Chapter 2

Principle

2.1 Introduction

A dielectric grating with its period smaller than wavelength of incident light can be treated as an effectively birefringent material. Region O is a homogeneous dielectric with index of refraction n_O; region S is a homogeneous dielectric with index of refraction n_S; the grating region consists of a periodic distribution of two dielectric media with refractive indices n_1 and n_2, respectively, as shown in Fig. 2.1. In the case of surface-relief grating, $n_1 = n_O$, $n_2 = n_S$. For simplicity, both dielectric media are considered as lossless media. The grating profile can be arbitrary since any arbitrary grating profile can be approximated by separating the grating region into slabs of rectangular one. Therefore, the theory of sub-wavelength grating is developed for rectangular profile only in the following sections.

Effective Medium Theory (EMT) is the most familiar theory used to calculate the optical properties of sub-wavelength grating. EMT treats the grating region as a unaxial film and can derive the values of effective refractive indices: $n_{//}$ and $n_{\perp}$. Then the reflectance and transmittance of optical wave with its electric vector parallel and perpendicular to the grating bar are determined by thin film theory with $n_{//}$ and $n_{\perp}$. It is discussed in detailed in the following.

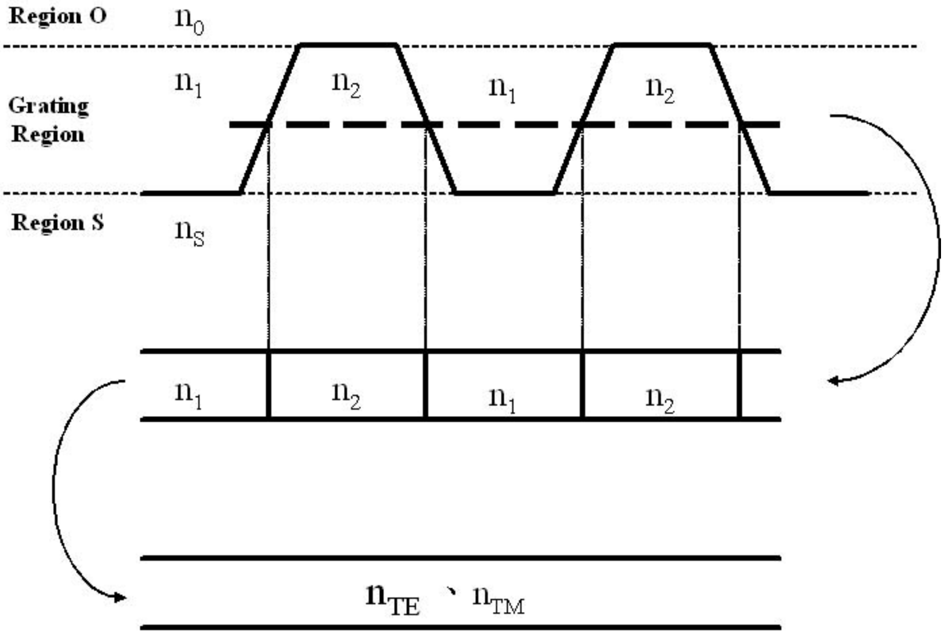

Fig. 2.1 A dielectric grating.

2.2 EMT by Average Weighting Method

The birefringence properties of crystals may be explained in terms of the anisotropic electrical properties of molecules of which the crystals are composed. Birefringence may, however, arise from anisotropy on a scale much larger then molecular, namely when there is an ordered arrangement of similar particles of optically isotropic material whose size is large compared with the dimensions of molecules, but small compared with the wavelength of light.

We shall explain the principle of the method by considering the grating shown in Fig. 2.2. The grating region is composed by dielectric 1 and 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 $\frac{t_1}{p}$ [15][16].

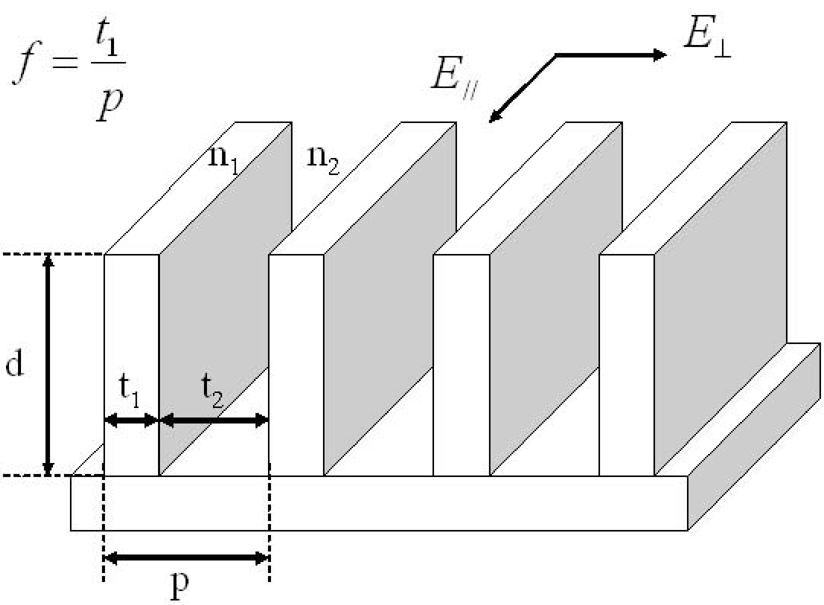

Fig. 2.2 Schematic of a laminar zero-order grating（$p << \lambda$）with the orientations of the incident electric wavefield and definitions of rectangular grating parameters. The fill factor f is defined as $\frac{t_1}{p}$.

Suppose that the grating period p is much smaller than the wavelength of incident light λ, the field in the grating region may be considered as uniform in dielectric 1 and 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 $n_{//}$ and $n_{\perp}$ under normal incidence are derived in sections 2.2.1 and 2.2.2 [16].

2.2.1 Effective Refractive Index $n_{//}$

Suppose that a plane monochromatic wave is incident on the grating and its electric vector is parallel to the grating bar. From the boundary conditions of Maxwell's equations, the tangential component of the electric vector is continuous across a discontinuity surface [17], so that the electric vector 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 the grating bar and the environment 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 $\varepsilon_{//}$ is, therefore,

$$\begin{aligned} \varepsilon_{//} &= \frac{\vec{D}}{\vec{E}} \\ &= \frac{t_1 \varepsilon_1 + t_2 \varepsilon_2}{t_1 + t_2} \\ &= f\varepsilon_1 + (1-f)\varepsilon_2 \end{aligned} \qquad 2.2.4$$

With the refractive index $n = \sqrt{\varepsilon}$, we have effective refractive index of the electric vector parallel to the grating bar

$$n_{//} = \sqrt{f n_1^2 + (1-f) n_2^2} \qquad 2.2.5$$

2.2.2 Effective Refractive Index $n_{\perp}$

Suppose next that the incident field has its electric vector perpendicular to the grating bar. According to boundary conditions of Maxwell's equations, the normal component of electric displacement $\vec{D}$ must be continuous across the boundary. Hence, vectors $\vec{D}$ are the same in both dielectric regions. The corresponding electric field $\vec{E}$ in each dielectric region is

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

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

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

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

Hence the effective dielectric constant $\varepsilon_\perp$ is now given by

$$\begin{aligned} \varepsilon_\perp &= \frac{\vec{D}}{\vec{E}} \\ &= \frac{(t_1 + t_2)\varepsilon_1\varepsilon_2}{t_1\varepsilon_2 + t_2\varepsilon_1} \\ &= \frac{\varepsilon_1\varepsilon_2}{f\varepsilon_2 + (1-f)\varepsilon_1} \end{aligned} \tag{2.2.9}$$

Again, we have the effective refractive index of the electric vector perpendicular to the grating bar

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

We, therefore, find that the sub-wavelength grating which has different indices, $n_{//}$ and $n_\perp$, for different polarization angles of the incident light. Since the amount of birefringence, described by $\Delta n = \sqrt{\varepsilon_\perp} - \sqrt{\varepsilon_{//}}$ depends on the grating profile, this phenomenon is so-called *form birefringence*.

The approximations of the refractive indices described by Eqs 2.2.5 and 2.2.10 are the base of the effective medium approximation to zero-order gratings. These equations describe the fact that upon transmission through a sub-wavelength grating, the zeroth order experiences an effective refractive index resulted from the averaging of the dielectric constants of the grating media.

2.2.3 Properties of $n_{//}$ and $n_{\perp}$

The validity of Eqs. 2.2.5 and 2.2.10 can be verified by setting fill factor *f* equals to 1 or 0. For these two special cases, the grating region is made of either dielectric 1 or dielectric 2. Consequently, $n_{//}$ and $n_{\perp}$ are of the same value and are reduced to n_1 or n_2. The relation of $n_{//}$ and $n_{\perp}$ versus fill factor *f* is plotted in Fig. 2.3, and several interesting properties of sub-wavelength gratings are observed. First, the values of $n_{//}$ and $n_{\perp}$ 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, $n_{//}$ is always larger than $n_{\perp}$. It can be easily verified that

$$n_{\perp}^2 - n_{//}^2 = -\frac{f(1-f)\left(n_1^2 - n_2^2\right)^2}{(1-f)n_1^2 + fn_2^2} \le 0 \qquad 2.2.11$$

implying that sub-wavelength grating behaves as a negative uniaxial crystal.

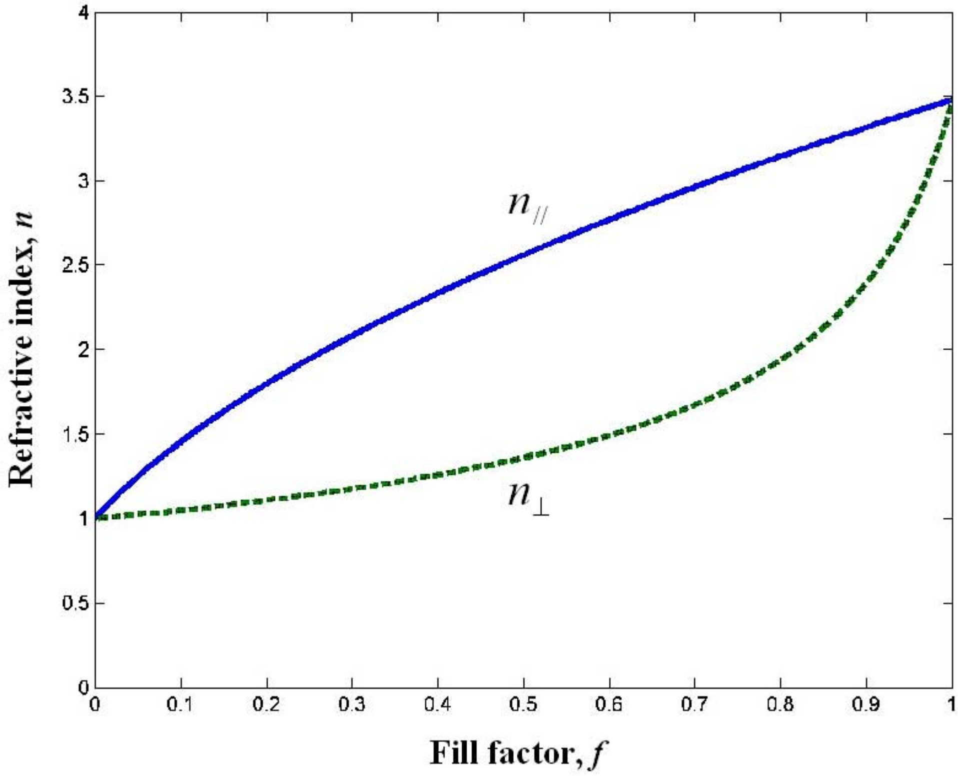

Fig. 2.3 Diagram of $n_{//}$ and $n_{\perp}$ versus fill factor *f*. n_1 is equal to 3.48, and n_2 is equal to 1.

2.3 EMT by Bloch Solution Method

The equations of $n_{//}$ and $n_{\perp}$ deduced by averaging weighting method is quite simple; and these equations are valid for grating period much smaller than the wavelength of incident light. Therefore, it is necessary to develop new equations that are suitable 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.

Before deriving the effective refractive indices, the coordinates have to be defined to describe the components of field vectors *E* and *H* that will be used in derivation. Assume the light is normally incident on the grating, we then define the direction of incident light as x-axis, and the directions parallel and perpendicular to the grating bar are defined as y-axis and z-axis, respectively, as shown in Fig. 2.4. The effective refractive indices of wave field parallel and perpendicular to the grating bar, $n_{//}$ and $n_{\perp}$, will be derived by the Bloch method in the following two sections [19].

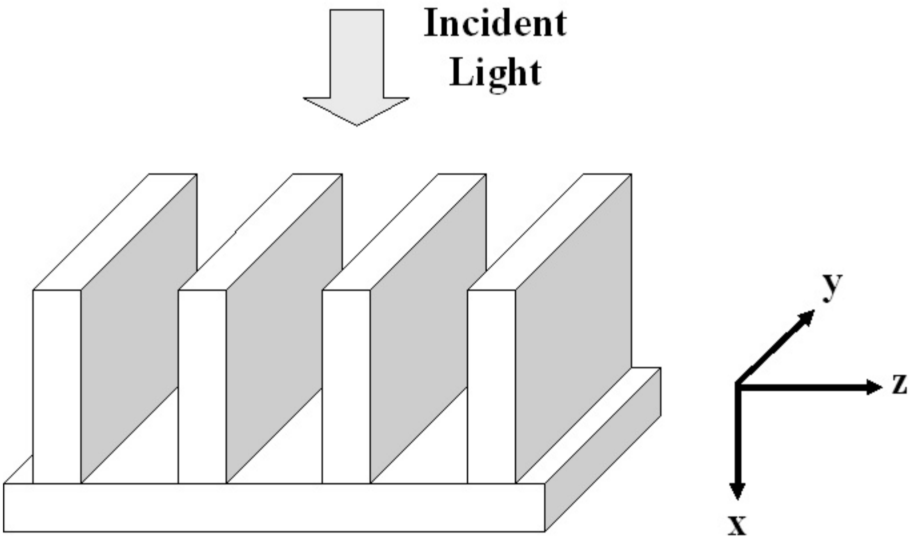

Fig. 2.4 Coordinate definition for deriving effective refraction indices.

2.3.1 Effective Refractive Index $n_{//}$

For optical wave of its polarization state parallel to the grating bar, the field vectors $\vec{E}$ and $\vec{H}$ are

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

and

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

From Maxwell's equation,

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

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

Three differential equations are given as

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

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

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

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

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

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

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

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

$$U(z+p) = U(z) \qquad 2.3.12$$

$$V(z+p) = V(z) \qquad 2.3.13$$

$$W(z+p) = W(z) \qquad 2.3.14$$

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

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

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

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

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 $-t_1 < z < 0$,

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

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

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

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

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

For $0 < z < t_2$,

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

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

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

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

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

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

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

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

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

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

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

$$B = xD \qquad 2.3.32$$

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

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

By setting the determinant of the system of Eqs. 2.3.30~2.3.31 to be zero, the dispersion equation, n as function of k, is obtained

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

Then, solve Eq. 2.3.35 for x,

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

or

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

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. 1.4.2）.

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

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

2.3.2 Effective Refractive Index $n_{\perp}$

For optical wave of its polarization state perpendicular to the grating bar, 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 steps of deriving effective refractive index $n_{\perp}$ are almost the same as that of deriving effective refractive index $n_{//}$, 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 electric field perpendicular to grating bar can be derived by replacing h, e, ε, μ in Eqs. 2.3.36~2.3.38 with e, $-h$, μ, ε. Hence, Eq. 2.3.36 is transformed into

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

and the effective refractive index of electric field perpendicular to the grating bar $n_{\perp}$ is

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

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. In consequence, Eqs. 2.3.38 and 2.3.45 will reduce to Eqs. 2.3.5 and 2.3.10, respectively. Therefore, the equations derived by weighting method can be regarded as the first order approximation of that by Bloch Solution Method.

2.4 EMT of Double-Layered Structure

In the previous two sections, the effective refraction indices, $n_{//}$ and $n_{\perp}$, of sub-wavelength grating with one material only were fully derived. The efficiency of separating polarized light of a sub-wavelength grating can be further increased by adopting multi-layered structure. In this thesis, the attention will be focused on the sub-wavelength grating with double-layered structure.

Assume that the grating structure is composed of a dielectric layer and a metal layer on glass substrate, and the width of the grating structure is W, period of the sub-wavelength grating is P, as shown in Fig. 2.5. Generally speaking, W is related to P by the following inequality

$$0.1P \le W \le 0.9P \qquad 2.4.1$$

In order to obtain a higher efficient light separation, period of the sub-wavelength grating and wavelength of incident light λ should be satisfied

$$\frac{0.5\lambda}{n+\sin\theta} \le P \le \frac{2\lambda}{n+\sin\theta} \qquad 2.4.2$$

where n is the refractive index of substrate, θ is the incident angle of the incident light.

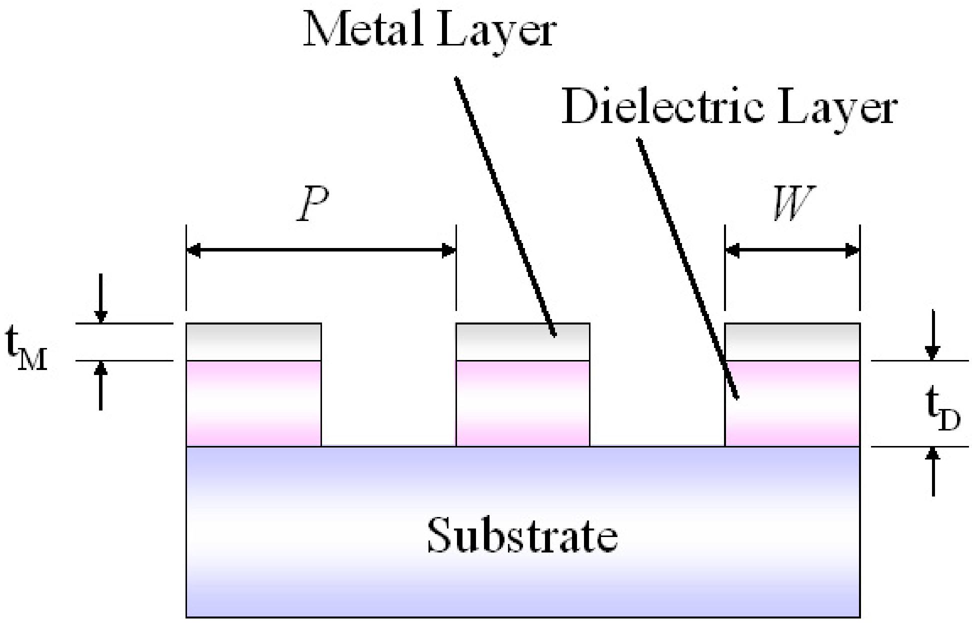

Fig. 2.5 Structure of double-layered sub-wavelength grating

Both effective refractive indices, $n_{//}$ and $n_{\perp}$, can be derived from the boundary conditions of Maxwell's equations. For S rays, defined as the electric field parallel to the grating bar, the relationship between effective refractive index $n_{//}$ and refractive indices of dielectric layer and metal layer, n_D and n_M, is

$$n_{//}^2 = \frac{a}{P} n_M^2 + \frac{b}{P} n_D^2 \qquad 2.4.3$$

For P rays, defined as the electric field perpendicular to the grating bar, the relationship between effective refractive index $n_{\perp}$ and refractive indices of dielectric layer and metal layer, n_D and n_M, is

$$\frac{1}{n_{\perp}^2} = \frac{a}{P \times n_M^2} + \frac{b}{P \times n_D^2} \qquad 2.4.4$$

Due to refractive index of metal layer n_M is much larger than that of dielectric layer, Eqs. 2.4.3 and 2.4.4 can be approximated as

$$n_{//} \cong n_M \times \left(\frac{a}{P} \right)^{1/2} \qquad 2.4.5$$

and

$$n_{\perp} \cong n_D \times \left(\frac{b}{P}\right)^{-1/2} \qquad 2.4.6$$

Some interesting phenomena are noticed from Eqs. 2.4.5 and 2.4.6. When light is incident on the sub-wavelength grating, it is as if S rays and P rays are incident on the metal layer and dielectric layer, respectively. Therefore, lots of S rays are reflected with very high reflection efficiency and most of P rays are transmitted.

2.5 Summary

As discussed above, the EMT derived can fully describe the phenomenon of form birefringence. It can be applied in most conditions with the period of grating much smaller than wavelength of incident light, i.e., the period is a factor of 5 smaller than wavelength of incident light or more. The efficiency of light separation of sub-wavelength grating with multi-layer will be higher than that of sub-wavelength grating with single layer. The sub-wavelength grating with double layer will, therefore, be focused on in this thesis.

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 results calculated will 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.