always larger than n_{TM}. It is easy to verify that

$$n_{TM}^2 - n_{TE}^2 = -\frac{f(1-f)\left(n_1^2 - n_2^2\right)^2}{fn_1^2 + (1-f)n_2^2} \leq 0 \qquad 2.2.11$$

implying that sub-wavelength grating behaves as a negative uniaxial crystal. Third, the ratio of n_{TE} over n_{TM} is also varied with f, and reaches to a maximum when f equals to 0.5.

2.3 EMT by Bloch Solution Method

The equations of n_{TE} and n_{TM} derived by averaging weighting method is quite simple; however, these equations are only valid for grating period much smaller than the wavelength of incident light. Therefore, it is necessary to develop new equations for gratings with larger period, which is much easier to be fabricated.

F. Bloch has proved the important theorem that the wave function for an infinite periodic potential must be of a special form [18]:

$$\varphi_K(\vec{r}) = u_K(\vec{r}) \cdot e^{i\vec{K}\cdot\vec{r}} \qquad 2.3.1$$

where $u_K(\vec{r}) = u_K(\vec{r} + p)$. Eqs. 2.3.1 expresses that the eigenfunctions of the wave equation for a periodic potential are the product of a plane wave $e^{i\vec{K}\cdot\vec{r}}$ times a function $u_K(\vec{r})$ with the periodicity of the grating. In the following sections, the effective refractive indices, n_{TE} and n_{TM}, shall be derived by the Block solution method [19].

Before deducing the effective refractive indices, the Cartesian coordinates have to be defined to describe the components of field vectors *E* and *H*. Assume the light is normally incident on the grating, we then define the direction of incident light as x-axis, and the directions parallel to the grating vector $\vec{K}$ as z-axis, respectively, as shown in Fig. 2.2.

2.3.1 Effective Refractive Index n_{TE}

In TE mode, the field vectors $\vec{E}$ and $\vec{H}$ are

$$\vec{E} = (0, e, 0) \qquad 2.3.2$$

and

$$\vec{H} = (h_x, 0, h_z) \qquad 2.3.3$$

First, from Maxwell's equation,

$$\nabla \times \vec{E} = -i\omega\mu\vec{H} \qquad 2.3.4$$

$$\nabla \times \vec{H} = i\omega\varepsilon\vec{E} \tag{2.3.5}$$

Three differential equations are given as

$$\frac{\partial e}{\partial z} = i\omega\mu h_x \tag{2.3.6}$$

$$\frac{\partial e}{\partial x} = -i\omega\mu h_z \tag{2.3.7}$$

$$\frac{\partial h_x}{\partial z} - \frac{\partial h_z}{\partial x} = i\omega\varepsilon e \tag{2.3.8}$$

As mentioned above, the wave functions in grating must be in Bloch form; therefore, e, h_x, and h_z are assumed as:

$$e = U(z)e^{-inkx} \tag{2.3.9}$$

$$h_x = V(z)e^{-inkx} \tag{2.3.10}$$

$$h_z = W(z)e^{-inkx} \tag{2.3.11}$$

where $U(z)$, $V(z)$, and $W(z)$ are periodic functions, i.e.,

$$U(z+p) = U(z) \tag{2.3.12}$$

$$V(z+p) = V(z) \tag{2.3.13}$$

$$W(z+p) = W(z) \tag{2.3.14}$$

Substituting Eqs. 2.3.9~2.3.11 into Eqs. 2.3.6~2.3.8, respectively,

$$\frac{dU}{dz} = i\omega\mu V \tag{2.3.15}$$

$$\frac{n}{c}U = \mu W \tag{2.3.16}$$

$$\frac{dV}{dz} + iknW = i\omega\varepsilon U \tag{2.3.17}$$

Then, we solve the simultaneous equations 2.3.15~2.3.17 for U, V, and W. There are two regions that are taken into account.

For $0 < z < t_1$,

$$U = A\cos(\alpha_1 z) + B\sin(\alpha_1 z) \tag{2.3.18}$$

$$V = -\frac{\alpha_1}{i\mu_1\omega}\left[A\cos(\alpha_1 z) + B\sin(\alpha_1 z)\right] \tag{2.3.19}$$

$$W = \frac{n}{\mu_1 c}\left[A\cos(\alpha_1 z) + B\sin(\alpha_1 z)\right] \tag{2.3.20}$$

$$\alpha_1 = k\sqrt{n_1^2 - n^2} \tag{2.3.21}$$

$$n_1^2 = \varepsilon_1\mu_1 \tag{2.3.22}$$

For $-t_2 < z < 0$,

$$U = C\cos(\alpha_2 z) + D\sin(\alpha_2 z) \tag{2.3.23}$$

$$V = -\frac{\alpha_2}{i\mu_2\omega}[C\cos(\alpha_2 z) + D\sin(\alpha_2 z)] \tag{2.3.24}$$

$$W = \frac{n}{\mu_2 c}[C\cos(\alpha_2 z) + D\sin(\alpha_2 z)] \tag{2.3.25}$$

$$\alpha_2 = k\sqrt{n_2^2 - n^2} \tag{2.3.26}$$

$$n_2^2 = \varepsilon_2\mu_2 \tag{2.3.27}$$

After applying the four conditions of continuity and periodicity of e and h_x with respect to z,

$$U(+0) = U(-0) \qquad U(t_1) = U(-t_2) \tag{2.3.28}$$

$$V(+0) = V(-0) \qquad V(t_1) = V(-t_2) \tag{2.3.29}$$

we obtain four homogeneous equations for A, B, C, D

$$A = C \tag{2.3.30}$$

$$A\cos(\alpha_1 t_1) + B\sin(\alpha_1 t_1) = C\cos(\alpha_2 t_2) - D\sin(\alpha_2 t_2) \tag{2.3.31}$$

$$B = xD \tag{2.3.32}$$

$$-x[A\cos(\alpha_1 t_1) + B\sin(\alpha_1 t_1)] = C\cos(\alpha_2 t_2) - D\sin(\alpha_2 t_2) \tag{2.3.33}$$

$$x = \frac{\mu_2\alpha_1}{\mu_1\alpha_2} \tag{2.3.34}$$

By setting the determinant of the system of Eqs. 2.3.30~2.3.33 equal to zero, the dispersion equation, n as function of k, is obtained

$$(1 + x^2)\sin(\alpha_1 t_1)\sin(\alpha_2 t_2) + 2x[1 - \cos(\alpha_1 t_1)\cos(\alpha_2 t_2)] = 0 \tag{2.3.35}$$

Then, solving Eq. 2.3.35 for x,

$$\frac{\tan\left(\frac{\alpha_2 t_2}{2}\right)}{\tan\left(\frac{\alpha_1 t_1}{2}\right)} = -x = -\frac{\alpha_1\mu_2}{\alpha_2\mu_1} \tag{2.3.36}$$

or

$$\frac{\tan\left(\frac{\alpha_2 t_2}{2}\right)}{\tan\left(\frac{\alpha_1 t_1}{2}\right)} = -\frac{1}{x} = -\frac{\alpha_2 \mu_1}{\alpha_1 \mu_2} \qquad 2.3.37$$

Eq. 2.3.37 is of no interest because the mean field in the grating region never satisfies the condition of zero-order grating（Eq. 1.2.2）.

Finally, replacing α_1 and α_2 with Eq. 2.3.21 and Eq. 2.3.26, t_1 and t_2 with $(1-f)\cdot p$ and $f \cdot p$, respectively, and setting μ equal to 1, which is suitable for most optical materials, then, the effective refractive index n_{TE} is

$$\frac{\tan\left(\pi\sqrt{n_2^2 - n^2}\cdot\frac{f\cdot p}{\lambda}\right)}{\tan\left(\pi\sqrt{n_1^2 - n^2}\cdot\frac{(1-f)\cdot p}{\lambda}\right)} = -\frac{\sqrt{n_1^2 - n^2}}{\sqrt{n_2^2 - n^2}} \qquad 2.3.38$$

2.3.2 Effective Refractive Index n_{TM}

In TM mode, the field vectors $\vec{E}$ and $\vec{H}$ are

$$\vec{E} = (e_x, 0, e_z) \qquad 2.3.39$$

and

$$\vec{H} = (0, h, 0) \qquad 2.3.40$$

The derived steps are almost the same as that of TE mode, except the conditions of continuity are imposed on h and e_x. The three differential equations are

$$\frac{\partial h}{\partial z} = -i\omega\varepsilon e_x \qquad 2.3.41$$

$$\frac{\partial h}{\partial x} = i\omega\mu e_z \qquad 2.3.42$$

$$\frac{\partial e_x}{\partial z} - \frac{\partial e_z}{\partial x} = -i\omega\mu h \qquad 2.3.43$$

It is interesting to find out that the equations of TM mode can be derived by replacing h, e, ε, μ in Eqs. 2.3.6~2.3.8 with e, $-h$, μ, ε. Hence, Eq. 2.3.36 is transformed into

$$\frac{\tan\left(\frac{\alpha_2 t_2}{2}\right)}{\tan\left(\frac{\alpha_1 t_1}{2}\right)} = -x = -\frac{\alpha_1 \varepsilon_2}{\alpha_2 \varepsilon_1} \qquad 2.3.44$$

and the effective refractive index n_{TM} is

$$\frac{\tan\left(\pi\sqrt{n_2^2 - n^2}\cdot\frac{f\cdot p}{\lambda}\right)}{\tan\left(\pi\sqrt{n_1^2 - n^2}\cdot\frac{(1-f)\cdot p}{\lambda}\right)} = -\frac{n_2^2\sqrt{n_1^2 - n^2}}{n_1^2\sqrt{n_2^2 - n^2}} \qquad 2.3.45$$

In the case of grating period p much smaller than λ, the $\tan(x)$ in Eqs. 2.3.38 and 2.3.45 can be approximated by x. As a result, Eqs. 2.3.38 and 2.3.45 will reduce to Eqs. 2.2.5 and 2.2.10, respectively. Therefore, the equations derived by average weighting method can be regarded as the first order approximation of that by Bloch Solution Method.

2.4 Summary

The EMT derived can fully describe the phenomenon of form birefringence, which is applicable for the most conditions with the period of grating much smaller than wavelength of incident light. However, the period designed in this thesis is close to wavelength of incident light. The results calculated by EMT derived above are then not so accurate. Thus, another theory, said *Rigorous Coupled Wave Analysis* (RCWA), is more suitable for our analysis. RCWA is an exact solution of Maxwell's equations, the calculated results will be more accurate than EMT in principle. Since package software based on RCWA is already available, we use the software, GAOLVER, to perform the simulation which will be introduced in detail in chapter 4.

Sub-wavelength grating can be treated as a uniaxial medium, and its effective indices can be derived by Average Weighting Method when the grating period is much smaller than the wavelength of incident light. The effective medium has large birefringence, which can be controlled by fill factor. Therefore, sub-wavelength grating is applicable for AR coating and phase plate which requires specific index of refraction. In the case of grating with larger period, the accuracy of n_{TE} and n_{TM} can be improved by Bloch Solution Method.