Coordinate Transformation Formulation of Two-Dimensional Scattering from Apodized Surface-Relief Gratings

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1. Introduction

Electromagnetic scattering from periodic structures with finite extent has been extensively studied as wavelength and polarization selective components in microwave, millimeter-wave, and optical wave regions. As well know, when a plane wave is incident on a perfectly periodic structure, the Floquet theorem claims that the scattered fields are pseudo-periodic (namely, each field component is a product of a periodic function and an exponential phase factor) and the analysis region can be reduced to one periodicity cell. However, in case of periodic structure with finite extent, the Floquet theorem is no longer applicable and the computation has been mainly performed with the finite difference timedomain method, the finite element method, the time-domain beam propagation method, etc., in which the structural periodicity is not utilized.

This paper deals with the two-dimensional electromagnetic scattering from an apodized surfacerelief grating with finite extent. The basic idea of the formulation is the same with Ref. [1]. Namely, the present formulation is based on the differential method of Chandezon *et al.* [2] (referred to as the C-method) with the help of the pseudo-periodic Fourier transform (PPFT) [3]. Let f(x) be a function of x and d be a positive real constant. Then the PPFT and the inverse transform are defined by

$$\overline{f}(x;\xi) = \sum_{m=-\infty}^{\infty} f(x-m\,d)\,e^{i\,m\,d\,\xi}, \qquad \qquad f(x) = \frac{d}{2\,\pi} \int_{-\pi/d}^{\pi/d} \overline{f}(x;\xi)\,d\xi. \tag{1}$$

The transformed function $\overline{f}(x;\xi)$ has a pseudo-periodic property with the pseudo-period d in terms of x: $\overline{f}(x-d;\xi) = \overline{f}(x;\xi) e^{-id\xi}$. Also, $\overline{f}(x;\xi)$ is a periodic function of the transform parameter ξ with period $2\pi/d$. Maxwell's equations and the constitutive relations are transformed and the benefit of the pseudo-periodicity makes us possible to express the transformed fields in the generalized Fourier series [4]. Also, we introduce a discretization of the transform parameter, and then the problem can be solved by the standard matrix operation.

2. Settings of the Problem

Figure 1 shows an example of apodized surface-relief gratings. We consider time-harmonic fields assuming a time-dependence in $e^{-i\omega t}$. The grating structure is uniform in the z-direction, and the y-axis is perpendicular to the grating-plane. The grating surface is given by a known function $g(x) = g_a(x) g_p(x)$, where $g_p(x)$ is a periodic function with a period d and $g_a(x)$ is an apodization factor. For simplification,



Figure 1: Apodized surface-relief grating.

g(x) is supposed to be a continuous function with continuous derivative. The region y > g(x) is filled with a homogeneous and isotropic material described by a permittivity ε_c and a permeability μ_c , and the incident field illuminates the grating surface from this region. The substrate region y < g(x) is also homogeneous and isotropic, and the material is described by a permittivity ε_s and a permeability μ_s . The incident field, which does not need to be plane wave, is supposed to be dependent on x and yonly. Consequently, the electromagnetic fields are uniform in the z-direction and two-dimensional scattering problem is considered. Two fundamental polarizations are expressed by TE and TM, in which the electric and the magnetic fields are respectively parallel to the z-axis. The Cartesian components of the fields is denoted by $(\phi_x, \phi_y, \psi_z) = (H_x, H_y, E_z)$ for TE polarization and $(\phi_x, \phi_y, \psi_z) = (E_x, E_y, H_z)$ for TM polarization. Also, the regions above and below the grating surface are both homogeneous, and we consider the electromagnetic fields in each region separately. We use a notation r = c, s to deal with the both regions simultaneously, and the regions y > g(x) and y < g(x) are denoted by r = c and r = s, respectively.

3. Formulation

The formulation of the problem follows the same process with that in Ref. [1]. We introduce a curvilinear coordinate system O-uvz, which is related to the original coordinate system O-xyz by continuously differentiable transformation equations: u = x and v = y - g(x). Introducing PPFT with respect to u, the transformed fields have pseudo-periodic property in terms of u, and they can be approximately expanded in the truncated generalized Fourier series. For example, the z-component of the field can be written as

$$\overline{\psi}_{z}(u;\xi,v) \approx \sum_{n=-N}^{N} \overline{\psi}_{z,n}(\xi,v) e^{i\,\alpha_{n}(\xi)\,u}, \qquad \qquad \alpha_{n}(\xi) = \xi + n\,k_{d} \tag{2}$$

where N denotes the truncation order and $\overline{\psi}_{z,n}(\xi, v)$ are the *n*th-order generalized Fourier coefficients. We take L sample points $\{\xi_l\}_{l=1}^L$ to discretize the transfer parameter ξ , and the convolutions yielded from the products of functions of u are approximated by an appropriate numerical integration scheme. Then we may obtain a coupled differential-equation set as

$$\begin{pmatrix} \tilde{\psi}_{z}(v) \\ -i\frac{d}{dv}\tilde{\psi}_{z}(v) \end{pmatrix} = -iM_{r}\frac{d}{dv}\begin{pmatrix} \tilde{\psi}_{z}(v) \\ -i\frac{d}{dv}\tilde{\psi}_{z}(v) \end{pmatrix}$$
(3)

with

$$\boldsymbol{M}_{r} = \begin{pmatrix} -\left(k_{r}^{2}\boldsymbol{I} - \widetilde{\boldsymbol{X}}^{2}\right)^{-1} \left(\widetilde{\boldsymbol{X}} \begin{bmatrix} \overline{\boldsymbol{j}} \end{bmatrix} + \begin{bmatrix} \overline{\boldsymbol{j}} \end{bmatrix} \widetilde{\boldsymbol{X}} \right) & \left(k_{r}^{2}\boldsymbol{I} - \widetilde{\boldsymbol{X}}^{2}\right)^{-1} \left(\begin{bmatrix} \overline{\boldsymbol{j}} \end{bmatrix}^{2} + \boldsymbol{I} \right) \\ \boldsymbol{I} & \boldsymbol{0} \end{pmatrix}$$
(4)

$$[\![\bar{g}]\!] = \begin{pmatrix} \frac{w_1}{k_d} [\![\bar{g}]\!] (\xi_1 - \xi_1) & \cdots & \frac{w_L}{k_d} [\![\bar{g}]\!] (\xi_1 - \xi_L) \\ \vdots & \ddots & \vdots \\ \frac{w_1}{k_d} [\![\bar{g}]\!] (\xi_L - \xi_1) & \cdots & \frac{w_L}{k_d} [\![\bar{g}]\!] (\xi_L - \xi_L) \end{pmatrix}, \quad ([\![\bar{g}]\!] (\xi))_{n,m} = \frac{1}{d} \int_{-\infty}^{\infty} \dot{g}(u) \, e^{-i\,\alpha_{n-m}(\xi)\,u} \, du$$
(5)

where $\widetilde{\psi}_z(v)$ denotes a column matrix generated by the generalized Fourier coefficients $\{\overline{\psi}_{z,n}(\xi_l, v)\}$, $k_r = \omega \sqrt{\varepsilon_r \mu_r}$ denotes a wavenumber in the region r, \widetilde{X} denotes a diagonal matrix whose diagonal elements are $\{\alpha_n(\xi_l)\}$, $\dot{g}(u)$ denotes the derivative of g(u), and $\{w_l\}_{l=1}^L$ denotes the weight determined by the numerical integration scheme.

Since the coefficient matrix M_r is constant, the general solution to the coupled equation set (3) is obtained by solving an eigenvalue-eigenvector problem. Let $\eta_{r,n}$ be the reciprocal of the *n*theivenvalue of M_r and $p_{r,n}$ be the corresponding eigenvector. The order of M_r is 2L(2N + 1), and the 2L(2N + 1) eigenvalues are numbered in such a way that $\{\eta_{r,n}\}_{n=1}^{L(2N+1)}$ contains real values with negative value and complex values with positive imaginary parts and that $\{\eta_{r,n}\}_{n=L(2N+1)+1}^{2L(2N+1)}$ contains values with the opposite signs. Then, the general solution to Eq. (3) is written in the following form:

$$\widetilde{\psi}_{z}(v) = P_{r,11} a_{r}^{(-)}(v) + P_{r,12} a_{r}^{(+)}(v)$$
(6)

where $P_{r,nm}$ (n, m = 1, 2) are $L(2N + 1) \times L(2N + 1)$ block matrices contained in the eigenvector matrix, in which the *n*th-eigenvector of M_r is stored in the *n*th-column. The *v*-dependences of the column matrices $a_r^{(\pm)}(v)$ are expressed as

$$\boldsymbol{a}_{r}^{(\pm)}(v) = \boldsymbol{U}_{r}(\pm (v - v')) \, \boldsymbol{a}_{r}^{(\pm)}(v'), \qquad (\boldsymbol{U}_{r}(v))_{n,m} = \delta_{n,m} \, e^{i \, \eta_{r,n} \, v} \tag{7}$$

for a constant v', and $a_r^{(+)}(v)$ and $a_r^{(-)}(v)$ gives therefore the amplitudes of the eigenmodes propagating in the positive and negative v-direction, respectively.

We denote the covariant component of fields in terms of u by $\phi_t = \phi_x + \dot{g} \phi_y$, which gives the tangential component of the field on the grating surface y = g(x). Then the generalized Fourier coefficients of $\overline{\phi}_t(u;\xi_l,v)$ are expressed in the following form:

$$\widetilde{\phi}_t(v) = Q_{r,1} a_r^{(-)}(v) + Q_{r,2} a_r^{(+)}(v)$$
(8)

$$\boldsymbol{Q}_{r,m} = \begin{cases} -\frac{1}{\omega\,\mu_r} \left[\left[\overline{\boldsymbol{j}} \overline{\boldsymbol{j}} \right] \, \widetilde{\boldsymbol{X}} \, \boldsymbol{P}_{r,1m} - \left(\left[\overline{\boldsymbol{j}} \overline{\boldsymbol{j}} \right] \,^2 + \boldsymbol{I} \right) \, \boldsymbol{P}_{r,2m} \right] & \text{for TE-polarization} \\ \frac{1}{\omega\,\varepsilon_r} \left[\left[\overline{\boldsymbol{j}} \overline{\boldsymbol{j}} \right] \, \widetilde{\boldsymbol{X}} \, \boldsymbol{P}_{r,1m} - \left(\left[\overline{\boldsymbol{j}} \overline{\boldsymbol{j}} \right] \,^2 + \boldsymbol{I} \right) \, \boldsymbol{P}_{r,2m} \right] & \text{for TM-polarization} \end{cases}$$
(9)

for m = 1, 2. The general solutions separately obtained in the regions c and s are matched at the grating surface v = 0 by equating the ψ_z and ϕ_t . Then the amplitudes of the incident and the scattered fields are related by

$$\begin{pmatrix} \boldsymbol{a}_{c}^{(+)}(+0) \\ \boldsymbol{a}_{s}^{(-)}(-0) \end{pmatrix} = \begin{pmatrix} \boldsymbol{S}_{11} \\ \boldsymbol{S}_{21} \end{pmatrix} \boldsymbol{a}_{c}^{(-)}(+0)$$
(10)

where the scattering matrices are given as follows:

$$S_{11} = -\left(P_{s,11} Q_{s,1}^{-1} Q_{c,2} - P_{c,12}\right)^{-1} \left(P_{s,11} Q_{s,1}^{-1} Q_{c,1} - P_{c,11}\right)$$
(11)

$$S_{21} = Q_{s,1}^{-1} \left(Q_{c,1} + Q_{c,2} S_{11} \right).$$
(12)

The relation (10) makes possible to calculate the scattered fields for known incident fields.

4. Numerical Results

To validate the present formulation, this section shows some numerical results for a specific example of apodized surface-relief grating. The grating profile is determined as

$$g_p(x) = h \cos\left(\frac{2\pi}{d}x\right), \qquad g_a(x) = \begin{cases} 1 & \text{for } |x| \le w_1 \\ \sin^2\left(\frac{\pi}{2}\frac{x-w_2}{w_2-w_1}\right) & \text{for } 0 < |x| \le w_2 \\ 0 & \text{for } |x| > w_2 \end{cases}$$
(13)

Also, the electromagnetic fields are excited by a line source located parallel to the z-axis at $(x, y) = (x_0, y_0)$, and the incident field is then given as

$$\psi_z^{(i)}(x,y) = H_0^{(1)}(k_c \,\rho(x-x_0,y-y_0)), \qquad \rho(x,y) = \sqrt{x^2 + y^2}. \tag{14}$$

The parameters are chosen as follows: $\lambda_0 = 0.6328 \,\mu\text{m}$, $h = 0.2 \,\lambda_0$, $d = 0.6 \,\lambda_0$, $w_1 = 1.5 \,d$, $w_2 = 3 \,d$, $\varepsilon_c = \varepsilon_0$, $\varepsilon_s = (1.3 + i \,7.6)^2 \,\varepsilon_0$, $\mu_c = \mu_s = \mu_0$, and $(x_0, y_0) = (0, 2 \,d)$. An observation point is chosen at

(x,y) = (d,d) without deliberation and the intensity of ψ_z is computed. The obtained results are plotted as functions of the number of sample points for the transform parameter in Fig. 2. The computation is performed with the truncation order N = 3, and the periodic interval of the transform parameter ξ is split into two subintervals at the Wood-Rayleigh anomalies [3]. The number of sample points L is divided in the ratio of the subinterval widths, and apply the Gauss-Legendre scheme for each subinterval to decide the sample points $\{\xi_l\}_{l=1}^L$ and the weights $\{w_l\}_{l=1}^L$. The results show reliable convergence though TM polarization converges slower. Also, the field intensity distribution near the grating surface is computed for N = 3 and L = 100 and shown in Fig. 3.

5. Conclusions

This paper presents a novel approach to the electromagnetic scattering from apodized surface-relief gratings. The formulation is based on C-method with the help of PPFT. The near field analysis requires a numerical integration with respect to the transform parameter, and the sample points are determined by considering the Wood-Rayleigh anomalies. Numerical experiments of an apodized sinusoidal grating made of conducting material show reliable results and the present formulation seems to be no problem.

References

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Figure 2: Convergence of the field intensity at an observation point (x, y) = (d, d) with respect to the number of sample points L.



(a) TE polarization



(b) TM polarization

Figure 3: Field intensity near a apodized sinusoidal grating with a line source excitation.