Polynomial Expansion of Electromagnetic Fields for Grating Diffraction Analysis

Maysam Reza Chamanzar, Khashayar Mehrany, Bizhan Rashidian*
Department of Electrical Engineering, Sharif University of Technology,
P.O. Box 11365-9363, Tehran, Iran
Rashidia@sharif.edu

1. Introduction

Analysis of wave propagation behavior in periodic structures due to its wide range of applications is faced in various systems and design processes appearing in electromagnetics, optics, acoustics, and telecommunications [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 the grating. Different approaches have been reported for analysis of gratings in literature, rigorous coupled wave [1], coupled mode [2], two wave methods [3], Raman-Nat [4], etc. just to name a few. Of many methods for analysis of volume 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, it should be noticed that RCWA steps could be applied without numerical difficulty only when evanescent orders corresponding to real eigenvalues do not appear in the solution of Maxwell's equations. In general, if some evanescent orders are present, in imposing boundary conditions some extremely large coefficients are involved which are the cause of overflow in calculations. But evanescent orders cannot always be discarded especially in such cases as multiple grating structures. These methods are also vulnerable to numerical instability when the ratio of thickness over grating periodicity is large, or large number of spatial harmonics is retained. In the proposed method, the field expressions inside the grating are expanded in terms of orthogonal polynomials such as Legendre polynomials where the solution is examined in a Hilbert space spanned by polynomials. The method yields numerically stable results. This paper is arranged as follows: Polynomial expansion formulation of electromagnetic fields for the general case slanted gratings is given in Section 2. Section 3 involves a comparison of the results with the RCWA eigenvector expansion results. Finally, Section 4 deals with the conclusion.

2. Polynomial Expansion Analysis of general case Slanted Gratings

In this section, the field expressions inside grating are expanded in terms of orthogonal polynomials e.g. Legendre Polynomials [12]-[13]. Starting with Maxwell equations, Helmholtz equation is derived and the Floquet expansion in the grating direction is modified in terms of orthogonal Legendre polynomials. Then this form of the solution is substituted in Helmholtz equation and the boundary conditions are applied to find the unknown coefficients. It should be noticed that expansion of the field expressions in an orthogonal complete space of polynomials is a nonharmonic expansion [13], i.e. it isn't a linear combination of intrinsic eigenvectors. Nonetheless, it has many advantages over eigenvector expansion and other previously mentioned methods. First, the equations become algebraic so that they can be manipulated easier. Second, this approach works properly in some special cases where other methods may fail. There is not any numerical instability as the matrices involved are not very sparse and also there is no need to keep many digits because the large and the small numbers involved are not highly at either extreme. Also solving in polynomial Hilbert space, can be interpreted as the projection of the other solutions e.g. eigenvector expansions on the new polynomial bases. This means that each polynomial contains the projection of all of electromagnetic eigenmodes of the system in it

A general form of a slanted grating is shown in Fig.1. Here, Permittivity is assumed to be a periodic function of x':

$$\varepsilon(x') = \varepsilon_0 + \varepsilon_1 \cos(K_G x'), \tag{1}$$

* The author to whom the correspondence should be made

ISBN: 4-88552-206-4 C3055©IEICE

where $K_G = \frac{2\pi}{\Lambda_G}$ and Λ_G is the grating period. Inside the grating, the Helmholtz equation can be easily derived for TE incidence as follows [14]

$$\nabla^2 E_y(x',z') + k^2 \varepsilon(x') E_y(x',z') = 0\,, \tag{2}$$

The relation between (x,z) coordinates and (x',z') is simply a clockwise rotation of coordinates.
Following the Floquet solution in x' direction, the general form of the solution may be obtained as [1]

$$E_y(x,z) = \sum_{i=-\infty}^{+\infty} S_i(z) e^{-j(\vec{K_2} - i\vec{K_G}).\vec{r}}\,, \tag{3}$$

where $\vec{K_2} = K_{2x}\hat{x} + K_{2z}\hat{z}$ and $\vec{K_G} = \frac{2\pi}{\Lambda_G}[\sin(\phi)\hat{x} + \cos(\phi)\hat{z}]$.

Substituting this form of solution into wave equation and doing appropriate manipulations we have [1]

$$\frac{d^2 S_i(z)}{dz^2} - j2[K_2\cos(\theta) - iK_G\cos(\phi)]\frac{dS_i}{dz} + i(m'-i)K_G^2 S_i(z) + K_2^2 \tfrac{\varepsilon_1}{\varepsilon_0}[S_{i-1}(z) + S_{i+1}(z)] = 0\,, \tag{4}$$

where $m' = \frac{2\Lambda\sqrt{\varepsilon_0}}{\lambda}\cos(\theta - \phi)$, and λ is the wavelength of light at free space.

To solve the above equation we assume the answer is expanded in terms of Legendre Polynomials as

$$S_i(z) = \sum_{m=0}^{+\infty} q_m^i P_m(\xi) \quad , \quad \xi = \frac{2z-d}{d}\,, \tag{5}$$

Here $P_m(\xi)$'s are normalized Legendre Polynomials and q_m^i are the expansion coefficients to be determined later. It should be noticed that the space of Legendre polynomials is complete [13] and $S_i(z)$'s can be expanded in terms of them. However, computationally one has to truncate the previous expansion and retain only first M_i terms of expansion and this leads to truncation error. Minimizing this truncation error leads to [13]:

$$r_m^i - jN_i g_m^i + \gamma_i q_m^i + \frac{d^2}{4}K_2^2\frac{\varepsilon_1}{\varepsilon_0}(q_m^{i-1} + q_m^{i+1}) = 0\,, \tag{6}$$

where $r_n^i = \frac{2n+1}{2}\sum_{\substack{p=n+2t \\ t=1,2,3,..}}^{M_i}(p+n+1)(p-n)q_p^i$, and $g_n^i = (2n+1)\sum_{\substack{p=n+1 \\ p+n \ odd}}^{M_i} q_p^i$.

Equation (6) rsults in a set of $M_i - 1$ equations with $M_i + 1$ unknowns. Therefore, one needs two further equations obtained by applying boundary conditions at z = 0 and z = d [14]. Appropriate boundary conditions can be applied by using field expressions in regions I and III given in (7), and (8), respectively [1].

$$E_1 = e^{-j\vec{K_1}.\vec{r}} + \sum_{i=-\infty}^{+\infty} R_i e^{-j\vec{K_{1i}}.\vec{r}}\,, \tag{7}$$

$$E_3 = \sum_{i=-\infty}^{+\infty} T_i e^{-j\vec{K_{3i}}.(\vec{r} - d\ \hat{z})}\,, \tag{8}$$

Here R_i and T_i are the reflection and the transmission coefficients of each order.
Applying continuity conditions of tangential electromagnetic fields by using equations (3),(7-8), eliminating R_i and T_i coefficients, and doing further algebraic manipulations results in:

$$\sum_{m=0}^{M_i}(-1)^m q_m^i\left[\frac{m(m+1)}{d} + j(K_{1iz} + C_i)\right] = 2jK_{1z}\delta_{i0}\,, \tag{9}$$

$$\sum_{m=0}^{M_i} q_m^i\left[\frac{m(m+1)}{d} + j(K_{3iz} - C_i)\right] = 0\,, \tag{10}$$

where $C_i = K_2\cos(\theta) - iK_G\cos(\phi)$. Now equations (6), (9) and (10) forms a set of $M_i + 1$ equations through which $q_m^i{}'s$ can be obtained. Consequently, R_i, T_i, and corresponding diffraction efficiencies would be determined from boundary conditions where

$$DE_{1i} = \text{Re}(\frac{K_{1iz}}{K_{1z}})R_i R_i^*, \quad (11)$$

$$DE_{3i} = \text{Re}(\frac{K_{3iz}}{K_{1z}})T_i T_i^*, \quad (12)$$

3. Numerical Results

As a first numerical example, a reflection grating is analyzed where the grating slant angle is $\phi = 150°$, $\varepsilon_I = \varepsilon_{III} = \varepsilon_0 = 2.25$, the grating modulation is $\varepsilon_1/\varepsilon_0$=0.33, and the angle of incidence satisfies first Bragg condition at $\theta' = 20°$. Fig. 2 shows variations of different diffraction efficiencies versus normalized thickness (d / Λ_G) obtained by using RCWA (solid line) and polynomial expansion method proposed in this paper (dashed line) where five space harmonics are retained. Our results show an excellent consistency with those obtained by Gaylord et. al. [1]. However, it should be noticed that RCWA eigenvector expansion method fails when the thickness is increased beyond $5\Lambda_G$ where numerical instability occurs. As another example, a transmission grating with permittivities of $\varepsilon_I = \varepsilon_{III} = \varepsilon_0 = 2.25$, grating modulation of $\varepsilon_1/\varepsilon_0$=0.12, slant angle of $\phi = 120°$, and the angle of incidence satisfies first Bragg condition at $\theta' = 42°$, is considered. Similarly Fig. 3 shows variations of different diffraction efficiencies versus normalized thickness (d / Λ_G) obtained by using RCWA (solid line) and polynomial expansion method proposed in this paper (dashed line). Again, our results show good agreement with those reported by Gaylord et. al. in [1]. However, it should be noticed that conventional RCWA analysis fails to handle more than five spatial orders (i > 4) while polynomial expansion method works good enough to work out this problem.

Conclusion:

In this paper, a polynomial expansion of electromagnetic fields for grating diffraction analysis is reported and the formulation of the general case of slanted grating is derived. This new method is based on Legendre polynomial expansion rather than conventional modal analysis. To verify the proposed method, the results of our analysis are compared with results reported previously. Besides, it is shown that our proposed polynomial expansion method yields more reliable and stable results especially when conventional RCWA method fails to get stable numerical results for thick gratings, and increased numbers of space harmonics. 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 field in Hilbert space spanned by Legendre polynomials is truncated, each of the polynomials that remains in the calculation contains the projection of all of electromagnetic eigenmodes of the system in it. Thus no modal information on the system is lost in the truncation process.

References:

[1] T. K. Gaylord, and M. G. Moharam, “Analysis and applications of optical diffraction by gratings,” *Proceedings of the IEEE*, vol. 73, pp. 894-937, May 1985.

[2] B. Momeni, and B. Rashidian, “Improved coupled mode analysis of planar diffraction gratings,” *Proc. SPIE.*, vol. 4581, pp. 68-78, Oct 2001.

[3] P. St. J. Russel, “Optical volume holography,” *Phys. Rep.*, vol. 71, pp. 209-312, May 1981.

[4] C. V Raman, and N. S. K. Nath, “The diffraction of light by high frequency sound waves: part IV,” *Proc. Ind. Acad. Sci. A*, vol. 2, pp.119-125, Feb 1936.

[5] M. G. Moharam, and T. K. Gaylord, “Rigorous coupled-wave analysis of planar-grating diffraction,” *J. Opt. Soc. Am.*, vol. 71, pp. 811-818, July 1981.

[6] M. G. Moharam, and T. K. Gaylord, “Three-dimensional vector coupled-wave analysis of planar-grating diffraction,” *J. Opt. Soc. Am.*, vol. 73, pp. 1105-1112, Sept 1983.

[7] E. N. Glytsis, and T. K. Gaylord, “Three-dimensional (vector) rigorous coupled-wave analysis of anisotropic grating diffraction,” *J. Opt. Soc. Am. A*, vol. 7, pp. 1399-1420, Aug 1990.

[8] M. G. Moharam, E. B. Grann, D. A. Pommet, and T. K. Gaylord, "Formulation for stable and efficient implementation of the rigorous coupled-wave analysis of binary gratings," *J. Opt. Soc. Am. A*, vol. 12, pp. 1068-1076, May 1995.

[9] M. G. Moharam, D. A. Pommet, E. B. Grann, and T. K. Gaylord, "Stable Implementation of the Rigorous Coupled-Wave Analysis for Surface-Relief Gratings: Enhanced Transmittance Matrix Approach," *J. Opt. Soc. Am. A*, vol. 12, pp. 1077-1086, May 1995.

[10] E. N. Glytsis, and T. K. Gaylord, "Rigorous 3-D coupled wave diffraction analysis of multiple superposed gratings in anisotropic media," *Applied Optics*, vol. 28, pp. 2401-2421, June 1989.

[11] E. J. Restall, and A. C. Walker, "Rigorous coupled-wave method applied to fan-out gratings," *IEE Proceedings-Optoelectronics*, vol. 145, pp. 165-169, Jan 1998.

[12] "Special Functions of Mathematical Physics : A Unified Introduction with Applications" Nikiforov, AF. Boston 1988.

[13] K. Mehrany and B. Rashidian, "Polynomial expansion for extraction of electromagnetic eigenmodes in layered structures," *J. Opt. Soc. Am. B.*, vol.20, No. 12, Dec 2003.

[14] A. Ishimaru, "Electromagnetic wave propagation, radiation, and scattering," Prentice Hall, 1991.

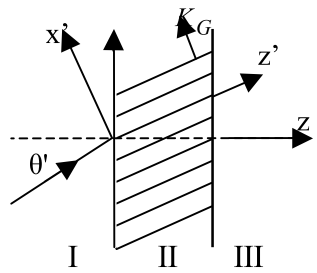

Fig. 1. Slanted grating

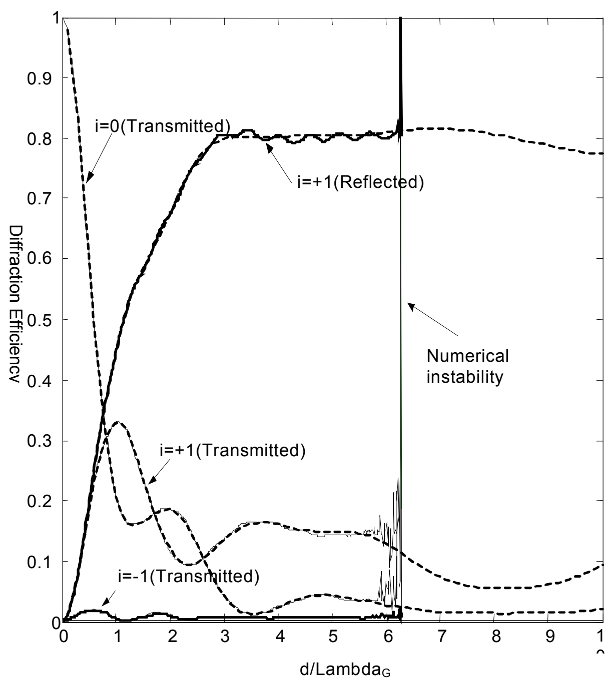

Fig.2. Diffraction efficiency computed by polynomial expansion (dashed line) and RCWA method (solid line) As the grating thickness increases, eigenvector analysis (solid lines) fails due to numerical instability, while polynomial expansion (dashed lines) works well.

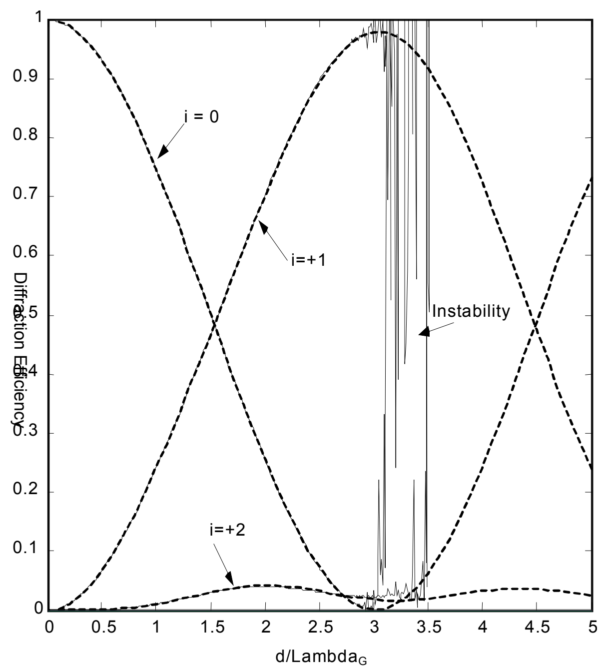

Fig. 3. Diffraction efficiency computed by polynomial expansion (dashed line) and RCWA method (solid line). While the proposed polynomial expansion works well with seven space harmonics (i=7), the conventional RCWA analysis fails to handle only five orders (i=5).