# Numerical Analysis of Three-dimensional Gratings Using the Method of Integral Functionals

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## 1. Introduction

Periodic dielectric or metallic structures have been a subject of continuing interest because of their wide applications to frequency selective or polarization selective components in microwaves to optical wave regions. Among them, three-dimensional gratings, sometimes referred to as crossed-gratings, have many applications such as antireflection layers, beam splitters, phase plates, narrow-band filters, substrates for radiating elements, and so on. The three-dimensional grating is formed by arranging the diffractive elements periodically in two non-collinear directions on a planar structure. To date, various numerical techniques have been developed to model the electromagnetic scattering from periodic structures, such as the differential method, the Fourier modal method, the method of moments, the mode-matching method, the finite-element method, and the time-domain method.

In this paper, we shall discuss a novel numerical method in the frequency domain that applies to both of dielectric gratings and metallic gratings under the same algorithm. The method uses a concept of the double periodic magneto-dielectric layer [1] to a three-dimensional grating and formulates a set of volume integral equations [2] for the equivalent electric and magnetic polarization currents of the assumed periodic layer in vectorial form. The integral equations are solved using the integral functionals [3] characterizing the spectral amplitudes of the polarization currents distributions. Once the integral functionals are determined, the scattered fields outside the layer can be calculated accordingly without performing the modal analysis of the electric and magnetic fields inside the grating layer. The proposed method is quite general and applies to various grating geometries distributed periodically along any two coordinates. We shall present numerical examples for a two layered gratings consisting of crossed rectangular dielectric rods. It is shown that the polarization of the scattered field can be controllable by properly choosing the crossing angle between the rods.

## 2. Formulation

To illustrate the formulation process, we consider a single layer of doubly periodic magneto-dielectric medium as shown in Fig. 1. A linearly polarized plane wave of unit amplitude is incident from the half space ($z<0$) on a double-periodic layer of magneto-dielectric medium at an angle $\theta$ with respect to the $z$-axis. The incident plane wave can be expressed as a superposition of the TE wave and the TM wave. For the TE (TM) wave, the electric (magnetic) field vector $\mathbf{E}_0(\mathbf{r})$ ($\mathbf{H}_0(\mathbf{r})$) of the incident wave is lying in the $x$-$y$ plane and polarized with an angle $\varphi$ with respect to the $x$-axis. The doubly periodic layer with a thickness $h$ is comprised of a periodic arrangement of parallelepipeds in the $x_1$-$y_1$-$z$ coordinates. The $x_1$-axis is parallel to the $x$-axis, whereas the $y_1$-axis forms an angle $\tilde{\beta}$ with respect to the $y$-axis. The unit cell with periods $L_{x_1}$ and $L_{y_1}$ along the $x_1$- and $y_1$-axes contains several parallelepiped blocks characterized by the complex-valued relative permittivity and permeability of step functions profiles. The relative permittivity and permeability of the $i$-th block in the $x_1$-direction and $j$-th block in the $y_1$-direction are denoted by $\varepsilon_{ij}$ and $\mu_{ij}$, respectively. Then the equivalent electric polarization currents $\mathbf{J}_{ij}^e(x_1, y_1, z)$ and magnetic polarization currents $\mathbf{J}_{ij}^h(x_1, y_1, z)$ in each of unit-cell segments are related to the electric and magnetic fields in the segments as follows:

$$\mathbf{J}_{ij}^e(x_1,y_1,z)=\begin{cases}(\varepsilon_{ij}-1)\mathbf{E}_{ij}(x_1,y_1,z), \\ \quad a_{i-1}\le x_1\le a_i \text{ and } b_{j-1}\le y_1\le b_j \\ 0, \text{ elesewhere on the unit cell}\end{cases}, \quad \mathbf{J}_{ij}^h(x_1,y_1,z)=\begin{cases}(\mu_{ij}-1)\mathbf{H}_{ij}(x_1,y_1,z), \\ \quad a_{i-1}\le x_1\le a_i \text{ and } b_{j-1}\le y_1\le b_j \\ 0, \text{ elesewhere on the unit cell}\end{cases} \quad (1)$$

Using the polarization current densities $\mathbf{J}_{ij}^{e}(\mathbf{r})$ and $\mathbf{J}_{ij}^{h}(\mathbf{r})$, the total electric field in the whole space are expressed as follows:

$$\mathbf{E}(\mathbf{r})=\mathbf{E}_0(\mathbf{r})+\frac{1}{4\pi}\int_V (k^2\mathbf{I}+\nabla\nabla)\cdot[G(\mathbf{r},\mathbf{r}')\mathbf{J}^e(\mathbf{r}')]d\mathbf{r}' + \frac{ik}{4\pi}\int_V \nabla G(\mathbf{r},\mathbf{r}')\times\mathbf{J}^h(\mathbf{r}')d\mathbf{r}' \qquad (2)$$

$$\mathbf{H}(\mathbf{r})=\mathbf{H}_0(\mathbf{r})+\frac{1}{4\pi}\int_V (k^2\mathbf{I}+\nabla\nabla)\cdot[G(\mathbf{r},\mathbf{r}')\mathbf{J}^h(\mathbf{r}')]d\mathbf{r}' - \frac{ik}{4\pi}\int_V \nabla G(\mathbf{r},\mathbf{r}')\times\mathbf{J}^e(\mathbf{r}')d\mathbf{r}' \qquad (3)$$

with

$$\mathbf{J}^{e(h)}(\mathbf{r}') = \sum_{i=1}^{M_x}\sum_{j=1}^{M_y}\mathbf{J}_{ij}^{e(h)}(\mathbf{r}') \qquad (4)$$

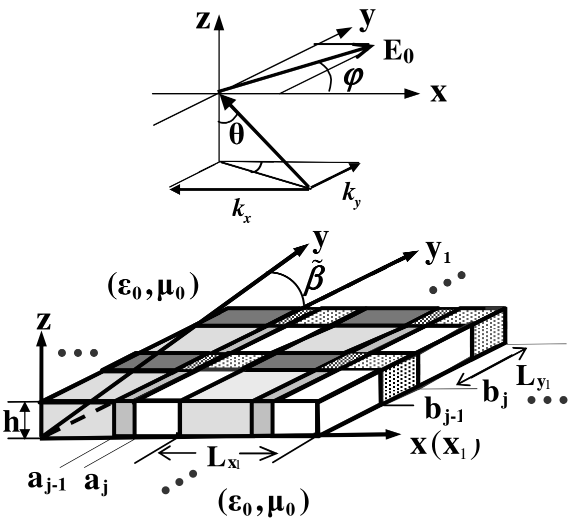


Fig. 1. A doubly periodic magneto-dielectric layer of thickness $h$ illuminated by an electromagnetic plane wave.

where $\mathbf{r}$ is an observation point, $\mathbf{r}'$ is the source point, $\mathbf{E}_0(\mathbf{r})$ and $k=2\pi/\lambda$ are the electric field and the wave number of excitation, $V$ is the scattering volume, $M_x$ and $M_y$ denote the total numbers of the segments per unit cell along the $x_1$- and $y_1$-axes, and $G(\mathbf{r},\mathbf{r}')$ denotes the Green's function in free space. Taking the observation point $\mathbf{r}$ inside the $(i,j)$-th segment of $V$, the coupled integral equations for the equivalent polarization currents $\mathbf{J}_{ij}^{e}(x_1,y_1,z)$ and $\mathbf{J}_{ij}^{h}(x_1,y_1,z)$ .are derived [2]. We define the unknown spectral amplitudes $\mathbf{F}_{ij,pq}^{e(h)}(z)$ of the polarization currents in the $(i,j)$-th segment as follows:

$$\mathbf{J}^{e(h)}(x_1,y_1,z)=\sum_{j=1}^{M_y}\sum_{i=1}^{M_x}\mathbf{J}_{ij}^{e(h)}(x_1,y_1,z)=\sum_{j=1}^{M_y}\sum_{i=1}^{M_x}\sum_{q=-\infty}^{\infty}\sum_{p=-\infty}^{\infty}\mathbf{F}_{ij,pq}^{e(h)}(z)\mathrm{e}^{ik_{x_1,p}x_1}\,\mathrm{e}^{ik_{y_1,q}y_1} \qquad (5)$$

$$\mathbf{F}_{ij,pq}^{e(h)}(z)=\frac{1}{L_{x_1}L_{y_1}}\int_{b_{j-1}}^{b_j}\int_{a_{i-1}}^{a_i}\mathrm{e}^{ik_{x_1,p}x_1}\,\mathrm{e}^{ik_{y_1,q}y_1}\,\mathbf{J}_{ij}^{e(h)}(x_1,y_1,z)dx_1dy_1 \qquad (6)$$

where $k_{x_1,p}=k_{x_1}+2\pi p/L_{x_1}$, $k_{y_1,q}=k_{y_1}+2\pi q/L_{y_1}$, $k_{x_1}=-k\sin\theta\sin\varphi,$, and $k_{y_1}=k\sin\theta\sin(\varphi+\tilde{\beta})$. Using the Floquet theorem and the Fourier integral representation of the Green's function, the integral equations are transformed into a set of coupled differential equations for the unknown integral functionals $\mathbf{I}_{ij,pq}^{e(h)}(z)$ as follows [3]:

$$\begin{pmatrix} \dfrac{\varepsilon_{ij}}{(\varepsilon_{ij}-1)}\nabla_{z,pq}^2 I_{x,ij,pq}^{e} \\ \dfrac{\varepsilon_{ij}}{(\varepsilon_{ij}-1)}\nabla_{z,pq}^2 I_{y,ij,pq}^{e} \\ \dfrac{1}{(\varepsilon_{ij}-1)}\nabla_{z,pq}^2) I_{z,ij,pq}^{e} \end{pmatrix} = 2i\alpha_{i,p}\alpha_{j,q}\mathbf{E}_0\mathrm{e}^{ik_z z}-\sum_{s=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}\alpha_{i,p-r}\alpha_{j,q-s}\mathbf{M}_{rs}^{e} \qquad (7)$$

$$\begin{pmatrix} \dfrac{\mu_{ij}}{(\mu_{ij}-1)}\nabla_{z,pq}^2 I_{x,ij,pq}^{h} \\ \dfrac{\mu_{ij}}{(\mu_{ij}-1)}\nabla_{z,pq}^2 I_{y,ij,pq}^{h} \\ \dfrac{1}{(\mu_{ij}-1)}\nabla_{z,pq}^2) I_{z,ij,pq}^{h} \end{pmatrix} = 2i\alpha_{i,p}\alpha_{j,q}\mathbf{H}_0\mathrm{e}^{ik_z z}-\sum_{s=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}\alpha_{i,p-r}\alpha_{j,q-s}\mathbf{M}_{rs}^{h} \qquad (8)$$

$$
\mathbf{M}_{rs}^{e(h)}(z)=\begin{pmatrix} \gamma_{rs}^2-\dfrac{\partial^2}{\partial z^2} & -\xi_r\gamma_{rs} & i\xi_r\dfrac{\partial}{\partial z} \\ -\gamma_{rs}\xi_r & \xi_r^2-\dfrac{\partial^2}{\partial z^2} & i\gamma_{rs}\dfrac{\partial}{\partial z} \\ i\xi_r\dfrac{\partial}{\partial z} & i\gamma_{rs}\dfrac{\partial}{\partial z} & k^2+\dfrac{\partial^2}{\partial z^2} \end{pmatrix}\begin{pmatrix} I_{x,rs}^{e(h)} \\ I_{y,rs}^{e(h)} \\ I_{z,rs}^{e(h)} \end{pmatrix} \pm ik\begin{pmatrix} 0 & -\dfrac{\partial}{\partial z} & i\gamma_{rs} \\ \dfrac{\partial}{\partial z} & 0 & -i\xi_r \\ -i\gamma_{rs} & i\xi_r & 0 \end{pmatrix}\begin{pmatrix} I_{x,rs}^{h(e)} \\ I_{y,rs}^{h(e)} \\ I_{z,rs}^{h(e)} \end{pmatrix} \tag{9}
$$

$$
I_{\nu,pq}^{e(h)}(z)=\sum_{j=1}^{M_y}\sum_{i=1}^{M_x} I_{\nu,ij,pq}^{e(h)}, \quad I_{\nu,ij,pq}^{e(h)}(z)=\frac{1}{\kappa_{pq}}\int_0^h F_{\nu,ij,pq}^{e(h)}(z')\,\mathrm{e}^{i|z-z'|\kappa_{pq}}\,dz' \quad (\nu=x,y,z) \tag{10}
$$

$$
\alpha_{i,p-r}=\frac{1}{L_{x_1}}\int_{a_{i-1}}^{a_i}\mathrm{e}^{-i\frac{2\pi(p-r)}{L_{x_1}}x_1}\,dx_1, \quad \alpha_{j,q-s}=\frac{1}{L_{y_1}}\int_{b_{j-1}}^{b_j}\mathrm{e}^{-i\frac{2\pi(q-s)}{L_{y_1}}y_1}\,dy_1 \tag{11}
$$

$$
\xi_r=k_{x_1,r}=k_x+\frac{2\pi r}{L_{x_1}}, \ \gamma_{rs}=k_{y_1}+\frac{2\pi}{\sin\tilde{\beta}}\left(\frac{s}{L_{y_1}}-\frac{r}{L_{x_1}}\cos\tilde{\beta}\right), \ \kappa_{pq}=\sqrt{k^2-\xi_p^2-\gamma_{pq}^2} \tag{12}
$$

where $\nabla_{z,pq}^2=\partial^2/\partial z^2+\kappa_{pq}^2$. The general solutions to the coupled differential equations (7) and (8) are given as a sum of the particular solutions and the solutions to the corresponding homogeneous differential equations. The particular solutions are directly related to the excitation by the incident plane wave of $(0,0)$-th spatial harmonic. The unknown constants contained in the homogeneous solutions are determined by the condition that the perturbed electric and magnetic fields inside the grating layer should vanish in the absence of the initial excitation ($\mathbf{E}_0=\mathbf{H}_0=0$). The spectral amplitudes $\mathbf{F}_{ij,pq}^{e(h)}(z)$ of the polarization currents are calculated through the relation:

$$
\mathbf{F}_{pq}^{e(h)}(z)=\frac{1}{2i}\left[\frac{\partial^2}{\partial z^2}\mathbf{I}_{pq}^{e(h)}(z)+\kappa_{pq}^2\mathbf{I}_{pq}^{e(h)}(z)\right]. \tag{13}
$$

Using the results in Eqs.(2) and (3), the reflected electric field in the region $z<0$ and the transmitted electric field in the region $z>h$ can be obtained [3] in terms of the spatial harmonics $\mathrm{e}^{i(\xi_p x+\gamma_{pq}y\mp\kappa_{pq}z)}$ as the basis. For a multilatered doubly periodic structure, we can apply the same algorithm as described above. For a $Q$-layered system, we have $Q$ sets of coupled differential equations for the integral functionals $\mathbf{I}_{s,pq}^{e(h)}(z)$ $(s=1,2,\cdots,Q)$ defined for each layer in the same form as Eqs.(7) and (8). The equations are solved under the condition that the perturbed electric and magnetic fields inside each of $Q$ layers should vanish separately in the absence of the initial excitation.

## 3. Numerical Examples and Discussions

We have developed a computer program based on the integral functional method for analyzing various kinds of three-dimensional gratings. The accuracy of the calculated diffraction efficiencies depends on the truncation size $N$ of the double spatial harmonics in the field expansions. We have confirmed that the energy conservation law for the lossless periodic layer is usually satisfied with the accuracy of $10^{-8}$. The desktop CPU run-time on the 1800 MHz AMD (3000+) with 1 Gb RAM was approximately 7.5 minutes per one frequency point when $(2N+1)^2=625$ which was the maximum in our numerical test, and 2 seconds when $(2N+1)^2=121$. We have used the method to analyze the scattering of electromagnetic plane waves by a two layered gratings consisting of crossed rectangular dielectric rods as shown in Fig. 2. The lower grating consists of the rods with thickness $h_1$, width $w_1$, and relative permittivity $\varepsilon_{r1}$, which are parallel to $y_1$-axis and periodically spaced with a distance $L_{x_1}(=L)$ along the $x$-axis. The upper grating consists of the rods with thickness $h_2$, width $w_2$, and relative permittivity $\varepsilon_{r2}$, which are parallel to $x$-axis and periodically spaced with a distance $L_{y_1}(=L/\sin\tilde{\beta})$ along the $y_1$-axis. The crossing angle between two gratings is denoted by $\beta\,(=90°-\tilde{\beta})$. The transmission coefficient $|T_{00y}|$

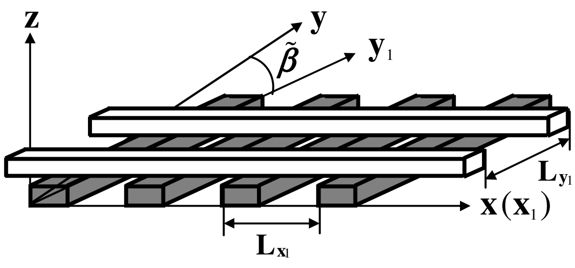


Fig. 2. Two layered crossed gratings formed by rectangular dielectric rods.

of the zero-th order diffraction into the $y$-polarized wave for the normal incidence of $x$-polarized wave on the two layered crossed grating is plotted as functions of the normalized frequency, where $h_1 = h_2 = 0.5L$, $w_1 = w_2 = w = 0.5L$, $\varepsilon_{r1} = \varepsilon_{r2} = \varepsilon = 5.0$, $\theta = \varphi = 0°$, and four different crossing angles $\beta$ are considered. The truncation number of spatial harmonics is $(2N+1)^2 = 361$ It is known that if $\beta = 90°$, the reflected and transmitted waves are always polarized in the $x$- direction and $|T_{00y}| = 0$ for the normal incidence of $x$-polarized wave. Figure 3 shows that if the crossing angle changes from $\beta = 90°$, there appears a significant transmission into the cross-polarized component even for the normal incidence. This feature is useful for designing a polarization converter based on the layered crossed-gratings.


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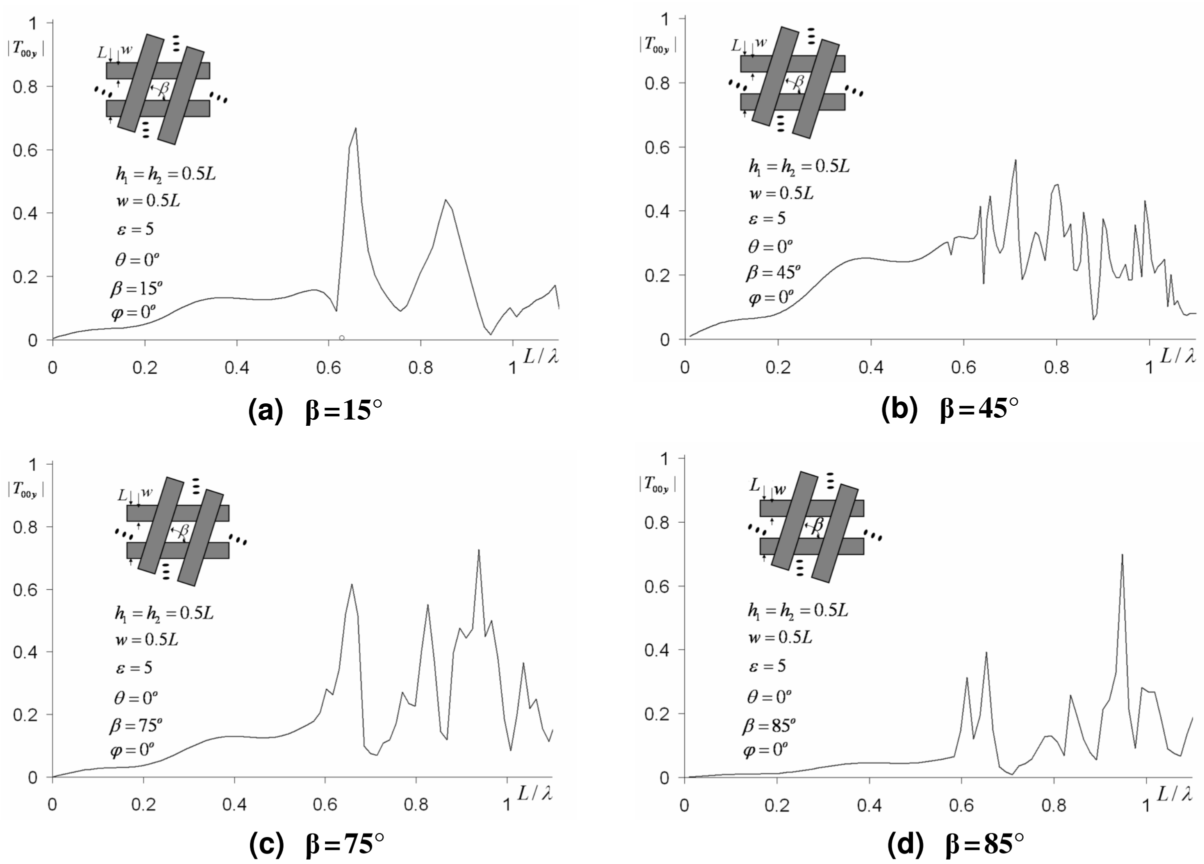


Fig. 3. Transmission coefficient $|T_{00y}|$ of the zero-th order diffraction into the $y$-polarized wave for the normal incidence of $x$-polarized wave on the two layered crossed grating as shown in Fig. 2