Efficient and Stable Implementation of RCWA for Ultrathin Multilayer Gratings: *T*-Matrix Approach Without Solving Eigenvalues

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***Abstract*—Based on the transmittance matrix (*T*-matrix) approach, an efficient and stable rigorous coupled-wave analysis (RCWA) method for ultrathin multilayer gratings without solving eigenvalues is proposed in this letter. The numerical instability caused by the inversion of an ill-conditioned matrix in the traditional *T*-matrix approach is solved by implementing the proposed method. Besides, compared with the traditional RCWA method, the proposed method does not need to solve the eigenvalues and eigenvectors of the eigenmatrix, which avoids the numerical problems and time-consuming problems caused by this process. A numerical example shows that the results of CST simulations are consistent with the results obtained by the proposed method.**

***Index Terms*—Eigenvalues, rigorous coupled-wave analysis (RCWA), transmittance matrix (*T*-matrix) approach, ultrathin multilayer gratings.**

I. Introduction

MULTILAYER gratings, especially ultrathin multilayer gratings, are widely used in terahertz and microwave bands. Chao *et al.* proposed an ultrathin plasmonic multilayer structure containing a metallic grating as a light trap for the PV cell. The results calculated by the rigorous coupled-wave analysis (RCWA) method show that compared with the ITO/α-Si/Ag structure, the number of photons absorbed by this structure increases by 28.7% under a normal incident transverse magnetic (TM) polarized wave [1]. Wu *et al.* fabricated and tested a wideband reflector consisting of a multilayer-based grating structure with a multisubpart profile. The reflector can offer the combined merits of high reflectivity over a wideband spectrum and good angular bandwidth [2]. Liu *et al.* demonstrated a designable infrared narrowband absorber by using an ultrathin Al/Si multilayer grating structure [3], [4]. Mao *et al.* presented a THz polarizer with high-polarization extinction ratio and transmittance by using multilayer subwavelength metal gratings filled in a polyimide film [5]. Huang *et al.* proposed a low optical contrast multilayer grating to develop highly efficient narrow-bandwidth multilayer optics for the soft X-ray spectroscopy [6]. In the methods of analyzing ultrathin multilayer gratings, RCWA is the most widely used one [7]–[13]. According to the different boundary condition equations, the RCWA method for analyzing multilayer gratings can be divided into the *R*-matrix propagation algorithm [11], [13], the enhanced transmittance matrix (*T*-matrix) approach [12], *S*-matrix propagation algorithm [13], [14], and *H*-matrix algorithm [15]. The *S*-matrix and *R*-matrix algorithms have inherent stability for avoiding the exponential growth submatrices in the recursive formulas. However, when factorization is impossible, the *S*-matrix and *R*-matrix algorithms are stable only when the layer thicknesses and the truncation order are low. The *T*-matrix algorithm for RCWA itself is numerically unstable, so Moharam *et al.* [12] proposed the enhanced *T*-matrix approach to improve its numerical stability. Tan [15] puts forward the *H*-matrix algorithm based on the above methods, and the *H*-matrix algorithm can be derived from the enhanced *T*-matrix approach. It is worth noting that for ultrathin multilayer gratings, especially for those with metal grating layers, a large truncation order is needed for obtaining more accurate calculation results. This means that the dimension of the eigenmatrix will be so large that it will become very difficult and time-consuming or even impossible to solve the eigenvalues of the eigenmatrix. Unfortunately, all the above methods need to solve the eigenvalues of the eigenmatrix.

In this letter, an efficient and stable RCWA method for ultrathin multilayer gratings without solving eigenvalues is proposed. In Section II, the basic formulations of RCWA for multilayer gratings using the *T*-matrix approach are presented. In Section III, the first-order Taylor expansion is used to simplify the original executive equation. A more efficient and stable method is proposed, which involves nor eigenvalues but only the eigenmatrix. Section IV provides numerical evidence that the new method is effective and is consistent with CST simulations. Finally, concluding remarks are given in Section V.

II. Basic Formulations of RCWA

In this section, the basic formulations of RCWA based on the *T*-matrix approach for multilayer gratings are given. The geometry of the multilayer grating diffraction problem is depicted in Fig. 1. A linearly polarized electromagnetic wave is incident at an angle θ. The grating periodic along the x-direction with Λ as a period and f_l as the duty cycle of the lth layer with depth d_l. The z-axis is perpendicular to the boundaries, and the

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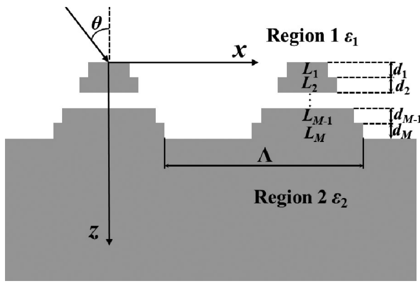

Fig. 1. Geometry for the multilayer grating diffraction problem.

diffraction problem is invariant in the *y*-direction. The grating region is bound by two different media with relative permittivity ε_1 and ε_2, and the permeability is μ_0.

A linearly polarized electromagnetic wave can be decomposed into transverse electric (TE) and TM components. TE polarization is taken as an example in this section (extension to TM polarization is straightforward), and the RCWA is derived as follows. The incident reflected diffracted and transmitted diffracted fields in Regions 1 and 2 are given by

$$E_{1,y} = e^{-jk_0 n_1(\sin\theta x - \cos\theta z)} + \sum_{i=-\infty}^{+\infty} R_i(z) e^{-j(k_{xi}x - k_{1,zi}z)}$$

$$E_{2,y} = \sum_{i=-\infty}^{+\infty} T_i(z) e^{-j(k_{xi}x + k_{2,zi}(D^M - z))} \tag{1}$$

where k_0 is the wavenumber in air, R_i and T_i are unknown components and

$$k_{p,zi} = \begin{cases} (k_0^2 n_p^2 - k_{xi}^2)^{0.5} & k_0 n_p > k_{xi} \\ -j(k_{xi}^2 - k_0^2 n_p^2)^{0.5} & k_0 n_p < k_{xi}. \end{cases}, p = 1, 2. \tag{2}$$

k_{xi} is determined from the Floquet condition and is given by

$$k_{xi} = k_0 n_1 \sin\theta - i^{2\pi}/_{\Lambda}. \tag{3}$$

The periodic relative permittivity of the *l*th grating layer region can be expanded to a Fourier series of the form as follows:

$$\varepsilon^l(x) = \sum_{h=-\infty}^{+\infty} \varepsilon_h^l e^{j\frac{2\pi}{\Lambda}hx}, D^l - d_l < z < D^l = \sum_{p=1}^{l} d_l \tag{4}$$

where $\varepsilon^l{}_h$ is the *h*th Fourier coefficient of $\varepsilon^l(x)$.

Using the Fourier expansion in terms of space harmonic fields, the tangential electric field $E^l{}_{gy}$ and magnetic field $H^l{}_{gx}$ in the *l*th grating layer region may be expressed as

$$E_{gy}^l = \sum_{i=-\infty}^{+\infty} S_{yi}^l(z) e^{-jk_{xi}x} \tag{5}$$

$$H_{gx}^l = -j\sqrt{\varepsilon_0/\mu_0} \sum_{i=-\infty}^{+\infty} U_{xi}^l(z) e^{-jk_{xi}x} \tag{6}$$

where $S^l{}_{yi}$ and $U^l{}_{xi}$ represent the normalized amplitudes of the *i*th space harmonic fields of $E^l{}_{gy}$ and $H^l{}_{gx}$, respectively, and *j* is the imaginary unit.

Maxwell's curl equations in *l*th grating layer region are

$$\partial E_{gy}^l / \partial z = j\omega\mu_0 H_{gx}^l \tag{7}$$

$$\partial H_{gx}^l / \partial z - \partial H_{gz}^l / \partial x = j\omega\varepsilon_0\varepsilon^l(x) E_{gy}^l. \tag{8}$$

Substituting (5) and (6) into (7) and (8) and eliminating $H^l{}_{gz}$, the coupled-wave equations can be expressed as

$$\left[\partial^2 S_y^l \middle/ \partial(z')^2\right] = \left[\Phi^l\right]\left[S_y^l\right] \tag{9}$$

where $z' = k_0 z$ and

$$\Phi^l = K_x^2 - E^l \tag{10}$$

where K_x is an $N \times N$ diagonal matrix with the elements k_{xi}/k_0, and E^l is an $N \times N$ Toeplitz matrix with the *i, p* element being equal to $\varepsilon^l{}_{i-p}$, *N* is the number of truncation orders.

Solving (9), $S^l{}_{yi}$ and $U^l{}_{xi}$ in the *l*th grating layer region are given by

$$S_{yi}^l(z) = \sum_{m=1}^{N} \omega_{i,m}^l \left\{ e^{-k_0 q_m^l (z - D^l + d_l)} \cdot \varphi_m^{l+} + e^{k_0 q_m^l (z - D^l)} \cdot \varphi_m^{l-} \right\} \tag{11}$$

$$U_{xi}^l(z) = \sum_{m=1}^{N} \nu_{i,m}^l \left\{ -e^{-k_0 q_m^l (z - D^l + d_l)} \cdot \varphi_m^{+} + e^{k_0 q_m^l (z - D^l)} \cdot \varphi_m^{-} \right\} \tag{12}$$

where $\omega^l{}_{i,m}$ and $q^l{}_m$ are the components of eigenvector matrix Ω^l and diagonal matrix Q^l composed by positive square roots of eigenvalues of eigenmatrix Φ^l, respectively. $\nu^l{}_{i,m}$ is the element of matrix N^l, where $N^l = \Omega^l Q^l$. The quantities $\varphi^{l+}{}_m$ and $\varphi^{l-}{}_m$ are unknown constants to be determined from boundary conditions.

By matching the tangential electric-field and magnetic-field components at different boundaries, the following equations can be obtained. At the boundary $z = 0$, we have

$$\begin{bmatrix} \delta_{i0} \\ jn_1\cos\theta\delta_{i0} \end{bmatrix} + \begin{bmatrix} I \\ -jZ_1 \end{bmatrix}[R] = \begin{bmatrix} \Omega^1 & \Omega^1\Gamma^1 \\ N^1 & -N^1\Gamma^1 \end{bmatrix} \begin{bmatrix} \varphi^{1+} \\ \varphi^{1-} \end{bmatrix} \tag{13}$$

at the boundaries between the (*l*–1)th and the *l*th grating layers

$$\begin{bmatrix} \Omega^{l-1}\Gamma^{l-1} & \Omega^{l-1} \\ N^{l-1}\Gamma^{l-1} & -N^{l-1} \end{bmatrix} \begin{bmatrix} \varphi^{(l-1)+} \\ \varphi^{(l-1)-} \end{bmatrix} = \begin{bmatrix} \Omega^l & \Omega^l\Gamma^l \\ N^l & -N^l\Gamma^l \end{bmatrix} \begin{bmatrix} \varphi^{l+} \\ \varphi^{l-} \end{bmatrix} \tag{14}$$

at the boundary $z = D^M$

$$\begin{bmatrix} I \\ jZ_2 \end{bmatrix}[T] = \begin{bmatrix} \Omega^M\Gamma^M & \Omega^M \\ N^M\Gamma^M & -N^M \end{bmatrix} \begin{bmatrix} \varphi^{M+} \\ \varphi^{M-} \end{bmatrix} \tag{15}$$

where Γ^l is a diagonal matrix with the diagonal elements exp($-k_0 d_l q^l{}_m$). Z_1, Z_2 are diagonal matrices with elements $k_{1,zi}/k_0$ and $k_{2,zi}/k_0$. *I* is an identity matrix, $\delta_{i0} = 1$ for $i = 0$, and $\delta_{i0} = 0$ for $i \neq 0$. The standard *T*-matrix method solves the unknown components by cascading (13)–(15) as

$$\begin{bmatrix} \delta_{i0} \\ jn_1\cos\theta\delta_{i0} \end{bmatrix} + \begin{bmatrix} I \\ -jZ_1 \end{bmatrix}[R] = \prod_{l=1}^{M} \begin{bmatrix} \Omega^l & \Omega^l\Gamma^l \\ N^l & -N^l\Gamma^l \end{bmatrix} \begin{bmatrix} \Omega^l\Gamma^l & \Omega^l \\ N^l\Gamma^l & -N^l \end{bmatrix}^{-1} \begin{bmatrix} I \\ jZ_2 \end{bmatrix}[T]. \tag{16}$$

It should be noted that the inversion of ill-conditioned transmittance matrices cannot be represented with sufficient accuracy due to the finite precision of common computers. This problem is caused by very small terms in the diagonal matrix Γ^l when some of the generally complex eigenvalues have a large or small positive real part.

III. New Formulation of the Proposed Method

Attempts to solve (16) for determining [T] and [R] will probably cause numerical instability. This problem restricts the development of the T-matrix method in RCWA. In this section, based on the first-order Taylor expansion, a new method for ultrathin multilayer gratings without solving eigenvalues will be proposed to implement the coupled-wave formulation.

Equation (16) can be rewritten as

$$\begin{bmatrix} \delta_{i0} \\ jn_1\cos\theta\delta_{i0} \end{bmatrix} + \begin{bmatrix} I \\ -jZ_1 \end{bmatrix}[R] = \prod_{l=1}^{M}\begin{bmatrix} \Omega^l & \Omega^l \\ N^l & -N^l \end{bmatrix}\begin{bmatrix} \Gamma^{l^{-1}} & \\ & \Gamma^l \end{bmatrix}\begin{bmatrix} \Omega^l & \Omega^l \\ N^l & -N^l \end{bmatrix}^{-1}\begin{bmatrix} I \\ jZ_2 \end{bmatrix}[T]. \quad (17)$$

Generally, when $k_0d<<1$, the depth d can be regarded as ultrathin. When $d<10^{-3}\lambda_0$, where λ_0 is the wavelength in air, the method proposed in this letter is applicable. Of course, when the required accuracy of the calculation results is reduced, $d<10^{-2}\lambda_0$ can also be regarded as ultrathin. Considering ultrathin multilayer gratings, $\exp(\pm k_0d_lq^l{}_m)$ can be expanded as

$$e^{\pm k_0d_lq_m^l} \sim 1 \pm k_0d_lq_m^l. \quad (18)$$

Therefore, matrix Γ^l and its inverse can be replaced by

$$\Gamma^l = I - k_0d_lQ^l, \quad \Gamma^{l^{-1}} = I + k_0d_lQ^l. \quad (19)$$

The right-hand side of (17) can be rewritten as

$$\begin{bmatrix} \Omega^l & \Omega^l \\ N^l & -N^l \end{bmatrix}\begin{bmatrix} \Gamma^{l^{-1}} & \\ & \Gamma^l \end{bmatrix}\begin{bmatrix} \Omega^l & \Omega^l \\ N^l & -N^l \end{bmatrix}^{-1} = \frac{1}{2}\begin{bmatrix} \Omega^l\left(\Gamma^{l^{-1}}+\Gamma^l\right)\Omega^{l^{-1}} & \Omega^l\left(\Gamma^{l^{-1}}-\Gamma^l\right)N^{l^{-1}} \\ N^l\left(\Gamma^{l^{-1}}-\Gamma^l\right)\Omega^{l^{-1}} & N^l\left(\Gamma^{l^{-1}}+\Gamma^l\right)N^{l^{-1}} \end{bmatrix}. \quad (20)$$

According to the relationship between the eigenmatrix and its eigenvalues, the submatrix of (20) can be simplified as

$$\begin{aligned} \Omega^l\left(\Gamma^{l^{-1}}+\Gamma^l\right)\Omega^{l^{-1}} &= \Omega^l(2I)\Omega^{l^{-1}} = 2I \\ \Omega^l\left(\Gamma^{l^{-1}}-\Gamma^l\right)N^{l^{-1}} &= \Omega^l\left(2k_0d_lQ^l\right)Q^{l^{-1}}\Omega^{l^{-1}} = 2k_0d_lI \\ N^l\left(\Gamma^{l^{-1}}-\Gamma^l\right)\Omega^{l^{-1}} &= \Omega^lQ^l\left(2k_0d_lQ^l\right)\Omega^{l^{-1}} = 2k_0d_l\Phi^l. \end{aligned} \quad (21)$$

Substituting (21) into (20), there is

$$\frac{1}{2}\begin{bmatrix} \Omega^l\left(\Gamma^{l^{-1}}+\Gamma^l\right)\Omega^{l^{-1}} & \Omega^l\left(\Gamma^{l^{-1}}-\Gamma^l\right)N^{l^{-1}} \\ N^l\left(\Gamma^{l^{-1}}-\Gamma^l\right)\Omega^{l^{-1}} & N^l\left(\Gamma^{l^{-1}}+\Gamma^l\right)N^{l^{-1}} \end{bmatrix} = \begin{bmatrix} I & k_0d_lI \\ k_0d_l\Phi^l & I \end{bmatrix}. \quad (22)$$

Substituting (22) into (17) and (17) may be reformulated as

$$\begin{bmatrix} \delta_{i0} \\ jn_1\cos\theta\delta_{i0} \end{bmatrix} + \begin{bmatrix} I \\ -jZ_1 \end{bmatrix}[R] = \prod_{l=1}^{M}\begin{bmatrix} I & k_0d_lI \\ k_0d_l\Phi^l & I \end{bmatrix}\begin{bmatrix} I \\ jZ_2 \end{bmatrix}[T]. \quad (23)$$

Comparing (23) with (16), the following points can be drawn.

1) There is no inverse process on the right-hand side of (23), which can effectively avoid the numerical error caused by the inverse process on the right-hand side of (16).
2) Equation (23) is only related to the eigenmatrix Φ^l of each grating layer, it has nothing to do with its eigenvalues and eigenvectors.
3) The matrix cascade part on the right-hand side of (23) can be calculated quite easily by matrix multiplication, which is much simpler than the executive equation formed by the traditional T-matrix approach.

The advantage of this execution equation is that it does not need to solve eigenvalues and eigenvectors. Thus, it will be more efficient and stable to solve R_i and T_i by solving (23). Then, the diffraction efficiency of each diffraction order can be obtained by using

$$\begin{aligned} DE_{ri} &= R_iR_i^*\mathrm{Re}\left(\frac{k_{1,zi}}{k_0n_1\cos\theta}\right) \\ DE_{ti} &= T_iT_i^*\mathrm{Re}\left(\frac{k_{2,zi}}{k_0n_1\cos\theta}\right) \end{aligned} \quad (24)$$

where DE_{ri} and DE_{ti} represent the forward and backward diffraction efficiency of the ith order, respectively, R_i^* and T_i^* denote the conjugate amplitudes of the diffracted fields R_i and T_i.

For lossless gratings, conservation of energy is a necessary criterion for the numerical stability of the algorithm and is defined by

$$\sum_i DE_{ri} + DE_{ti} = 1. \quad (25)$$

It is worth pointing out that the accuracy of the diffraction efficiency of each order cannot be guaranteed by satisfying the condition of energy conservation. The accuracy of a single order diffraction efficiency depends on the number of spatial harmonics retained in the field expansion. For lossy gratings, the condition that the diffraction efficiency of each order remains constant with the increase of the truncation orders is a better criterion to judge the numerical stability.

IV. Numerical Validation

To validate the accuracy of the proposed algorithm, a three-layers ultrathin multilayer grating is selected to compare the calculation results of the proposed method of this letter with the results of the CST simulations. The three-layers ultrathin multilayer grating is surrounded by air and the geometry is illustrated in Fig. 2. To prove the effectiveness of the proposed method, the forward and backward diffraction coefficients of TE polarization and TM polarization under normal and oblique incidence ($\theta = 30°$) calculated by the proposed method are used

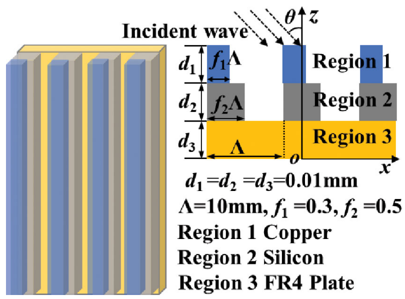

Fig. 2. Geometry of the three-layers ultrathin multilayer grating.

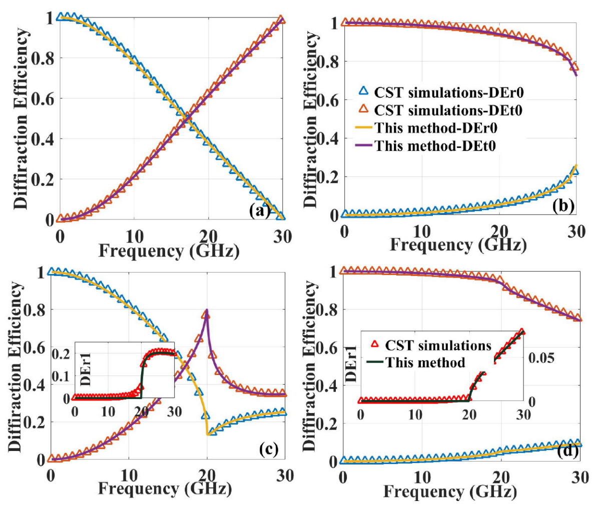

Fig. 3. Diffraction efficiency of the three-layers ultrathin multilayer grating. Solid line, the method proposed in this letter. Triangular, the CST simulations. (a) TE polarization under normal incidence. (b) TM polarization under normal incidence. (c) TE polarization under oblique incidence. (d) TM polarization under oblique incidence.

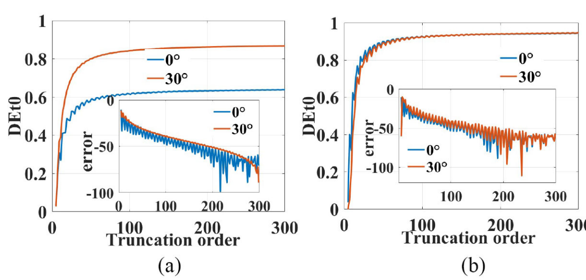

Fig. 4. Zero-order forward diffraction efficiency of the three-layers ultrathin multilayer grating. (a) TE polarization. (b) TM polarization.

to compare with that of the CST simulations. Fig. 3 shows the results of the proposed method and CST simulations.

To quantify the convergence rate and numerical stability of the proposed method, the zero-order forward diffraction efficiency DE_{t0} of 20 GHz is chosen as an example and the error shown in Fig. 4 is defined as

$$\mathrm{error}(N) = 20\lg\left|{DE_{t0}}^{N} - {DE_{t0}}^{N\max}\right| \tag{26}$$

where ${DE_{t0}}^{N}$ denotes the zero-order forward diffraction efficiency corresponding to N and ${DE_{t0}}^{N\max}$ is a reference value that is calculated when $N = 301$. The specific values of DE_{t0} under different truncation orders and the comparison with CST simulation results are shown in Table I.

TABLE I
DIFFRACTION EFFICIENCY UNDER DIFFERENT TRUNCATION ORDER

Polarization	TE		TM	
Incident angle	0	30	0	30
N=21	0.4808	0.6590	0.8180	0.7687
N=51	0.5916	0.8002	0.8998	0.8934
N=101	0.6146	0.8432	0.9247	0.9238
N=201	0.6321	0.8618	0.9418	0.9408
N=301	0.6352	0.8675	0.9453	0.9439
CST Simulations	0.6347	0.8159	0.9458	0.9440

As shown in Fig. 3 and Table I, the results yielded by the method proposed in this letter and CST simulations are in good agreement with each other. It can be found that the calculated data in Table I show that when TE polarization is obliquely incident, the results obtained by CST are slightly different from those obtained by the proposed method. The main reason for this is that the results of high-order diffraction efficiency are different, as clearly shown in Fig. 3(c). Judging from the conditions to produce high-order diffraction efficiency, when θ is 30° and Λ is 10 mm, the first-order diffraction will only occur when the frequency is greater than 20 GHz. From this judgment condition, the method proposed in this letter is more accurate than that of CST simulations. Similarly, from the results provided in Fig. 4 and Table I, for such a three-layers ultrathin grating, a large N is needed to obtain more accurate results. This means that the dimension of the eigenmatrix Φ^{l} will be so large that it will be quite difficult and challenging to solve its eigenvalues and eigenvectors. In this case, the advantage of the proposed algorithm that it does not solve the eigenvalues is obvious.

V. CONCLUSION

In this letter, based on the T-matrix approach and the first-order Taylor expansion, a stable and efficient RCWA algorithm for ultrathin multilayer gratings without solving eigenvalues is proposed. The proposed algorithm solves the forward and backward diffraction efficiency of each order by using the eigenmatrix, which can effectively solve the problem that solving eigenvalues is time-consuming and difficult when a large truncation order is needed. Compared with the traditional method, the proposed method is relatively simple and does not involve the inverse process of the cascade matrix, so it can stably solve the diffraction problem of ultrathin multilayer gratings. The calculation results of the three-layers ultrathin multilayer grating show that the proposed method is in good agreement with those obtained by the CST simulations.

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