REFORMULATION OF THE DIFFERENTIAL METHOD FOR ANISOTROPIC CROSSED GRATINGS WITH SMOOTH PROFILE

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Abstract: This paper presents a fast converging formulation of the differential theory for smooth profiled cross gratings made of anisotropic materials. A coupled first-order differential equation set is derived by taking into account Li’s Fourier factorization rules [J. Opt. Soc. Am. A, Vol. 13, 1996, pp. 1870–1876.], but the present formulation uses the Laurent rule only. Numerical results show that convergence of the present formulation is superior to that of the conventional one.

STATEMENT OF THE PROBLEM

We shall investigate the diffraction problem on a crossed surface-relief gratings schematically shown in Fig. 1. The structure is periodic in two directions which are perpendicular to each other, and we introduce a rectangular Cartesian coordinate system $O-xyz$, in which $x$ and $y$-axes are parallel to two periodic directions. Also, the $z$-axis is perpendicular to the grating plane and the origin is assumed to be at the bottom boundary of the grating layer. The periods in the $x$ and $y$-directions are denoted by $d_x$ and $d_y$, respectively and the grating depth is denoted by $h$. We consider time harmonic fields assuming a time-dependence in $e^{-i\omega t}$, and deal with the plane incident wave propagating in the direction of polar angle $\theta$ ($0 \leq \theta < \pi / 2$) and azimuth angle $\phi$ ($-\pi < \phi \leq \pi$). The surface of the grating is defined by an equation $z = p(x, y)$, where $p(x, y)$ is a known periodic and smooth function. The region 1: $z > p(x, y)$ is filled with a lossless, homogeneous, and isotropic material described by the permittivity $\varepsilon_1$ and the permeability $\mu_1$, and the region 2: $z < p(x, y)$ is filled with a homogeneous and anisotropic material described by the permittivity tensor $\varepsilon_2$ and the permeability tensor $\mu_2$.

FAST CONVERGING FORMULATION

The differential method [1] is one of the most commonly used approaches in the analyses of gratings. Thanks to the periodicity, the Cartesian components of electromagnetic fields can be expressed by the generalized Fourier series, and then Maxwell’s curl equations are transformed into a coupled ordinary differential equation set. Outside the groove region, the fields can be expressed in Rayleigh expansions, and thus the solution inside the groove region can be matched to them. Then the diffraction problem is reduced to the numerical integration problem of a coupled differential-equation set with the boundary conditions at the top and the bottom of the groove region. This theory is widely used because of the simplicity and wide applicability. However, gratings that are deep and made of conducting materials sometimes cause serious problems of poor convergence [2]. The origin of poor convergence is recently explained by Li’s Fourier factorization rules [3], and they gave an idea for accelerating the convergence. Let $\varepsilon_{l,pq}$ and $\mu_{l,pq}$ ($l = 1, 2$ and $p, q = x, y, z$) be the $(p, q)$-entries of the permittivity and the permeability matrices in the region $l$. Then, the constitutive relations in the original space are written as follows:

$$
\begin{pmatrix}
  D_x \\
  D_y \\
  D_z
\end{pmatrix} = \sum_{l=1}^{2} w_l \begin{pmatrix}
  \varepsilon_{l,xx} & \varepsilon_{l,xy} & \varepsilon_{l,xz} \\
  \varepsilon_{l,yx} & \varepsilon_{l,yy} & \varepsilon_{l,yz} \\
  \varepsilon_{l,zx} & \varepsilon_{l,zy} & \varepsilon_{l,zz}
\end{pmatrix} \begin{pmatrix}
  E_x \\
  E_y \\
  E_z
\end{pmatrix},
\begin{pmatrix}
  B_x \\
  B_y \\
  B_z
\end{pmatrix} = \sum_{l=1}^{2} w_l \begin{pmatrix}
  \mu_{l,xx} & \mu_{l,xy} & \mu_{l,xz} \\
  \mu_{l,yx} & \mu_{l,yy} & \mu_{l,yz} \\
  \mu_{l,zx} & \mu_{l,zy} & \mu_{l,zz}
\end{pmatrix} \begin{pmatrix}
  H_x \\
  H_y \\
  H_z
\end{pmatrix}
$$

(1)
with

\[ w_1(x, y, z) = \begin{cases} 1 & \text{for } z > p(x, y) \\ 0 & \text{for } z \leq p(x, y) \end{cases}, \quad w_2(x, y, z) = 1 - w_1(x, y, z). \]  

(2)

To derive the coupled differential equation set, an expression of the constitutive relations in Fourier space. All the pseudo-periodic functions are replaced by the generalized Fourier series that are truncated from \(-N_x\)th to \(N_x\)th-orders for the \(x\)-direction and from \(-N_y\)th to \(N_y\)th-order for the \(y\)-direction, and then the electric relation yields the following relations:

\[
\begin{bmatrix} D_x \\ D_y \\ D_z \end{bmatrix} = \sum_{l=1}^{2} \begin{bmatrix} \varepsilon_{l,xx} I & \varepsilon_{l,xy} I & \varepsilon_{l,xz} I \\ \varepsilon_{l,yx} I & \varepsilon_{l,yy} I & \varepsilon_{l,yz} I \\ \varepsilon_{l,zx} I & \varepsilon_{l,zy} I & \varepsilon_{l,zz} I \end{bmatrix} \begin{bmatrix} w_l E_x \\ w_l E_y \\ w_l E_z \end{bmatrix}
\]  

(3)

where \([f]\) is the \((2N_x + 1)(2N_y + 1) \times 1\) column matrices constructed with the generalized Fourier coefficients of doubly periodic function \(f\). The conventional formulations applied the Laurent rule, which is a discrete style of the convolution rule, to factorize the coefficients of products \(w_l E_p\) \((p = x, y, z)\) without any care of the continuity properties. Li pointed out that the Laurent rule is valid only for a product of two periodic functions that have no concurrent discontinuities. \(w_l\) and \(E_p\) have concurrent jump discontinuities on the grating surface \(z = p(x, y)\), and the direct use of the Laurent rule causes poor convergence in many cases.

To resolve this difficulty, we introduce intermediary functions \(E_t, E_s,\) and \(D_n\) that combine concurrently discontinuous functions [4]. Let \(p_x(x, y)\) and \(p_y(x, y)\) be the partial derivatives of \(p(x, y)\) by \(x\) and \(y\), respectively. Then, these functions are defined as follows:

\[
\begin{bmatrix} E_t \\ E_s \\ D_n \end{bmatrix} = \sum_{l=1}^{2} w_l \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ -\varepsilon_{l,xx}p_x - \varepsilon_{l,xy}p_y + \varepsilon_{l,xz} \\ -\varepsilon_{l,xz}p_x - \varepsilon_{l,zz}p_y + \varepsilon_{l,zz} \\ -\varepsilon_{l,xz}p_x - \varepsilon_{l,zz}p_y + \varepsilon_{l,zz} \\ \varepsilon_{l,zz}p_x - \varepsilon_{l,zz}p_y + \varepsilon_{l,zz} \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}
\]  

(4)

where \(E_t, E_s, D_n\) respectively give the tangential components of electric field and the normal component of electric displacement on the boundary \(z = p(x, y)\) and they are continuous everywhere. Multiplying Eq. (4) by \(w_l(x, y)\), we have the following relation:

\[
w_l \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} = w_l \begin{bmatrix} a^{(e)}_{l,xt} & a^{(e)}_{l,xs} & a^{(e)}_{l,xn} \\ a^{(e)}_{l,yt} & a^{(e)}_{l,ys} & a^{(e)}_{l,yn} \\ a^{(e)}_{l,zt} & a^{(e)}_{l,zn} & a^{(e)}_{l,zn} \end{bmatrix} \begin{bmatrix} E_t \\ E_s \\ D_n \end{bmatrix}
\]  

(5)

where the expressions of \(a^{(e)}_{l,pq}\) \((p, q = x, y, z)\) are obtained by inverting the square matrix in Eq. (4).

Here, we express the Laurent rule as \([f g] = [f] [g]\) where \([f]\) is a square matrix generated by the Fourier coefficients. Since \(w_l\) and \(E_t, E_s, E_z\) are concurrently discontinuous on the boundary \(z = p(x, y)\), the products on the left-hand side of Eq. (5) cannot be Fourier factorized by the Laurent rule. On the other hand, \(a^{(e)}_{l,pq}\) and \(E_t, E_s, D_n\) are continuous everywhere, and therefore the products on the right-hand side can be Fourier factorized by the Laurent rule. Then, we obtain

\[
\begin{bmatrix} [w_l E_x] \\ [w_l E_y] \\ [w_l E_z] \end{bmatrix} = C^{(e)}_l \begin{bmatrix} [E_t] \\ [E_s] \\ [D_n] \end{bmatrix}, \quad C^{(e)}_l = \begin{bmatrix} [w_l] [a^{(e)}_{l,xt}] & [w_l] [a^{(e)}_{l,xs}] & [w_l] [a^{(e)}_{l,xn}] \\ [w_l] [a^{(e)}_{l,yt}] & [w_l] [a^{(e)}_{l,ys}] & [w_l] [a^{(e)}_{l,yn}] \\ [w_l] [a^{(e)}_{l,zt}] & [w_l] [a^{(e)}_{l,zn}] & [w_l] [a^{(e)}_{l,zn}] \end{bmatrix}.
\]  

(6)

Since \([E_p]\) \((p = x, y, z)\) are equal to \([w_l E_p]\) + \([w_2 E_p]\), Eq. (6) gives the following relation:

\[
\begin{bmatrix} [w_l E_x] \\ [w_l E_y] \\ [w_l E_z] \end{bmatrix} = C^{(e)}_l \left( \sum_{m=1}^{2} C^{(e)}_m \right)^{-1} \begin{bmatrix} [E_x] \\ [E_y] \\ [E_z] \end{bmatrix}.
\]  

(7)

Substituting this relation into Eq. (3), we obtain the electric constitutive relations in Fourier space. Similarly, the magnetic constitutive relations in Fourier space can be also derived in the same way.
NUMERICAL EXAMPLE

Numerical experiments using the derived coupled differential-equation set may show that in many cases instabilities occur, especially for deep grating and/or for conducting materials. The origin of troubles is the accumulation of contamination linked with growing exponential functions, when computing the field over the entire groove region. We use the S-matrix propagation algorithm [5] to get rid of this problem, which can be easily adapted to the differential method. To validate the proposed formulation, we consider a specific example. The values of geometrical parameters are chosen as \( \lambda_0 = 0.6328 \, \mu m \), \( \theta = 30^\circ \), \( \phi = 20^\circ \), \( d_x = d_y = 0.6 \, \mu m \), \( h = 0.2 \, \mu m \), \( p(x, y) = (h/4) \, [1 + \cos(2 \pi x/d_x)] \, [1 + \cos(2 \pi y/d_y)] \), 
\( \varepsilon_1 = \varepsilon_0 \), \( \varepsilon_{2,xx} = \varepsilon_{2,yy} = \varepsilon_{2,zz} = (-8.19 + i \, 16.38) \, \varepsilon_0 \), \( \varepsilon_{2,yx} = -\varepsilon_{2,xy} = (0.495 + i \, 0.106) \, \varepsilon_0 \), \( \varepsilon_{2,zz} = \varepsilon_{2,yz} = \varepsilon_{2,zx} = \varepsilon_{2,zy} = 0 \), \( \mu_1 = \mu_0 \), \( \varepsilon_{2,zz} = \mu_2 = \mu_0 I \), and the TM polarized incident wave. Figure 2 shows the efficiencies of (0,0)th and (-1,0)th-order diffraction waves as a function of the truncation order \( N \) which truncates the Fourier series expansion from \(-N\)th to \(N\)-th-order for both \( x \) and \( y \)-directions, namely, \( N_x = N_y = N \). The solid and the dotted curves are obtained by the present and the conventional formulations, respectively. It is seen that the present formulation provides a significant improvement of convergence.

CONCLUSION

In this paper, we presented a fast converging formulation of the differential theory for anisotropic cross grating with smooth profile. The formulation is based on Li’s Fourier factorization rules and we introduced continuous intermediary functions that combine discontinuous functions. Then the coupled differential equation set was derived by the Laurent rule only and the use of inverse rule is suppressed. Numerical experiment showed the validity of the present formulation and the convergence was greatly improved by comparing with the conventional one.

REFERENCES


Fig. 2: Comparison of convergences of the diffraction efficiencies computed by the conventional and the present formulations.