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Three-dimensional Diffraction Analysis of Phase and Amplitude Gratings Based on Legendre Expansion of Electromagnetic Fields

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ABSTRACT

Three-dimensional vectorial diffraction analysis of phase and amplitude gratings in conical mounting is presented based on Legendre expansion of electromagnetic fields. In the so-called conical mounting, different fields components are coupled and the solution is not separable in terms of independent TE and TM cases. In contrast to conventional RCWA in which the solution is obtained using state variables representation of the coupled wave amplitudes by expanding space harmonic amplitudes of the fields in terms of the eigenfunctions and eigenvectors of the coefficient matrix defined by rigorous coupled wave equations, here the solution of first order coupled Maxwell's equations is expanded in terms of Legendre polynomials. This approach yields well-behaved algebraic equations for deriving diffraction efficiencies and electromagnetic field profiles. It can nicely handle the cases in which conventional methods face the problem of numerical instability and inevitable round off errors; also, it yields accurate results to any desired level of accuracy. The method is applied to phase and amplitude gratings in conical mountings, comparison to other methods already reported in the literature is made, and the presented approach is justified and its usefulness in cases that other methods usually fail is demonstrated. This general method applies well even in such cases as thick gratings, non-Bragg incidence, and cases in which higher diffracted orders are needed to be retained, or evanescent orders corresponding to real eigenvalues have to be included. The efficacy of the proposed method relies on the fact that although Legendre polynomials span a complete space, they are not eigensolutions and hence each polynomial basis function bears a weighted projection of all eigenfunctions. Thus no modal information is completely missed in the ineluctable truncation process. In deriving the formulation, a rigorous approach is followed.

Keywords: Grating, Diffraction, Legendre Polynomials, Coupled Waves, Periodic Media

1. INTRODUCTION

Analysis of wave propagation in periodic structures, due to its wide range of applications, is faced in various systems and design processes appearing in telecommunications, electromagnetism, optics, and acoustics[1]. Consequently, it is essential to have an exact, efficient, and stable way to find reflection and transmission coefficients, diffraction efficiencies and field profiles inside and outside of gratings. Different approaches have been reported for grating analysis in literature such as rigorous coupled wave[1], coupled mode [2], two wave methods [3], and Raman-Nath approach [4]. Of many methods proposed for analysis of volume diffraction gratings, rigorous coupled wave analysis, or RCWA, is the most precise, the most general, and the most widely used method. It has been successfully applied to the analysis of two-dimensional and three-dimensional isotropic and anisotropic structures [5-9], as well as multiple grating structures [10-11]. However, the presence of evanescent orders corresponding to real eigenvalues appearing in the solution of Maxwell's equations usually leads to numerical difficulties in applying RCWA method. This problem is also encountered in applying other conventional approaches which are based on modal expansion, where Maxwell's equations lead to an eigenvalue problem. This is due to the fact that evanescent orders result in the simultaneous appearance of extremely large and extremely small coefficients in the equations obtained by imposing the boundary conditions and, consequently cause numerical overflow and ill-conditioned matrices in calculations. Therefore, a robust method capable of handling evanescent orders is mandatory, especially in cases such as multiple grating structures or metallic corrugated gratings,

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where evanescent or complex diffracted orders cannot always be discarded. Modal expansion methods are also vulnerable to numerical instability whenever the ratio of the thickness over the grating periodicity is large, or large number of spatial harmonics is retained in the analysis [12]. This problem is more critical when analyzing diffraction gratings in conical mounting, since the TE and TM components of the electromagnetic field inside the grating are not separable and therefore three-dimensional vectorial analysis of Maxwell's equations is required [6].

Morf has reported a new mathematical method for the special case of lamellar gratings[13]. That method is based on the expansion of the eigenfunctions in terms of a set of polynomial basis functions. However, the polynomial expansion is applied only in transverse direction and at each region of constant refractive index separately. Even though the Gibbs phenomenon was avoided in following that approach, the method still needed a subtle and delicate handling of propagating electromagnetic fields where numerical instabilities similar to those usually encountered in applying transfer matrix methods were expected [13,14].

In this paper, similar yet fundamentally different approach is proposed. The electromagnetic field expressions, for each component inside the grating, which are the solutions of Maxwell's equations, are expanded in terms of orthogonal Legendre polynomials. Then the solution is examined in a Hilbert space spanned by the polynomials. The method yields numerically stable results [12].

This paper is arranged as follows: Legendre polynomial expansion formulation of electromagnetic fields for the analysis of gratings in conical mounting is discussed in Section 2. In Section 3, comparison of the polynomial expansion results with the three-dimensional vector coupled wave results is presented for some specific test cases. Finally, conclusions are made in Section 4.

2. FORMULATION

In this section, the electromagnetic field expressions inside the grating are expanded in terms of orthogonal Legendre polynomials [15, 16]. This novel electromagnetic field expression, in accordance with Floquet theorem, is then substituted in Maxwell's equations; appropriate boundary conditions are applied, and finally the unknown expansion coefficients and diffraction efficiencies are found. It should be noticed that expanding the electromagnetic field expressions in an orthogonal complete space of polynomials is a nonharmonic expansion [16], i.e. it isn't a linear combination of intrinsic eigenvectors. Nonetheless, it has some advantages over eigenvector expansion and other previously mentioned methods. First, the equations become algebraic rather than transcendental; therefore, they can be manipulated easier. Second, this approach works properly even in those special cases in which other methods usually fail. There is not any numerical instability, not only because the involved matrices are not very sparse, but also because the numbers constituting the matrices are neither extremely small nor extremely large, i.e. the condition numbers of the matrices are very good. It should be noticed that finding the solution in the Hilbert space spanned by polynomials can be interpreted as the projection of harmonic solutions, i.e. modal expansions, on the new bases formed by the polynomials. This means that each polynomial contains some information from all the infinite number of the natural modes of the system through their projection. This is an important advantage when inevitable truncation of the infinite expansion to finite terms could be counterbalanced by keeping the tracks of all eigenmodes in each member of the polynomial set that makes the basis of this Hilbert space.

A grating in conical mounting is shown in Fig. 1. Here, the permittivity is a periodic function:

$$\varepsilon(\boldsymbol{r} + \Lambda_G) = \varepsilon(\boldsymbol{r}), \tag{1}$$

where Λ_G is the grating periodicity. Inside the grating, the Maxwell's equations can be easily derived as [6]:

$$\nabla \times \boldsymbol{E} = -j\omega\mu\boldsymbol{H}\ . \tag{2}$$

$$\nabla \times \boldsymbol{H} = j\omega\varepsilon_0\varepsilon(x,z)\boldsymbol{E}\ . \tag{3}$$

In these equations, $\boldsymbol{E}$ and $\boldsymbol{H}$ can be expanded in terms of space harmonics as [6]:

$$\boldsymbol{E} = \sum_i \left[S_{xi}(z)\hat{x} + S_{yi}(z)\hat{y} + S_{zi}(z)\hat{z}\right]\exp[-j\sigma_i.r]\ . \tag{4}$$

$$\boldsymbol{H} = \sqrt{\frac{\varepsilon_0}{\mu_0}}\sum_i \left[U_{xi}(z)\hat{x} + U_{yi}(z)\hat{y} + U_{zi}(z)\hat{z}\right]\exp[-j\sigma_i.r], \tag{5}$$

where $\boldsymbol{\sigma}_i = k_{xi}\hat{x} + k_y\hat{y} + (k_z - iK_{Gz})\hat{z}$.

k_{xi} and k_y are determined from phase matching condition and k_z is the average wavevector in grating region which correspond to the average permittivity in that region, and $\boldsymbol{K}_G = \frac{2\pi}{\Lambda_G}[\sin(\phi)\hat{x} + \cos(\phi)\hat{z}]$ is the grating vector. The index i running from $-\infty$ to $+\infty$ denotes the i^{th} space harmonic corresponding to the i^{th} diffracted order in regions I and III. Numerically, expansion of the electromagnetic fields in terms of infinite number of space harmonics, i.e. Eqs. (4) and (5), is inevitably truncated. For dielectric gratings, all the space harmonics corresponding to propagating Floquet orders should be retained in the preceding expansion, where only a few of those terms corresponding to evanescent Floquet orders are needed to be included. In contrast, more space harmonics are needed to be kept for metallic gratings.

Since ε is a periodic function, it can be expanded in terms of its Fourier series as

$$\varepsilon(x,z) = \sum_h \tilde{\varepsilon}_h e^{jh\overrightarrow{K_G}.\overrightarrow{r}} \quad , \tag{6}$$

where $\tilde{\varepsilon}_h = \frac{2}{\Lambda_G}\int_{\Lambda_G} \varepsilon(r) e^{-jh\overrightarrow{K_G}.\overrightarrow{r}}\, dr$ is the Fourier component of the grating permittivity.

After substituting Eq. (4), Eq. (5), and Eq. (6) in Eq. (2) and Eq. (3) and eliminating the z component of the electromagnetic field, a set of four first order coupled differential equations is derived as:

$$\frac{dS_{xi}(z)}{dz} = -j\left\{iK_{Gz}S_{xi}(z) + \frac{k_{xi}}{k_0}\sum_p a_{i-p}\left[k_y U_{xp}(z) - k_{xp}U_{yp}(z)\right] + k_0 U_{yi}(z)\right\}. \tag{7}$$

$$\frac{dS_{yi}(z)}{dz} = -j\left\{iK_{Gz}S_{yi}(z) + \frac{k_y}{k_0}\sum_p a_{i-p}\left[k_y U_{xp}(z) - k_{xp}U_{yp}(z)\right] - k_0 U_{xi}(z)\right\}. \tag{8}$$

$$\frac{dU_{xi}(z)}{dz} = j\left\{-iK_{Gz}U_{xi}(z) + \frac{k_{xi}}{k_0}\left[k_y S_{xi}(z) - k_{xi}S_{yi}(z)\right] + k_0\sum_p \tilde{\varepsilon}_{i-p}S_{yp}(z)\right\}. \tag{9}$$

$$\frac{dU_{yi}(z)}{dz} = -j\left\{iK_{Gz}U_{yi}(z) - \frac{k_y}{k_0}\left[k_y S_{xi}(z) - k_{xi}S_{yi}(z)\right] + k_0\sum_p \tilde{\varepsilon}_{i-p}S_{xp}(z)\right\}. \tag{10}$$

where p=i-h and $\tilde{\varepsilon}_h$ is the hth Fourier component of the permittivity profile, i.e. ε, and a_h is the hth Fourier component of the ε^{-1} .

Each component of the space harmonic amplitudes is expanded in terms of Legendre polynomials:

$$S_{xi}(z) = \sum_{m=0}^{+\infty} q_m^i P_m(\xi) . \tag{11}$$

$$S_{yi}(z) = \sum_{m=0}^{+\infty} h_m^i P_m(\xi) . \tag{12}$$

$$U_{xi}(z) = \sum_{m=0}^{+\infty} t_m^i P_m(\xi) . \tag{13}$$

$$U_{yi}(z) = \sum_{m=0}^{+\infty} l_m^i P_m(\xi) . \tag{14}$$

Here, $\xi = \frac{2z-d}{d}$ and $P_m(\xi)$ are the normalized Legendre Polynomials and d is the grating thickness as is shown in Fig. 1.

It should be noticed that the vector space spanned by Legendre polynomials is a complete one[16] and each space harmonic amplitude can be expanded in terms of them. Although, truncating the polynomial expansions given in Eqs. (11-14) is inevitable, the introduced error is shown to be of no vital importance.

After substituting the above expansions in Eqs. (6-9), retaining the first M_i terms of the expansion, and minimizing the truncation error, a set of coupled algebraic equations is derived, representing the Maxwell's equations in the complete space spanned by Legendre polynomials:

$$\frac{2}{d}q'^{i}_{m}+j\left\{iK_{Gz}q^{i}_{m}+\frac{k_{xi}}{k_0}\sum_{p}a_{i-p}\left[k_y t^{p}_{m}-k_{xp}l^{p}_{m}\right]+k_0 l^{i}_{m}\right\}=0\,. \tag{15}$$

$$\frac{2}{d}h'^{i}_{m}+j\left\{iK_{Gz}h^{i}_{m}+\frac{k_{y}}{k_0}\sum_{p}a_{i-p}\left[k_y t^{p}_{m}-k_{xp}l^{p}_{m}\right]-k_0 t^{i}_{m}\right\}=0\,. \tag{16}$$

$$\frac{2}{d}t'^{i}_{m}+j\left\{iK_{Gz}t^{i}_{m}-\frac{k_{xi}}{k_0}\left[k_y q^{i}_{m}-k_{xi}h^{i}_{m}\right]-k_0\sum_{p}\widetilde{\varepsilon}_{i-p}h^{p}_{m}\right\}=0\,. \tag{17}$$

$$\frac{2}{d}l'^{i}_{m}+j\left\{iK_{Gz}l^{i}_{m}-\frac{k_{y}}{k_0}\left[k_y q^{i}_{m}-k_{xi}h^{i}_{m}\right]+k_0\sum_{p}\widetilde{\varepsilon}_{i-p}q^{p}_{m}\right\}=0\,. \tag{18}$$

In these equations, q'^{i}_{m} , h'^{i}_{m} , t'^{i}_{m} , and l'^{i}_{m} are the expansion coefficients of the first derivative of the Legendre expansion in terms of q^{i}_{m} , h^{i}_{m} , t^{i}_{m} , and l^{i}_{m} respectively, and are computed analytically as:

$$x'^{i}_{m}=(2m+1)\sum_{\substack{l=m+1\\ l+m\ odd}}^{M_i}x^{i}_{l}\ , \tag{19}$$

where x can be substituted by q, h, t, or l .

It should be noticed that each of Eqs. (15-19) result in a set of M_i equations, whereas each space harmonic expanded in Eqs. (11-14) is determined by M_i+1 unknown coefficients. Therefore, one needs four further equations, which can be obtained by applying boundary conditions[12] at $z = 0$ and $z = d$. Appropriate boundary conditions can be applied by using the electromagnetic field expressions in regions I and III given in Eq. (20), and Eq. (21), respectively [1].They are expanded in terms of plane waves corresponding to diffracted orders:

$$\boldsymbol{E}_1=\hat{u}e^{-j\overrightarrow{K_1}.\vec{r}}+\sum_{i=-\infty}^{+\infty}\boldsymbol{R}_i e^{-j\overrightarrow{K_{1i}}.\vec{r}}\ . \tag{20}$$

$$\boldsymbol{E}_3=\sum_{i=-\infty}^{+\infty}\boldsymbol{T}_i e^{-j\overrightarrow{K_{3i}}.(\vec{r}\ -\ d\hat{z})}\ . \tag{21}$$

Here $\boldsymbol{R}_i$ and $\boldsymbol{T}_i$ are reflection and transmission coefficients of each diffracted order, respectively, $\hat{u}$ is the incident wave polarization unit vector, and k_{1i} and k_{3i} are defined as:

$$k_{lxi}=k_{xi}=k_1\sin\alpha\cos\delta-iK_G\sin\phi \tag{22}$$

$$k_{lyi}=k_y=k_1\sin\alpha\sin\delta \tag{23}$$

$$k_{lzi}=\sqrt{k_l^2-k_{lxi}^2-k_y^2}\ , \tag{24}$$

for l=1,3 (representing region I or III).

Continuity of the electromagnetic fields at x=0 calls for:

$$u_x\delta_{i0}+R_{xi}=S_{xi}(0)\,. \tag{25}$$

$$u_y\delta_{i0}+R_{yi}=S_{yi}(0)\,. \tag{26}$$

$$\delta_{i0}(k_y u_z-k_1\cos\alpha u_y)-k_{z1i}R_{yi}+k_y R_{zi}=k_0 U_{xi}(0)\,. \tag{27}$$

$$\delta_{i0}(k_1\cos\alpha u_x-k_{x0}u_z)+k_{z1i}R_{xi}-k_{xi}R_{zi}=k_0 U_{yi}(0)\,. \tag{28}$$

and at x=d:

$$T_{xi}=S_{xi}(d)\exp(jiK_{Gz}d)\,. \tag{29}$$

$$T_{yi}=S_{yi}(d)\exp(jiK_{Gz}d)\,. \tag{30}$$

$$-k_{z3i}T_{yi}+k_y T_{zi}=k_0 U_{xi}(d)\exp(jiK_{Gz}d)\,. \tag{31}$$

$$k_{z3i}T_{xi}-k_{xi}T_{zi}=k_0 U_{yi}(d)\exp(jiK_{Gz}d)\,. \tag{32}$$

The divergence equation in region I and region III calls for:

$$k_{zi}R_{xi}+k_y R_{yi}+k_{z1i}R_{zi}=0\,. \tag{33}$$

$$k_{zi}T_{xi}+k_y T_{yi}+k_{z3i}T_{zi}=0\,. \tag{34}$$

Eliminating R_i and T_i components from these equations and substituting for space harmonic amplitudes, four equations are obtained as:

$$\sum_m \left[\frac{k_{z1i}^2 + k_{xi}^2}{k_{z1i}} q_m^i + \frac{k_{xi}k_y}{k_{z1i}} h_m^i - k_0 l_m^i \right] = (-1)^m \delta_{i0} \left[k_{x0}u_z - k_{1z}u_x + \frac{k_{z1i}^2 + k_{xi}^2}{k_{z1i}} u_x + \frac{k_{xi}k_y}{k_{z1i}} u_y \right]. \quad (35)$$

$$\sum_m \left[\frac{k_{z1i}^2 + k_y^2}{k_{z1i}} h_m^i + \frac{k_{xi}k_y}{k_{z1i}} q_m^i + k_0 t_m^i \right] = (-1)^m \delta_{i0} \left[k_y u_z - k_{1z}u_y + \frac{k_y^2 + k_{z1i}^2}{k_{z1i}} u_y + \frac{k_{xi}k_y}{k_{z1i}} u_x \right]. \quad (36)$$

$$\sum_m \left[\frac{k_{z3i}^2 + k_y^2}{k_{z3i}} h_m^i + \frac{k_{xi}k_y}{k_{z1i}} q_m^i + k_0 t_m^i \right] = 0. \quad (37)$$

$$\sum_m \left[\frac{k_{z3i}^2 + k_{xi}^2}{k_{z3i}} q_m^i + \frac{k_{xi}k_y}{k_{z3i}} h_m^i - k_0 l_m^i \right] = 0. \quad (38)$$

Now Eqs. (15-18) and (35-38) form a complete set equations, through which the unknown coefficients, i.e. q_m^i , h_m^i, t_m^i, and l_m^i are obtained. Consequently, $\boldsymbol{R}_i$, $\boldsymbol{T}_i$, and the corresponding diffraction efficiencies can be determined:

$$DE_{1i} = -\mathrm{Re}\left(\frac{K_{1iz}}{K_{1z}}\right) R_i R_i^* . \quad (39)$$

$$DE_{3i} = \mathrm{Re}\left(\frac{K_{3iz}}{K_{1z}}\right) T_i T_i^* . \quad (40)$$

For lossless dielectric gratings, as a result of energy conservation, one finds:

$$\sum_i DE_{1i} + DE_{3i} = 1. \quad (41)$$

3. NUMERICAL RESULTS

As an example, a transmission grating is analyzed. The parameters according to Fig.1 are: $\phi = 120^\circ$ (slant angle), $\alpha = 42^\circ$ (the angle of incidence), δ=45°(tilt angle), ψ=30°, and $\varepsilon(\boldsymbol{r}')=2.25(1+0.12\cos(\boldsymbol{K_G}.\boldsymbol{r}'))$ in region II, and $\varepsilon_I = \varepsilon_{III} = 2.25$. The incident wavelength is 0.6237μm and the grating period is 1 μm. In Fig. 2, diffraction efficiencies corresponding to the transmitted orders are plotted versus normalized thickness (d / Λ_G) by employing RCWA (solid line), and polynomial expansion method proposed in this paper (dashed line) by using 8 polynomial terms for each space harmonic. It should be noticed that conventional RCWA analysis becomes unstable for $d / \Lambda_G > 3$. In contrast, polynomial expansion method behaves well enough to handle such a problem. It is obvious that increasing the number of retained spatial orders improves the achieved accuracy of the truncated expansion of electromagnetic fields in terms of Legendre polynomials.

Another example is a lamellar grating with the following parameters: $\alpha = 42^\circ$ (the angle of incidence), δ=20°(tilt angle), ψ=30°, ε_I=1, $\varepsilon_{III} = 2.25$. Region II is a binary grating with 50% duty cycle. Permittivity of the ridge is 2.25 and that of the groove is 1. The incident wavelength is 0.6237μm and the grating period is 1 μm. In Fig. 3 , diffraction efficiencies corresponding to the transmitted orders are plotted versus normalized thickness (d / Λ_G) by employing RCWA (solid line), and polynomial expansion method proposed in this paper (dashed line) by using 20 polynomial terms for each space harmonic. It can be seen that near the normalized thickness of 1, the RCWA results become unstable**.**

4. CONCLUSIONS

In this paper, a Legendre polynomial expansion of electromagnetic fields for grating diffraction analysis in conical mounting has been reported. In this case TE and TM polarizations inside the grating are not separable and a vectorial three-dimensional analysis is required. In contrast to conventional modal analysis in which space harmonic amplitudes of the fields are expanded in terms of the eigenfunctions and eigenvectors of the coefficient matrix defined by rigorous coupled wave equations, the presented method is based on Legendre polynomial expansion. In this method, a set of algebraic equations is derived, which can be easily solved for diffraction efficiencies and electromagnetic field profiles. The method shows strong numerical stability. To verify the proposed method, the results of our analysis have been compared with that of RCWA and it has been shown that the presented approach yields numerically stable results. The physical intuition behind the accuracy of the proposed method can be described by the fact that, even though in practice the expansion of the electromagnetic fields in Hilbert space spanned by Legendre polynomials is truncated, each of the polynomials remaining in the calculation contains the projection of all electromagnetic eigenmodes of the system. Thus, no modal information of the system is fully lost in the truncation process.

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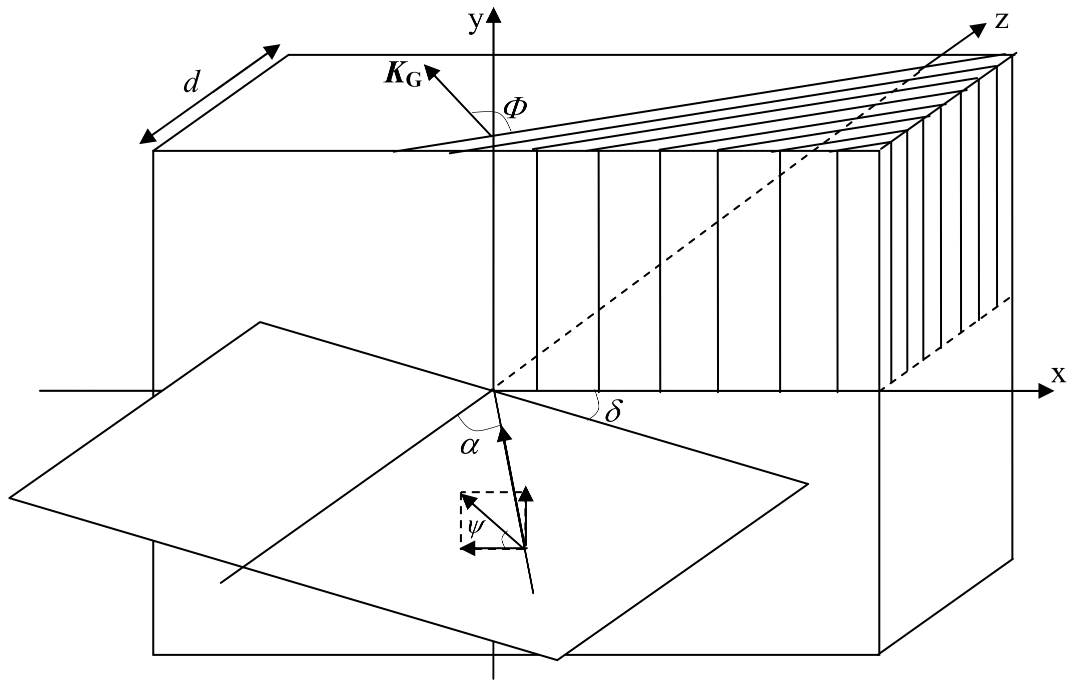

Fig.1 The general form of a slanted grating in conical mounting

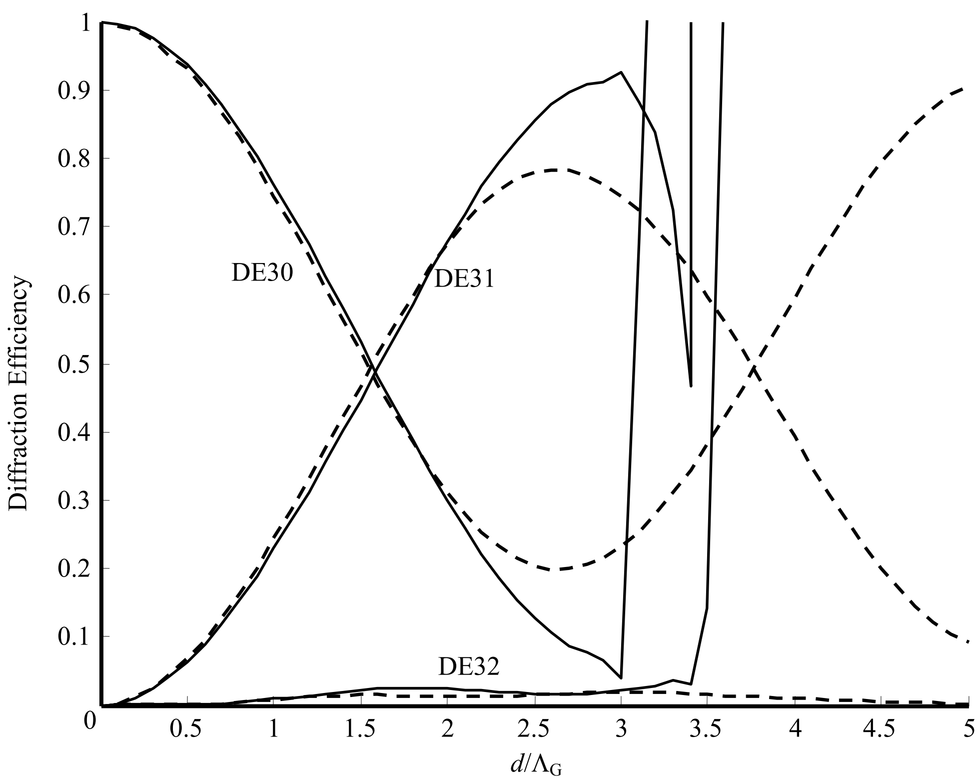

Fig.2 Diffraction efficiency for forward transmitted waves (Phase Grating). The proposed method (Dashed Lines) and conventional RCWA (Solid Lines).

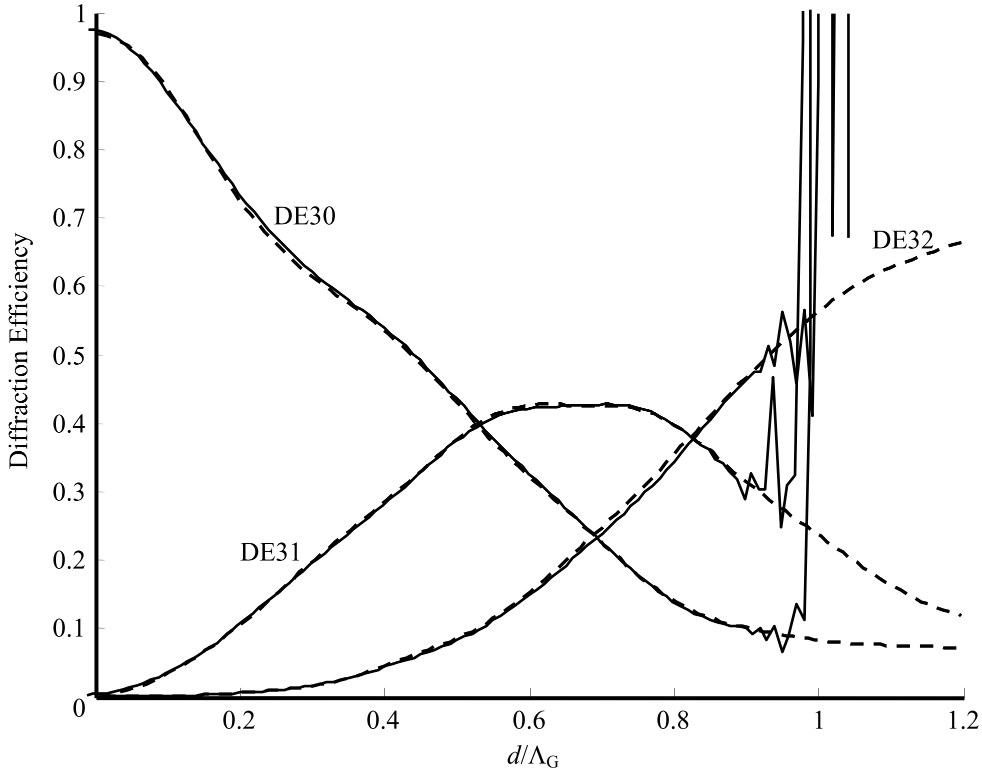

Fig.3 Diffraction efficiency for forward transmitted waves(Lamellar Grating). The proposed method (Dashed Lines) and conventional RCWA (Solid Lines).