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Periodical Structures and International Research Cooperation

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ABSTRACT: *The highest academic degree awarded is the Doctor of Engineering. The high quality doctoral degree requires the research projects at a professional level. At Department of Physics of Technical University in Ostrava we try to solve the theoretical and experimental doctoral research projects in the framework of international collaboration.*

The paper is devoted to the study of electromagnetic wave interaction with deep one- and two dimensional high periodicity structures. This study has been realized in the frame of international cooperation of three groups. Modelling of wave scattering on 1D deep gratings has been done independently at Fukuoka Institute of Technology (FIT) in Fukuoka and Research Institute of Electronics (RIE) in Hamamatsu. The model for the description of diffraction properties of 2D high periodicity gratings has been created at Technical University in Ostrava.

1 INTRODUCTION

The lamellar and binary optic periodical structures bring the new possible applications in the integrated optics, magneto-optic memories, and in sensor technique [1,2]. The special attention is at the present devoted to the metallic gratings [3,4,5], magnetic dots and nanostructures [6,7].

There are several different approaches to solve the problem of electromagnetic field propagation in periodical systems. The efficient method to calculate the lattice sums for 1 D periodic array of line sources [8], the differential theory for anisotropic gratings [9,10], and the recursive matrix algorithms for modeling layered diffraction gratings [11] have been presented. The reformulated coupled wave method (CWM) has been described and applied to isotropic and anisotropic periodical structures (including the metallic gratings) [12,13,14] and the systematic comparison of the scalar diffraction analysis and CWM has been published for two dimensional periodic systems [15]. The rigorous differential method has been used on the study of the influence of the height of grating on the diffraction hysteresis loop diagram [16]. The modal transmission-line theory of 3D periodic structures with arbitrary lattice configurations is described in [17]. The relationship between wavelength and periodicity of grating is an important parameter in the diffraction analysis of periodic system. This relation together with the influence of finite incident beam on the efficiency of gratings is studied in [18]. The resonant grating reflection filters operating at normal incidence are demonstrated in [19].

The phase modulated spectroscopic ellipsometry (PMSE) is the excellent experimental technique for the specification of optical and geometrical parameters of thin films and multilayer dielectric coatings. This technique has been applied ex situ and in situ for the growth control of transparent films with varying composition [20]. The recent advances in PMSE instrumentation are summarized in [21].

2 THEORETICAL

1D gratings

a) Separate themes method (STM – Research Institute of Electronics)

We first consider the diffraction of a time-harmonic plane wave by a lamellar dielectric isotropic grating. The Cartesian coordinate system is chosen such that y-axis is in the direction of periodicity and z-axis is normal to the interfaces. All the field components in this paper are assumed to have time dependence of $\exp(i\omega t)$.

Let the incident wave have a shape of transversal electric (TE), or s-polarized, plane wave

$$\boldsymbol{E}_{\mathrm{i}} = \hat{\boldsymbol{x}} \exp\left[-i\left(q_0 y + s_0^{\mathrm{i}} z\right)\right], \tag{1}$$

where $\hat{\boldsymbol{x}}$ is a unit vector of polarization in the direction of x-axis, y and z are Cartesian spatial coordinates scaled by the wave number of vacuum $k_0 = \frac{2\pi}{\lambda}$ and $[q_0, s_0^{\mathrm{i}}] = [\sin\vartheta_{\mathrm{i}}, \cos\vartheta_{\mathrm{i}}]$ is a normalized wave vector of a wave with an angle of incidence ϑ_{i}. Then the diffracted fields have a form of Rayleigh expansion

$$\begin{aligned} \boldsymbol{E}_{\mathrm{r}} &= \hat{\boldsymbol{x}} \sum_{n=-\infty}^{+\infty} r_n \exp\left[-i\left(q_n y - s_n^{\mathrm{r}} z\right)\right], \\ \boldsymbol{E}_{\mathrm{t}} &= \hat{\boldsymbol{x}} \sum_{n=-\infty}^{+\infty} t_n \exp\left[-i\left(q_n y + s_n^{\mathrm{t}} z\right)\right], \end{aligned} \tag{2}$$

where r_n and t_n denote amplitudes of terms of Rayleigh series for reflected and transmitted fields, respectively. The components of wavevectors are determined by equations

$$\begin{aligned} q_n &= q_0 + nq = q_0 + n\tfrac{\lambda}{\Lambda}, \\ s_n^{\mathrm{r}} &= \sqrt{1-q_n^2}, \quad s_n^{\mathrm{t}} = \sqrt{\varepsilon - q_n^2}, \end{aligned} \tag{3}$$

where Λ is the grating period and ε denotes permittivity of the substrate. Bivalent complex square root is chosen such that $s_n^{\mathrm{r,t}}$ have physical meaning of propagation numbers in the direction of z-axis.

As well as outside the grating, we can formally write the series of eigen-modes in the periodic medium using the Floquet theorem

$$\begin{aligned} \boldsymbol{E}_{\mathrm{d}} &= \hat{\boldsymbol{x}} \sum_j d_j v_j(y) \exp\left(-is_j^{\mathrm{d}} z\right), \\ \boldsymbol{E}_{\mathrm{u}} &= \hat{\boldsymbol{x}} \sum_j u_j v_j(y) \exp\left[-is_j^{\mathrm{d}}(-z)\right], \end{aligned} \tag{4}$$

for down- and up-going modes, respectively. Here d_j and u_j mean amplitudes of the modes, whereas $v_j(y)$ and s_j^{d} are propagation eigen-functions and eigen-numbers of the modes. Therefore, the propagation matrix in representation of eigen-modes for both directions is a diagonal matrix with elements of

$$P_{jj}^{[\mathrm{eig}]} = e^{-is_j^{\mathrm{d}} d}, \tag{5}$$

where d is a distance of propagation. In representation of Fourier modes corresponding to the Rayleigh modes n up to sufficient values $\pm n_{\max}$, the propagation matrix is

$$\mathbf{P} = \mathbf{T}\mathbf{P}^{[\mathrm{eig}]}\mathbf{T}^{-1}, \tag{6}$$

where $\mathbf{T}$ is a transformation matrix between both representations.

We will now divide the entire problem of RCWA into three separate themes: the scattering on a boundary between uniform and periodic media, propagation through the periodic medium, and final series of internal reflections. The solution of the first theme can be easily written in the matrix form

$$\begin{aligned} \boldsymbol{r}^{(0\to1)} &= \mathbf{R}_{01}\boldsymbol{i}, \quad \boldsymbol{t}^{(0\to1)} = \mathbf{T}_{01}\boldsymbol{i}, \\ \boldsymbol{r}^{(1\to0)} &= \mathbf{R}_{10}\boldsymbol{i}, \quad \boldsymbol{t}^{(1\to0)} = \mathbf{T}_{10}\boldsymbol{i}, \\ \boldsymbol{r}^{(1\to2)} &= \mathbf{R}_{12}\boldsymbol{i}, \quad \boldsymbol{t}^{(1\to2)} = \mathbf{T}_{12}\boldsymbol{i}, \end{aligned} \tag{7}$$

where $\boldsymbol{i}$ denotes a vector of amplitudes of a wave incident on the *J–K* boundary. This vector is transformed by reflection and transmission matrices $\mathbf{R}_{JK}$ and $\mathbf{T}_{JK}$ into the corresponding vectors of reflected and transmitted amplitudes.

If we now apply the propagation matrix $\mathbf{P}$ from Eqs. (6) together with an infinite number of internal reflections, we obtain the Airy-style formulas

$$\begin{aligned} \mathbf{R}_{02} &= \mathbf{R}_{01} + \mathbf{T}_{10}\mathbf{P}\mathbf{R}_{12}\left(\mathbf{1}+\mathbf{Q}+\mathbf{Q}^2+\ldots\right)\mathbf{P}\mathbf{T}_{01}, \\ \mathbf{T}_{02} &= \mathbf{T}_{12}\left(\mathbf{1}+\mathbf{Q}+\mathbf{Q}^2+\ldots\right)\mathbf{P}\mathbf{T}_{01}, \end{aligned} \tag{8}$$

where $\mathbf{Q} = \mathbf{P}\mathbf{R}_{10}\mathbf{P}\mathbf{R}_{12}$ is a factor of recursive internal reflections; **1** is a unit matrix. By using the rule of geometrical series in the matrix form, we can rewrite this result into the final form

$$\begin{aligned} \mathbf{R}_{02} &= \mathbf{R}_{01} + \mathbf{T}_{10}\mathbf{P}\mathbf{R}_{12}\left(\mathbf{1}-\mathbf{Q}\right)^{-1}\mathbf{P}\mathbf{T}_{01}, \\ \mathbf{T}_{02} &= \mathbf{T}_{12}\left(\mathbf{1}-\mathbf{Q}\right)^{-1}\mathbf{P}\mathbf{T}_{01}. \end{aligned} \tag{9}$$

By analogy with Eg. (1), we may derive formulas formally identical with Eqs. (9) for the case of transversal magnetic (TM), corresponding to *p*-polarized electric, incident wave

$$\boldsymbol{H}_{\mathrm{i}} = \hat{\boldsymbol{x}} \exp\left[-i\left(q_0 y + s_0^{\mathrm{i}} z\right)\right] \tag{10}$$

with different expression for reflection, transmission and propagation matrices acting on amplitudes of magnetic Fourier modes.

b) Fourier modal formulation (FMF – Fukuoka Institute of Technology)

The grating grooves are parallel to the *z*-axis and the direction of periodicity is parallel to the *x*-axis. We denote the grating period by *d*, the grating depth by *h*, and the groove breadth by *g*. We consider time-harmonic fields assuming a time dependence in $e^{-i\omega t}$, and the fields are therefore represented by complex vectors depending only on the space variables *x, y,* and *z*. A plane wave is supposed to be incident with the plane of incidence perpendicular to the *z*-axis and the incident angle is denoted by θ. The dielectric substrate under consideration is linear isotropic media with the relative permittivity $\varepsilon_{\mathrm{sub}}$ and the permeability of free space, and the cover region is assumed to be free space.

For simple expressions, we normalize the electromagnetic fields, namely, the electric field $\boldsymbol{E}$ by $\sqrt[4]{\mu_0/\varepsilon_0}$ and the magnetic field $\boldsymbol{H}$ by $\sqrt[4]{\varepsilon_0/\mu_0}$, where ε_0 and μ_0 denote the permittivity and the permeability in free space. Let $\varepsilon(x)$ be the relative permittivity distribution inside the groove region $0 < y < h$. Then the normalized Maxwell´s curl equations yield relations in terms of the electric and magnetic field components as follows:

$$\frac{\partial}{\partial_y} E_z = i\, k_0\, H_x \tag{11}$$

$$\frac{\partial}{\partial_x} E_z = -\, i\, k_0\, H_y \tag{12}$$

$$\frac{\partial}{\partial x} H_y - \frac{\partial}{\partial y} H_x = -\, i\, k_0\, \varepsilon\, E_z \tag{13}$$

$$\frac{\partial}{\partial y} H_z = -i k_0 \varepsilon E_x \tag{14}$$

$$\frac{\partial}{\partial x} H_z = i k_0 \varepsilon E_y \tag{15}$$

$$\frac{\partial}{\partial x} E_y - \frac{\partial}{\partial y} E_x = i k_0 H_z \tag{16}$$

The first three equations are connected to the s polarization and the other three equations are connected to the p polarization.

Since the structure is periodic in the x-direction, all the components of the electromagnetic fields are pseudoperiodic functions of x. Thus they can be approximately expanded in truncated generalized Fourier series; for example, the x-component of $\boldsymbol{E}$ can be written as

$$E_x(x, y) = \sum_{n=-N}^{N} E_{x,n}(y)\, e^{i k_0 \alpha_n x} \tag{17}$$

with

$$\alpha_n = \sin\theta + n \frac{\lambda_0}{d}, \tag{18}$$

where N denotes the truncation order, k_0 and λ_0 denote respectively the wavenumber and the wavelength in free space, and $E_{x,n}(y)$ are the nth-order generalized Fourier coefficients that are functions of y only. To treat the generalized Fourier coefficients systematically, we introduce column matrices; for example, the coefficients of E_x are expressed by a column matrix $\boldsymbol{e}_x$ that is defined by

$$e_x(y) = \left(E_{x,-N}(y) \ \ldots \ E_{x,N}(y)\right)^T, \tag{19}$$

where the superscript T denotes the transpose matrix. The generalized Fourier coefficients of the other field components are expressed in the same way.

Following Li´s Fourier factorization rules [12], Eqs. (11)-(16) are transformed into

$$\frac{d}{dy} \boldsymbol{e}_z = i k_0 \boldsymbol{h}_x \tag{20}$$

$$\boldsymbol{X} \boldsymbol{e}_z = -\boldsymbol{h}_y \tag{21}$$

$$i k_0 \boldsymbol{X} \boldsymbol{h}_y - \frac{d}{dy} \boldsymbol{h}_x = -i k_0 [\varepsilon] \boldsymbol{e}_z \tag{22}$$

$$\frac{d}{dy} \boldsymbol{h}_z = -i k_0 \left[\frac{1}{\varepsilon}\right]^{-1} \boldsymbol{e}_x \tag{23}$$

$$\boldsymbol{X} \boldsymbol{h}_z = [\varepsilon] \boldsymbol{e}_y \tag{24}$$

$$i k_0 \boldsymbol{X} \boldsymbol{e}_y - \frac{d}{dy} \boldsymbol{e}_x = i k_0 \boldsymbol{h}_z \tag{25}$$

where $\boldsymbol{X}$ is a diagonal matrix whose diagonal entries are given by α_n. After simple calculation, we obtain the following differential equation sets:

$$\frac{d^2}{dy^2} \boldsymbol{e}_z(y) = -k_0^2 \boldsymbol{C}_g^{(s)} \boldsymbol{e}_z(y) \tag{26}$$

$$\frac{d^2}{dy^2}\boldsymbol{h}_z(y) = -k_0{}^2\, \boldsymbol{C}_g^{(p)}\, \boldsymbol{h}_z(y) \tag{27}$$

with

$$\boldsymbol{C}_g^{(s)} = [\varepsilon] - \boldsymbol{X}^2 \tag{28}$$

$$\boldsymbol{C}_g^{(p)} = \left[\frac{1}{\varepsilon}\right]^{-1} \left(I - \boldsymbol{X}\,[\varepsilon]^{-1}\,\boldsymbol{X}\right), \tag{29}$$

These coupled differential equation sets can be solved as eigenvalues-eigenvector problems because the coefficient matrices $\boldsymbol{C}_g^{(s)}$ and $\boldsymbol{C}_g^{(p)}$ are constant. Let $\boldsymbol{p}_{g,n}^{(f)}$ ($f = s, p$ and $n = 1, \ldots, 2N+1$) be linearly independent eigenvectors of $\boldsymbol{C}_g^{(f)}$ corresponding to eigenvalues $\beta_{g,n}^{(f)}$, respectively. Then $\boldsymbol{C}_g^{(f)}$ can be diagonalized as

$$\boldsymbol{P}_g^{(f)^{-1}}\, \boldsymbol{C}_g^{(f)}\, \boldsymbol{P}_g^{(f)} = \boldsymbol{Y}_g^{(f)^2} \tag{30}$$

with

$$\boldsymbol{P}_g^{(f)} = \left(\boldsymbol{p}_{g,1}^{(f)}\ \cdots\ \boldsymbol{p}_{g,2N+1}^{(f)}\right) \tag{31}$$

$$\left(\boldsymbol{Y}_g^{(f)}\right)_{n,m} = \delta_{n,m}\, \beta_{g,n}^{(f)}, \tag{32}$$

where $(\cdot)_{n,m}$ denotes the (n, m)-entry of a matrix and $\delta_{n,m}$ is the Kronecker delta. Here, we introduce two columm matrices defined by

$$\boldsymbol{a}_g^{(s)}(y) = \boldsymbol{P}_g^{(s)^{-1}}\, \boldsymbol{e}_z(y) \tag{33}$$

$$\boldsymbol{a}_g^{(p)}(y) = \boldsymbol{P}_g^{(p)^{-1}}\, \boldsymbol{h}_z(y). \tag{34}$$

Then the coupled differential equation sets (26) and (27) are rewritten as

$$\frac{d^2}{dy^2}\boldsymbol{a}_g^{(f)} = -k_0{}^2\, \boldsymbol{Y}_g^{(f)^2}\, \boldsymbol{a}_g^{(f)} \tag{35}$$

for $f = s, p$.

Then, from Eqs. (20), (23), (33), and (34), we can derive the relations between the generalized Fourier coefficients of field components and the modal amplitudes as

$$\boldsymbol{f}^{(f)}(y) = \boldsymbol{Q}_g^{(f)} \begin{pmatrix} \boldsymbol{a}_{g-}^{(f)} & (y) \\ \boldsymbol{a}_{g+}^{(f)} & (y) \end{pmatrix} \tag{36}$$

with

$$\boldsymbol{f}^{(s)}(y) = \begin{pmatrix} \boldsymbol{e}_z & (y) \\ \boldsymbol{h}_x & (y) \end{pmatrix} \tag{37}$$

$$\boldsymbol{f}^{(p)}(y) = \begin{pmatrix} \boldsymbol{h}_z & (y) \\ \boldsymbol{e}_x & (y) \end{pmatrix} \tag{38}$$

$$\boldsymbol{Q}_g^{(s)} = \begin{pmatrix} \boldsymbol{P}_g^{(s)} & \boldsymbol{P}_g^{(s)} \\ -\boldsymbol{P}_g^{(s)}\boldsymbol{Y}_g^{(s)} & \boldsymbol{P}_g^{s}\boldsymbol{Y}_g^{(s)} \end{pmatrix} \tag{39}$$

$$\boldsymbol{Q}_g^{(p)} = \begin{pmatrix} \boldsymbol{P}_g^{(p)} & \boldsymbol{P}_g^{(p)} \\ \left[\dfrac{1}{\varepsilon}\right]\boldsymbol{P}_g^{(p)}\,\boldsymbol{Y}_g^{(p)} & -\left[\dfrac{1}{\varepsilon}\right]\boldsymbol{P}_g^{(p)}\,\boldsymbol{Y}_g^{(p)} \end{pmatrix}. \tag{40}$$

Outside the groove region, the electromagnetic parameters are constant, and therefore the electromagnetic fields can be approximately expressed by the truncated Rayleigh expansions. For numerical purposes, the truncation order of the Rayleigh expansion is assumed to be same as that of the generalized Fourier series introduced inside the groove region, namely, from $-N$th to Nth-orders. Each term of this expansion represents a plane wave and we include the exponential y dependence of each term in the Rayleigh coefficient. Then the relation between the generalized Fourier and Rayleigh coefficients can be written for the cover region $y > h$:

$$\boldsymbol{f}^{(f)}(y) = \boldsymbol{Q}_c^{(f)} \begin{pmatrix} \boldsymbol{a}_{c-}^{(f)}(y) \\ \boldsymbol{a}_{c+}^{(f)}(y) \end{pmatrix} \tag{41}$$

and for the substrate region $y < 0$:

$$\boldsymbol{f}^{(f)}(y) = \boldsymbol{Q}_s^{(f)}\,\boldsymbol{a}_{s-}^{(f)}(y), \tag{42}$$

where $\boldsymbol{a}_{r\pm}^{(f)}(y)$ ($f = s,p$ and $r = c,s$) are ($2N + 1$) x 1 column matrices constructed with the amplitudes of plane waves $\{a_{r\pm,n}^{(f)}(y)\}_{n=-N}^{N}$ in such a way that their nth-components are $a_{r\pm,n-N-1}^{(f)}(y)$. The first subscripts c and s denote the matrices defined in the cover and the substrate regions, and the second subscripts $-$ and $+$ denote the amplitude concerning the downward and upward waves, respectively. The ($4N + 2$) x ($4N + 2$) matrix $\boldsymbol{Q}_c^{(f)}$ and the ($4N + 2$) x ($2N + 1$) matrix $\boldsymbol{Q}_s^{(f)}$ are defined so that $\left|a_{r\pm,n}^{(f)}\right|^2$ give the powers carried by the nth-order plane waves. The expressions of these matrices are easily derived and omitted in this paper.

The boundary conditions on $y = h$ and $y = 0$ yield the following relations:

$$\begin{pmatrix} \boldsymbol{a}_{g-}^{(f)}(h) \\ \boldsymbol{U}_g^{(f)}(h)\,\boldsymbol{a}_{g+}^{(f)}(0) \end{pmatrix} = \boldsymbol{G}_c^{(f)} \begin{pmatrix} \boldsymbol{a}_{c-}^{(f)}(h) \\ \boldsymbol{a}_{c+}^{(f)}(h) \end{pmatrix} \tag{43}$$

$$\begin{pmatrix} \boldsymbol{U}_g^{(f)}(h)\,\boldsymbol{a}_{g-}^{(f)}(h) \\ \boldsymbol{a}_{g+}^{(f)}(0) \end{pmatrix} = \boldsymbol{G}_s^{(f)}\,\boldsymbol{a}_{s-}^{(f)}(0) \tag{44}$$

with ($r = c, s$)

$$\boldsymbol{G}_r^{(f)} = \boldsymbol{Q}_g^{(f)^{-1}}\,\boldsymbol{Q}_r^{(f)}. \tag{45}$$

To avoid the numerical instabilities due to the growing exponential functions, we use the amplitudes $\boldsymbol{a}_{g-}^{(f)}(h)$ and $\boldsymbol{a}_{g+}^{(f)}(0)$ in this relations. After simple calculation, we can obtain the relation between the coefficients concerning the incoming and outgoing plane waves as

$$\begin{pmatrix} \boldsymbol{a}_{c+}^{(f)}(h) \\ \boldsymbol{a}_{s-}^{(f)}(0) \end{pmatrix} = \begin{pmatrix} \boldsymbol{S}_{11}^{(f)} \\ \boldsymbol{S}_{21}^{(f)} \end{pmatrix} \boldsymbol{a}_{c-}^{(f)}(h) \tag{46}$$

with

$$\begin{pmatrix} \boldsymbol{S}_{11}^{(f)} \\ \boldsymbol{S}_{21}^{(f)} \end{pmatrix} = \begin{pmatrix} -\boldsymbol{G}_{c,22}^{(f)} & \boldsymbol{U}_g^{(f)}(h)\boldsymbol{G}_{s,21}^{(f)} \\ \boldsymbol{U}_g^{(f)}(h)\boldsymbol{G}_{c,12}^{(f)} & -\boldsymbol{G}_{s,11}^{(f)} \end{pmatrix}^{-1} \times \begin{pmatrix} \boldsymbol{G}_{c,21}^{(f)} \\ -\boldsymbol{U}_g^{(f)}(h)\boldsymbol{G}_{c,11}^{(f)} \end{pmatrix}, \tag{47}$$

The incident plane wave is assumed to carry unit power and then the *n*th-components of the column matrix $\boldsymbol{a}_{c-}^{(f)}(h)$ are $\delta_{n,N+1}$. Consequently, the complex amplitudes of the *n*th-order diffraction waves propagating upward are given by $\left(\boldsymbol{S}_{11}^{(f)}\right)_{n+N+1,N+1}$. The ellipsometric parameters are defined by a ratio of the complex amplitudes with the *s* and *p* polarized incidences and, for *n*th-order waves, they are expressed as follows:

$$\psi_n = \arctan\left|\frac{\left(\boldsymbol{S}_{11}^{(p)}\right)_{n+N+1,N+1}}{\left(\boldsymbol{S}_{11}^{(s)}\right)_{n+N+1,N+1}}\right| \tag{48}$$

$$\Delta_n = -\Im\left[Ln\left(\frac{\left(\boldsymbol{S}_{11}^{(p)}\right)_{n+N+1,N+1}}{\left(\boldsymbol{S}_{11}^{(s)}\right)_{n+N+1,N+1}}\right)\right], \tag{49}$$

where *Ln* denotes the principal natural logarithm function.

2D gratings with extremal periodicity

Rigorous coupled wave method (RCWM – Technical University Ostrava)

The coordinate system is introduced in Fig. 1. We suppose that the grating structure is created by binary modulated (in x-y plane) dielectric layer indexed as $\nu = 1$ located on buffer ultrathin layer of SiO_2 $(\nu = 2)$. The thickness of the $\nu -$th layer is $\mathrm{h}^{(\nu)}$. The discussed periodic system is sandwiched between two semi-infinite isotropic regions. One of them is the Si substrate ($\nu = 2$, $z \geq \sum_{\nu=1}^{2} \mathrm{h}^{(\nu)}$); the second air region (superstrate) is specified by $\nu = 0, z = 0$.

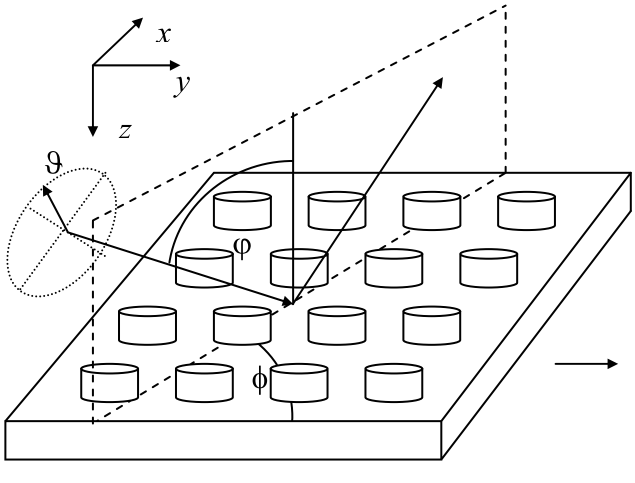

Figure 1 – Periodic structure, coordinate system, and plane of incidence geometry

In the FMM, both the electromagnetic fields and the permittivity function are expanded into two-fold Fourier series, thereby the boundary value problem for a system of partial differential equations is reformulated to an algebraic eigenvalue problem. According to the Floquet-Bloch theorem, the transformed expressions for amplitudes of field components in double periodic medium with period dimensions Λ_x, Λ_y take the form (we omit for the simplicity both the layer index (ν) and Rayleigh mode index q)

$$E_j(x_1,x_2,x_3)=\sum_m\sum_n e_{jmn}\exp\{-i(\alpha_m x_1+\beta_n x_2+\gamma x_3)\},$$
$$H_j(x_1,x_2,x_3)=\sum_m\sum_n h_{jmn}\exp\{-i(\alpha_m x_1+\beta_n x_2+\gamma x_3)\}, \tag{50}$$

where $\alpha_m = k_1 + \lambda\, m / \Lambda_x$, $\beta_n = k_2 + \lambda\, n / \Lambda_y$, m, n$\subset$ Z (the set of integers), $k_1 = n_0 \sin\varphi \sin\phi$, $k_2 = n_0 \sin\varphi \cos\phi$. **x** denotes the modified coordinates as **x** = (x_1,x_2,x_3) = $k_0(x,y,z)$. Moreover, the field propagation in x_3 direction characterized by γ, which does not follow from the Floquet theorem, has been included.

The Fourier transform of the permittivity tensor components can be written

$$\varepsilon_{ij} = \sum_k\sum_l c_{ij,kl}\exp\{-i(\lambda\, k\, x_1 / \Lambda_x + \lambda\, l\, x_2 / \Lambda_y)\}. \tag{51}$$

Substituting above expansions (50) and (51) into Maxwell's equations we obtain algebraic system for unknown Fourier coefficients e_{jmn}, h_{jmn} (j=1, 2, 3), where we apply the multiplications rule for the permittivity and electrical field Fourier series. We introduce in each layer the column vectors of Fourier coefficients $\mathbf{e}_j$ and $\mathbf{h}_j$ of the dimension d = (2M+1)(2N+1). On the base of tangential field component continuity we can create the single vector $\mathbf{g}$ = ($\mathbf{e}_1$, $\mathbf{h}_2$, $\mathbf{e}_2$, $\mathbf{h}_1$). Eliminating $\mathbf{e}_3$ and $\mathbf{h}_3$ from governing algebraic system we obtain eigenvalue problem of the dimension 4d, the solution of which leads to the eigenvalues γ_q (propagation constants) and square matrix $\mathbf{D}$ = ($\mathbf{g}_q$), q = 1,…,4d, of corresponding column eigenvectors (eigenpolarizations) in the relevant layer.

Denoting $\mathbf{u}^{(0)}$, $\mathbf{u}^{(s)}$ the 4d-dimensional vectors of amplitude coefficients in the superstrate and substrate, we can express the coupling condition of all layers as

$$\mathbf{u}^{(0)} = \mathbf{M}\, .\, \mathbf{u}^{(s)}, \tag{52}$$

where the total matrix of the structure **M** is the product of transfer and propagation matrices.

Reflection properties of the measured samples are described by complex ellipsometric ratio $\rho^{(0)}$ (we assume that the incident light is linearly polarized at azimuth $\theta = \pi/4$)

$$\rho_Q^{(0)} = u_{pp,Q}^{(0)\,-} / u_{ss,Q}^{(0)\,-}, \tag{53}$$

where Q = 1,…,4d; the sign "-" respects the negative direction considering z-axis.

In the case of magneto-optical gratings

$$\rho'^{(0)}_Q = \left(u_{pp,Q}^{(0)\,-} + u_{sp,Q}^{(0)\,-}\right) / \left(u_{ss,Q}^{(0)\,-} + u_{ps,Q}^{(0)\,-}\right). \tag{54}$$

The application of two last relations brings the possibility to specify the ellipsometric angles Ψ and Δ for isotropic and anisotropic binary gratings too. For a structure with magnetic ordering this process has been demonstrated in [21]. In the case we know the dispersion curves of permittivity we can analyze the spectral ellipsometry data.

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