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Coordinate Transformation Formulation of Two-Dimensional Scattering from Surface-Relief Grating with a Defect

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1. Introduction

Electromagnetic scattering from periodic structures has been extensively studied for a long time as wavelength and polarization selective components in microwave, millimeter-wave, and optical wave regions. As well known, 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. Recently, structures in which the periodicity is locally broken have also received much interest because they induce distinct properties; for example, the field localization induced by defects in the electromagnetic bandgap structures. In such structures, the Floquet theorem is no longer applicable, and the computation has been mainly performed with the finite differences time-domain method, the finite element method, the time-domain beam propagation method, the method of fictitious sources, etc. These approaches are limited to apply to the problems of scatterers with finite extent, and the analysis region has to cover whole scatterers under consideration.

This paper shows a new approach to the electromagnetic scattering problems from structures in which the periodicity is locally broken. As an example of the problems, we consider a surface-relief grating with a defect. The present formulation is based on a pseudo-periodic Fourier transform (PPFT) [1], which makes the field components pseudo-periodic and they are expanded in the generalized Fourier series [2] without introducing an approximation of artificial periodic boundary. 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

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

The transformed function $\overline{f}(x;\xi)$ has a pseudo-periodic property with the pseudo-period d in terms of x: $\overline{f}(x-d;\xi) = \overline{f}(x;\xi)\,e^{-i\,d\,\xi}$. 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. Also, we introduce a discretization of the transform parameter, and then the problem can be solved by using well-known differential method of Chandezon *et al.* [3] referred to as the C-method.

2. Setting of the Problem

Figure 1 shows an example of surface-relief gratings with a defect. 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 x-axis is parallel to the direction of periodicity (though the periodicity is locally collapsed). The equation of the grating surface is given by $y = g(x)$, where $g(x)$ is a known function. We decompose the surface profile function $g(x)$ into periodic and aperiodic parts: $g(x) = g_p(x) + g_a(x)$, where $g_p(x)$ is a periodic function with the period d and $g_a(x)$ has nonzero value only at the defect. For simplification, $g_p(x)$ and $g_a(x)$ are supposed to be continuous functions with continuous derivatives. The region defined

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by $y > g(x)$ is filled with a homogeneous and isotropic material described by the relative permittivity ε_c and the relative 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 the relative permittivity ε_s and the relative permeability μ_s. The incident field, which does not need to be plane wave, is supposed to be a function of x and y only. 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. For simple expressions, we normalize the fields, namely, the E field by $\sqrt[4]{\mu_0/\varepsilon_0}$, the H field by $\sqrt[4]{\varepsilon_0/\mu_0}$, and the D field by $\varepsilon_0\ \sqrt[4]{\mu_0/\varepsilon_0}$, where ε_0 and μ_0 denote the permittivity and the permeability in free space, respectively.

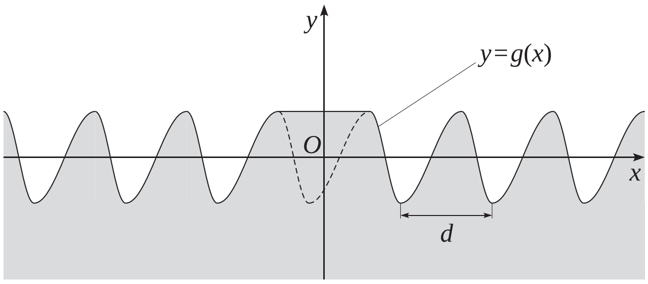

Figure 1: Surface-relief grating with a defect.

3. Formulation

The regions above and below the grating surface are both homogeneous, and we consider the electromagnetic fields in each region separately. We introduce 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.

First, we consider the TE polarized fields. 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 $v = y - g(x)$. Then, from normalized Maxwell's curl equations, we may obtain the relations of the Cartesian components of the fields as follows:

$$\frac{\partial}{\partial v} E_z(u, v) = i\, k_0\, \mu_r\, H_x(u, v) \tag{2}$$

$$\left(\frac{\partial}{\partial u} - \dot{g}(u)\, \frac{\partial}{\partial v}\right) E_z(u, v) = -i\, k_0\, \mu_r\, H_y(u, v) \tag{3}$$

$$\left(\frac{\partial}{\partial u} - \dot{g}(u)\, \frac{\partial}{\partial v}\right) H_y(u, v) - \frac{\partial}{\partial v} H_x(u, v) = -i\, k_0\, \varepsilon_r\, E_z(u, v) \tag{4}$$

where k_0 denotes the wavenumber in free space and $\dot{g}(u)$ denotes the derivative of $g(u)$. Introducing the PPFT defined by Eq. (1), Eqs. (2)–(4) are transformed into the following relations:

$$\frac{\partial}{\partial v} \overline{E}_z(u; \xi, v) = i\, k_0\, \mu_r\, \overline{H}_x(u; \xi, v) \tag{5}$$

$$\frac{\partial}{\partial u} \overline{E}_z(u; \xi, v) - \frac{d}{2\pi} \int_{-\pi/d}^{\pi/d} \bar{\dot{g}}(u; \xi - \xi')\, \frac{\partial}{\partial v} \overline{E}_z(u; \xi', v)\, d\xi' = -i\, k_0\, \mu_r\, \overline{H}_y(u; \xi, v) \tag{6}$$

$$\frac{\partial}{\partial u} \overline{H}_y(u; \xi, v) - \frac{d}{2\pi} \int_{-\pi/d}^{\pi/d} \bar{\dot{g}}(u; \xi - \xi')\, \frac{\partial}{\partial v} \overline{H}_y(u; \xi', v)\, d\xi' - \frac{\partial}{\partial v} \overline{H}_x(u; \xi, v) = -i\, k_0\, \varepsilon_r\, \overline{E}_z(u; \xi, v). \tag{7}$$

Since the transformed fields are pseudo-periodic in terms of u, they can be approximately expanded in the truncated generalized Fourier series. For example, the z-component of the E-field can be written as

$$\overline{E}_z(u; \xi, v) = \sum_{n=-N}^{N} \overline{E}_{z,n}(\xi, v)\, e^{i\, \alpha_n(\xi)\, u}, \qquad \alpha_n(\xi) = \xi + n\, \frac{2\pi}{d} \tag{8}$$

where N denotes the truncation order and $\overline{E}_{z,n}(\xi, v)$ are the nth-order generalized Fourier coefficients. To treat the coefficients systematically, we introduce $(2N + 1) \times 1$ column matrices; for example, the coefficients of $\overline{E}_z(u;\xi,v)$ are expressed by a column matrix $\overline{\boldsymbol{e}}_z(\xi,v)$ in such a way that nth-components are given by $\overline{E}_{z,n}(\xi,v)$. Then Eqs. (5)–(7) yield the following relations:

$$\frac{\partial}{\partial v}\,\overline{\boldsymbol{e}}_z(\xi,v) = i\,k_0\,\mu_r\,\overline{\boldsymbol{h}}_x(\xi,v) \tag{9}$$

$$\left(i\overline{\boldsymbol{X}}(\xi) - [\![\dot{g}_p]\!]\frac{\partial}{\partial v}\right)\overline{\boldsymbol{e}}_z(\xi,v) - \frac{d}{2\pi}\int_{-\pi/d}^{\pi/d}[\![\dot{\overline{g}}_a]\!](\xi-\xi')\,\frac{\partial}{\partial v}\,\overline{\boldsymbol{e}}_z(\xi',v)\,d\xi' = -i\,k_0\,\mu_r\,\overline{\boldsymbol{h}}_y(\xi,v) \tag{10}$$

$$\left(i\overline{\boldsymbol{X}}(\xi) - [\![\dot{g}_p]\!]\frac{\partial}{\partial v}\right)\overline{\boldsymbol{h}}_y(\xi,v) - \frac{d}{2\pi}\int_{-\pi/d}^{\pi/d}[\![\dot{\overline{g}}_a]\!](\xi-\xi')\,\frac{\partial}{\partial v}\,\overline{\boldsymbol{h}}_y(\xi',v)\,d\xi' - \frac{\partial}{\partial v}\,\overline{\boldsymbol{h}}_x(\xi,v) = -i\,k_0\,\varepsilon_r\,\overline{\boldsymbol{e}}_z(\xi,v) \tag{11}$$

where $\overline{\boldsymbol{X}}(\xi)$ is a diagonal matrix whose diagonal elements are $\alpha_n(\xi)$ and

$$\Big([\![\dot{g}_p]\!]\Big)_{n,m} = \frac{1}{d}\int_{-d/2}^{d/2}\dot{g}_p(u)\,e^{-i(n-m)\frac{2\pi}{d}\,u}\,du, \qquad \Big([\![\dot{\overline{g}}_a]\!](\xi)\Big)_{n,m} = \frac{1}{d}\int_{-d/2}^{d/2}\dot{\overline{g}}_a(u;\xi)\,e^{-i\,\alpha_{n-m}(\xi)\,u}\,du. \tag{12}$$

Equations (9)–(11) must be satisfied for arbitrary $\xi \in [-\pi/d, \pi/d]$. Here we take L sample points $\{\xi_l\}_{l=1}^{L}$ $(-\pi/d < \xi_1 < \xi_2 < \ldots < \xi_L \leqq \pi/d)$, and the convolution in Eqs. (10) and (11) is approximated by an appropriate numerical integration scheme. The sample points $\{\xi_l\}_{l=1}^{L}$ are chosen by the numerical integration scheme. Then Eqs. (9)–(11) give the following relations:

$$\frac{d}{dv}\,\widetilde{\boldsymbol{e}}_z(v) = i\,k_0\,\mu_r\,\widetilde{\boldsymbol{h}}_x(v) \tag{13}$$

$$i\,\widetilde{\boldsymbol{X}}\,\widetilde{\boldsymbol{e}}_z(v) - \widetilde{\boldsymbol{G}}\,\frac{d}{dv}\,\widetilde{\boldsymbol{e}}_z(v) = -i\,k_0\,\mu_r\,\widetilde{\boldsymbol{h}}_y(v) \tag{14}$$

$$i\,\widetilde{\boldsymbol{X}}\,\widetilde{\boldsymbol{h}}_y(v) - \widetilde{\boldsymbol{G}}\,\frac{d}{dv}\,\widetilde{\boldsymbol{h}}_y(v) - \frac{d}{dv}\,\widetilde{\boldsymbol{h}}_x(v) = -i\,k_0\,\varepsilon_r\,\widetilde{\boldsymbol{e}}_z(v) \tag{15}$$

with

$$\widetilde{\boldsymbol{e}}_z(v) = \begin{pmatrix}\overline{\boldsymbol{e}}_z(\xi_1,v)\\ \vdots \\ \overline{\boldsymbol{e}}_z(\xi_L,v)\end{pmatrix}, \qquad \widetilde{\boldsymbol{X}} = \begin{pmatrix}\overline{\boldsymbol{X}}(\xi_1) & & \boldsymbol{0}\\ & \ddots & \\ \boldsymbol{0} & & \overline{\boldsymbol{X}}(\xi_L)\end{pmatrix}, \tag{16}$$

$$\widetilde{\boldsymbol{G}} = \begin{pmatrix}\boldsymbol{G}_{1,1} & \cdots & \boldsymbol{G}_{1,L}\\ \vdots & \ddots & \vdots\\ \boldsymbol{G}_{L,1} & \cdots & \boldsymbol{G}_{L,L}\end{pmatrix}, \qquad \boldsymbol{G}_{l,l'} = \delta_{l,l'}\,[\![\dot{g}_p]\!] + \frac{d}{2\pi}\,w_{l'}\,[\![\dot{\overline{g}}_a]\!](\xi_l - \xi_{l'}), \tag{17}$$

where the definitions of $\widetilde{\boldsymbol{h}}_x(v)$ and $\widetilde{\boldsymbol{h}}_y(v)$ are similar to $\widetilde{\boldsymbol{e}}_z(v)$, and $\{w_l\}_{l=1}^{L}$ denotes the weight determined by the numerical integration scheme. After a simple calculation, Eqs. (13)–(15) yield the following differential equation set:

$$\begin{pmatrix}\widetilde{\boldsymbol{e}}_z(v)\\ -i\,\frac{d}{dv}\,\widetilde{\boldsymbol{e}}_z(v)\end{pmatrix} = -i\,\boldsymbol{M}_r\,\frac{d}{dv}\begin{pmatrix}\widetilde{\boldsymbol{e}}_z(v)\\ -i\,\frac{d}{dv}\,\widetilde{\boldsymbol{e}}_z(v)\end{pmatrix}, \qquad \boldsymbol{M}_r = \begin{pmatrix}-\widetilde{\boldsymbol{D}}_r\left(\widetilde{\boldsymbol{X}}\,\widetilde{\boldsymbol{G}} + \widetilde{\boldsymbol{G}}\,\widetilde{\boldsymbol{X}}\right) & \widetilde{\boldsymbol{D}}_r\left(\widetilde{\boldsymbol{G}}^2 + \boldsymbol{I}\right)\\ \boldsymbol{I} & 0\end{pmatrix} \tag{18}$$

where $\boldsymbol{I}$ denotes the identity matrix and $\widetilde{\boldsymbol{D}}_r = \left({k_0}^2\,\varepsilon_r\,\mu_r\,\boldsymbol{I} - \widetilde{\boldsymbol{X}}^2\right)^{-1}$. The general solution to the coupled differential equation set (18) is obtained by solving an eigenvalue-eigenvector problems because the $2L\,(2N+1)\times 2L\,(2N+1)$ matrices of coefficients $\boldsymbol{M}$ is constant. The $2L\,(2N+1)$ eigenvalues can be divided into two sets, each containing $L\,(2N+1)$ eigenvalues. The first set contains the negative real eigenvalues and the complex eigenvalues that have positive imaginary parts, and the second set contains those with the opposite signs. We denote the reciprocals of the eigenvalues of $\boldsymbol{M}$ by $\{\eta_{r,n}\}_{n=1}^{2L(2N+1)}$, in which $\{\eta_{r,n}\}_{n=1}^{L(2N+1)}$ is corresponding to the first set and $\{\eta_{r,n}\}_{n=L(2N+1)+1}^{2L(2N+1)}$ is corresponding to the second set. Here the covariant components of the H field in terms of u is given by $H_t = H_x + \dot{g}\,H_y$, which gives the tangential component of the H field on the grating surface $y = g(x)$. The generalized Fourier coefficients of $\overline{E}_z(u;\xi_l,v)$ and $\overline{H}_t(u;\xi_l,v)$ are expressed in the following form:

$$\begin{pmatrix}\widetilde{\boldsymbol{e}}_z(v)\\ \widetilde{\boldsymbol{h}}_t(v)\end{pmatrix} = \boldsymbol{Q}_{e,r}\begin{pmatrix}\boldsymbol{a}^{(-)}_{e,r}(v)\\ \boldsymbol{a}^{(+)}_{e,r}(v)\end{pmatrix} = \begin{pmatrix}\boldsymbol{Q}_{e,r,11} & \boldsymbol{Q}_{e,r,12}\\ \boldsymbol{Q}_{e,r,21} & \boldsymbol{Q}_{e,r,22}\end{pmatrix}\begin{pmatrix}\boldsymbol{a}^{(-)}_{e,r}(v)\\ \boldsymbol{a}^{(+)}_{e,r}(v)\end{pmatrix} \tag{19}$$

$$\boldsymbol{Q}_{e,r} = \begin{pmatrix}\boldsymbol{P}_{r,11} & \boldsymbol{P}_{r,12}\\ -\frac{1}{k_0\,\mu_r}\left[\widetilde{\boldsymbol{G}}\,\widetilde{\boldsymbol{X}}\,\boldsymbol{P}_{r,11} - \left(\boldsymbol{I}+\widetilde{\boldsymbol{G}}^2\right)\boldsymbol{P}_{r,21}\right] & -\frac{1}{k_0\,\mu_r}\left[\widetilde{\boldsymbol{G}}\,\widetilde{\boldsymbol{X}}\,\boldsymbol{P}_{r,12} - \left(\boldsymbol{I}+\widetilde{\boldsymbol{G}}^2\right)\boldsymbol{P}_{r,22}\right]\end{pmatrix} \tag{20}$$

where $\boldsymbol{a}^{(-)}_{e,r}(v)$ and $\boldsymbol{a}^{(+)}_{e,r}(v)$ are the amplitudes of the eigenmodes propagating in the positive and negative v-direction, respectively, and $\boldsymbol{P}_{r,nm}$ $(n,m = 1,2)$ are $L(2N+1)\times L(2N+1)$ block matrices contained in the eigenvector matrix, in which the nth eigenvector of $\boldsymbol{M}$, corresponding to the eigenvalue $1/\eta_{r,n}$, is stored in the nth column.

For the TM polarized fields, following the same manipulation with the TE case, the generalized Fourier coefficients of $\overline{E}_z(u;\xi_l,v)$ and $\overline{H}_t(u;\xi_l,v)$ are expressed in the following form:

$$\begin{pmatrix}\widetilde{\boldsymbol{h}}_z(v)\\ \widetilde{\boldsymbol{e}}_t(v)\end{pmatrix} = \boldsymbol{Q}_{h,r}\begin{pmatrix}\boldsymbol{a}^{(-)}_{h,r}(v)\\ \boldsymbol{a}^{(+)}_{h,r}(v)\end{pmatrix} = \begin{pmatrix}\boldsymbol{Q}_{h,r,11} & \boldsymbol{Q}_{h,r,12}\\ \boldsymbol{Q}_{h,r,21} & \boldsymbol{Q}_{h,r,22}\end{pmatrix}\begin{pmatrix}\boldsymbol{a}^{(-)}_{h,r}(v)\\ \boldsymbol{a}^{(+)}_{h,r}(v)\end{pmatrix} \tag{21}$$

$$\boldsymbol{Q}_{h,r} = \begin{pmatrix}\boldsymbol{P}_{r,11} & \boldsymbol{P}_{r,12}\\ \frac{1}{k_0\,\varepsilon_r}\left[\widetilde{\boldsymbol{G}}\,\widetilde{\boldsymbol{X}}\,\boldsymbol{P}_{r,11} - \left(\boldsymbol{I}+\widetilde{\boldsymbol{G}}^2\right)\boldsymbol{P}_{r,21}\right] & \frac{1}{k_0\,\varepsilon_r}\left[\widetilde{\boldsymbol{G}}\,\widetilde{\boldsymbol{X}}\,\boldsymbol{P}_{r,12} - \left(\boldsymbol{I}+\widetilde{\boldsymbol{G}}^2\right)\boldsymbol{P}_{r,22}\right]\end{pmatrix}. \tag{22}$$

In Eqs. (19)–(22), the subscripts e or h denotes the matrices depending on the polarization.

The general solutions separately obtained in the regions c and s can be matched at the grating surface: $v = 0$ $(y = g(x))$ by using the boundary conditions, which is given by the continuities of the tangential components of the electromagnetic fields. Then the scattering matrix that relate the amplitudes of the incident and the scattered fields is derived as

$$\begin{pmatrix}\boldsymbol{a}^{(+)}_{f,1}(0)\\ \boldsymbol{a}^{(-)}_{f,2}(0)\end{pmatrix} = \begin{pmatrix}\boldsymbol{S}_{f,11}\\ \boldsymbol{S}_{f,21}\end{pmatrix}\boldsymbol{a}^{(-)}_{f,1}(0) \tag{23}$$

with

$$\boldsymbol{S}_{f,11} = -\left(\boldsymbol{Q}_{f,2,11}\,\boldsymbol{Q}^{-1}_{f,2,21}\,\boldsymbol{Q}_{f,1,22} - \boldsymbol{Q}_{f,1,12}\right)^{-1}\left(\boldsymbol{Q}_{f,2,11}\,\boldsymbol{Q}^{-1}_{f,2,21}\,\boldsymbol{Q}_{f,1,21} - \boldsymbol{Q}_{f,1,11}\right) \tag{24}$$

$$\boldsymbol{S}_{f,21} = \boldsymbol{Q}^{-1}_{f,2,21}\left(\boldsymbol{Q}_{f,1,21} + \boldsymbol{Q}_{f,1,22}\,\boldsymbol{S}_{f,11}\right). \tag{25}$$

This relation make possible to calculate the scattered fields for known incident fields.

4. Conclusions

This paper has formulated the two-dimensional electromagnetic scattering from surface-relief grating with a defect. The formulation is based on the PPFT, which converts any function to a pseudo-periodic one, and the C-method. Numerical examples and discussions cannot be included in this paper because of page limitation, but they will be shown in the presentation. Anyway, the present formulation shows an ability of PPFT that enables the mediation between the electromagnetic problems on perfectly periodic and imperfectly periodic structures.

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