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COMPARATIVE STUDY OF INTEGRATION SCHEMES USED ON DIFFERENTIAL THEORY OF GRATINGS

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ABSTRACT

Several integration schemes are applied to the differential method for a sinusoidal-profiled surface-relief grating made of an anisotropic and conducting material. The numerical results show the importance of the numerical stability and the advantage of the implicit integration schemes.

DIFFERENTIAL THEORY OF GRATINGS

We investigate the diffraction problem on a surface-relief grating ruled on an anisotropic and homogeneous substrate schematically shown in Fig.1. The grating grooves are parallel to the z-axis and the equation of the grating surface is $y = p(x)$ where $p(x)$ is a known periodic function with the period d and the depth h. The region $y > p(x)$ is filled with a homogeneous and isotropic material described by the relative permittivity ε_1 and the relative permeability μ_1, and the homogeneous and anisotropic material that fills the region $y < p(x)$ is described by the relative permittivity matrix $\overline{\overline{\varepsilon_2}}$ and the relative permeability matrix $\overline{\overline{\mu_2}}$. We consider only time harmonic fields assuming a time-dependence in $\exp(-i\omega t)$, and deal with the plane incident wave propagating in the direction of polar angle θ and azimuth angle ϕ.

The differential theory [1,2] is one of the most commonly used approaches in the analyses of such gratings. Thanks to the periodic structure, the electromagnetic field compo

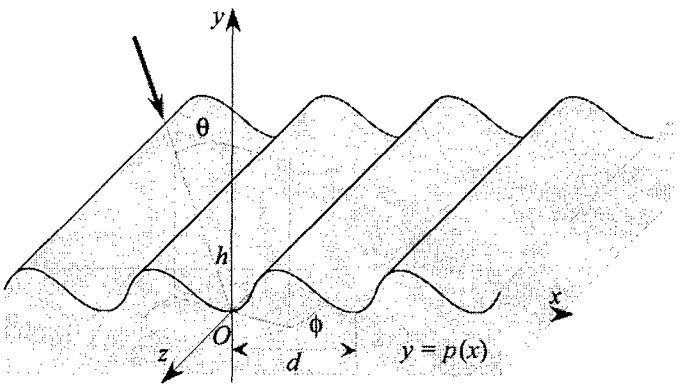


Figure 1: Geometry of the surface-relief grating under consideration.

nents can be approximately expanded in the truncated generalized Fourier series [2]; for example the x-component of $\boldsymbol{E}$ field can be written as

$$E_x(x,y,z) = \sum_{n=-N}^{N} E_{x,n}(y)\exp[i(\alpha_n x + \gamma z)] \tag{1}$$

with

$$\alpha_n = k_1 \sin\theta \cos\phi + n\frac{2\pi}{d}, \quad \gamma = k_1 \sin\theta \sin\phi \tag{2}$$

where N is the truncation order, k_1 is the wavenumber in the region $y > p(x)$, and $E_{x,n}(y)$ are the nth-order generalized Fourier coefficients which are functions of y only. Replacing all the periodic and the pseudo-periodic functions by their Fourier series and using the Fourier factorization rules [3], Maxwell's curl equations are transformed into a coupled differential equation set in the form of

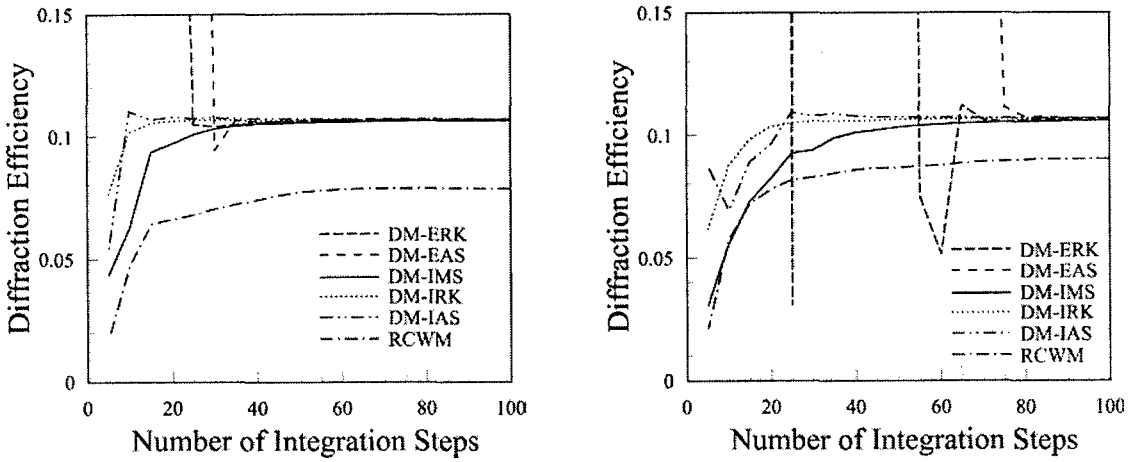
$$\frac{d}{dy}\begin{pmatrix} \boldsymbol{e}_x(y) \\ \boldsymbol{e}_z(y) \\ \boldsymbol{h}_x(y) \\ \boldsymbol{h}_z(y) \end{pmatrix} = \boldsymbol{M}(y)\begin{pmatrix} \boldsymbol{e}_x(y) \\ \boldsymbol{e}_z(y) \\ \boldsymbol{h}_x(y) \\ \boldsymbol{h}_z(y) \end{pmatrix} \tag{3}$$

where, for example, $\boldsymbol{e}_x(y)$ denotes a $(2N+1)\times 1$ column matrix generated by the Fourier coefficients of E_x and $\boldsymbol{M}(y)$ is the coupling coefficient matrix. Then, the scattering problem of grating is reduced to an integration problem of the coupled differential equation set with boundary conditions at the top and the bottom of the groove region.

NUMERICAL RESULTS OF VARIOUS INTEGRATION SCHEMES

One method for integrating the coupled differential equation set (3) is the rigorous coupled-wave method, which introduces the staircase approximation to describe arbitrary profiled gratings. The real profile in each step is replaced by the structure uniform in the y-direction, and then the boundary-value problem can easily be turned into an eigenvalue problem because of the absence of the y-dependence. Another approach is based on the shooting method, which can transform the boundary-value problem into the initial-value one. The initial-value problem can be solved by usual numerical integration schemes. In the narrow sense, this approach is called the differential method. In the method, the Runge-Kutta or the predictor-corrector Adams schemes are suggested for integration [2,4].

Here, several numerical integration schemes are applied to the differential method for a sinusoidal grating made of conducting material and the convergences of the TM diffraction efficiencies in -1st-order with respect to the number of the integration steps are compared in Fig.2. The grating parameters are chosen as follows: $\lambda_0 = 0.6328\,\mu m$, $\theta = 30°$, $\phi = 20°$, $d = 0.6\,\mu m$, $h = 0.5\,\mu m$, $p(x) = (h/2)[1+\cos(2\pi x/d)]$, $\varepsilon_1 = \mu_1 = 1$, $\varepsilon_{2,xx} = \varepsilon_{2,yy} = \varepsilon_{2,zz} = -8.19 + i16.38$, $\varepsilon_{2,xz} = -\varepsilon_{2,zx} = -0.495 - i0.106$, $\varepsilon_{2,xy} = \varepsilon_{2,yx} = \varepsilon_{2,yz} = \varepsilon_{2,zy} = 0$, $\overline{\overline{\boldsymbol{\mu}_2}} = \boldsymbol{I}$, and TM ($H_y = 0$) polarized incident plane wave. To avoid the numerical difficulty for deep gratings, we used the scattering matrix propagation al



(a) $N = 10$ (b) $N = 25$

Figure 2: Convergences of diffraction efficiencies computed using various integration schemes (DM: differential method, RCWM: rigorous coupled-wave method, ERK: classical fourth-order Runge-Kutta scheme, EAS: predictor-corrector Adams scheme, IMS implicit midpoint scheme, IRK: implicit fourth-order Runge-Kutta scheme, IAS: implicit Adams-Moulton scheme).

gorithm [5]. The rigorous coupled-wave method shows stable convergence but does not give reliable solutions for such a conductive grating as reported in Ref.[4,6]. The explicit schemes (ERK, EAS) show serious numerical instabilities and require large number of integration steps for reliable solutions. On the other hand, the implicit schemes (IMS, IRK, IAS) are numerically stable even when the number of integration steps is small. Consequently, the use of implicit schemes reduces greatly the computation time and is highly suggested.

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