SOME STUDIES ON THE DIFFERENTIAL THEORY OF HIGHLY CONDUCTING LAMELLAR GRATINGS

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1 Statement of the Problem

Let us consider plane wave diffraction by a lamellar grating ruled on a substrate schematically shown in Fig. 1. The grating grooves are parallel to the z-axis, and the direction of periodicity is parallel to the x-axis. We denote the grating period by d, the grating depth by h, and the groove width by g. We consider time-harmonic fields, assuming a time dependence in $\exp(-i\,\omega\,t)$, and the fields are therefore represented by complex vectors depending only on the space variables x, y, and z. A plane wave is assumed to be incident in the plane of incidence perpendicular to the z-axis, and the incident angle is denoted by θ. The substrate under consideration is a linear isotropic medium with the refractive index n_s and the permeability of free space, and the cover region is assumed to be free space.

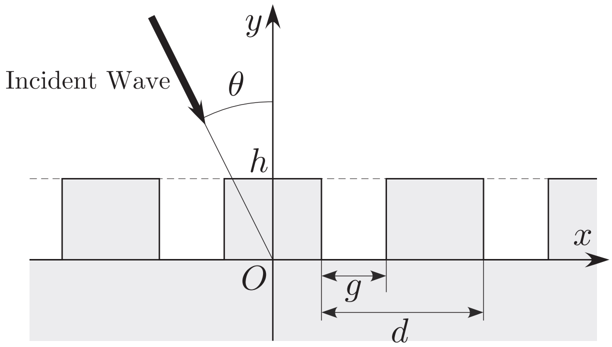

Fig. 1: Geometry of a lamellar grating under consideration.

This is a fundamental problem and many approaches have been proposed. One of the most commonly used approaches is the differential theory [1] because of its simplicity and wide applicability. The electromagnetic field components are pseudo-periodic functions, and they can be approximately expanded in truncated generalized Fourier series. Replacing all the periodic and pseudo-periodic functions by their Fourier series, the Maxwell equations yield a coupled differential equation set (CDES) for the Fourier coefficients of field components. The electromagnetic fields outside the groove region can be approximately expressed by the truncated Rayleigh expansions, and therefore the solution obtained inside the groove region is matched to the Rayleigh expansions at the top and the bottom of the grooves. This theory is very powerful and efficient for many types of grating. However, gratings that is deep and made of conducting materials cause problems because of the poor convergence. The origin of the difficulty, which was explained by Li [2], is the Fourier factorization rules applied to derive the CDES. He suggested three Fourier factorization rules and many papers have showed their validity.

However, Popov *et al.* [3] have recently discovered problems with use of silver and gold gratings in the near-infrared region even when the CDES is derived based on Li's Fourier factorization rules. The refractive index of gold reaches the value $0.1 + i\,10$ in the near-infrared region, and the real part of the value decreases for shorter wavelength. Figure 2 shows numerical results of a highly conducting grating made of artificial substrate with $n_s = 0 + i\,10$. The -1st-order diffraction efficiencies are computed by using the rigorous coupled-wave method (RCWM) [4, 5] as function of the groove width g. The grating parameters are same as Ref. [3]: $d = h = 500\,\text{nm}$, $\lambda_0 = 632.8\,\text{nm}$, $\theta = 30°$, and TM polarized (H-field is parallel to the z-axis) incident plane wave. We use the truncation order $N = 15$ that determines the number of

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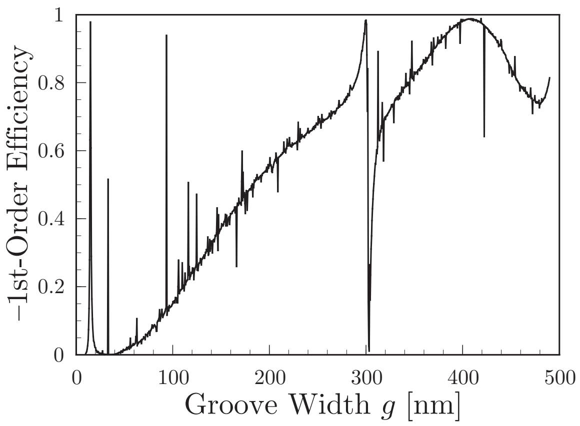

Fig. 2: −1st-order diffraction efficiency of a lamellar grating with refractive index of the material $n_s = 0 + i\,10$ as a function of the groove width g for the following parameters: $d = h = 500\,\mathrm{nm}$, $\lambda_0 = 632.8\,\mathrm{nm}$, $\theta = 30°$, $N = 15$, and TM incident plane wave.

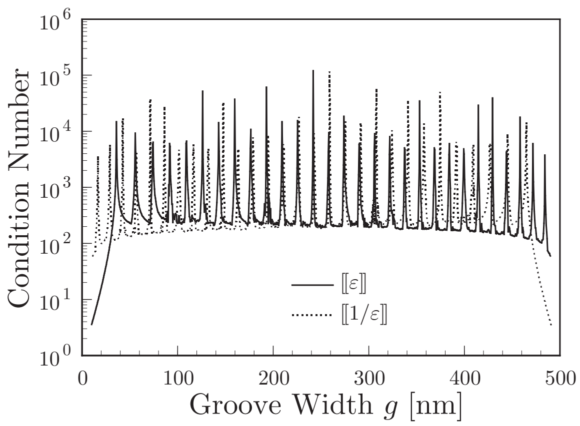

Fig. 3: Condition number of the Toeplitz matrices $[\![\varepsilon]\!]$ and $[\![1/\varepsilon]\!]$ as a function of the groove width g. All parameters are same as in Fig. 2.

Fourier coefficients (equal to $2N + 1$), and the efficiencies are computed for 1001 values of the groove width from 10 nm to 490 nm with identical intervals. The RCWM is a variant of the differential theory, in which the CDES is solved as an eigenvalue problem. Unfortunately, Popov *et al.* did not describe their computation procedure properly and it is impossible to obtain the same results. The RCWM procedure used in this paper is presented in Ref. [6], and then the numerical results in Fig. 2 are some different from those in Fig. 3(a) of Ref. [3]. Anyway, we observe similarly many unphysical artifacts due to numerical instability.

Let $\varepsilon(x)$ denote the relative permittivity distribution inside the groove region $0 < y < h$. Also, $[\![\varepsilon]\!]$ and $[\![1/\varepsilon]\!]$ denote $(2N + 1) \times (2N + 1)$ Toeplitz matrices generated by the Fourier coefficients of $\varepsilon(x)$ and $1/\varepsilon(x)$ in such a way that their (n, m)-entries are the $(n - m)$th-order Fourier coefficients. The RCWM based on Li's Fourier factorization rules requires inversion calculation of $[\![\varepsilon]\!]$ and $[\![1/\varepsilon]\!]$. Popov *et al.* calculated the condition number of $[\![\varepsilon]\!]$ (though they showed reciprocal values by mistake) and explained that its inversion calculation produces the numerical artifacts. Figure 3 shows estimated values of the L_1 condition number of the Toeplitz matrices $[\![\varepsilon]\!]$ and $[\![1/\varepsilon]\!]$ computed as function of the groove width g for the same parameters as Fig. 2. The condition numbers become certainly larger than 10^3 for many values of the groove width and sometimes go as large as 10^5. However, it is difficult to say that the inversion calculations are the direct reason of the numerical artifacts because the values in Fig. 2 are obtained by double-precision computation. Additionally, the positions of numerical artifacts do not agree with those with large condition number.

2 Stability of CDES Solvers with Large Truncation Order

It is well know that large truncation order is required in the analyses of conducting gratings. However, numerical experiments in Fig. 2 may abandon to overflow when the truncation order N is larger than 40. Trouble comes from the accumulation of contamination linked with growing exponential functions when the field is computed over the entire groove region. A simple way to get rid of this problem is to use the scattering-matrix propagation algorithm (SMPA) [7, 8]. The groove region $0 < y < h$ is decomposed into M layers so that the thickness of each layer is small enough to avoid the instability. Then, the scattering-matrix for the entire region can be derived by recursive calculation of the transmission matrices of the layers. Figure 4 shows the −1st-order diffraction efficiencies of the same grating as Fig. 2, but computed by the RCWM with the help of SMPA for $N = 100$ and $M = 100$. It is observed that number of the numerical

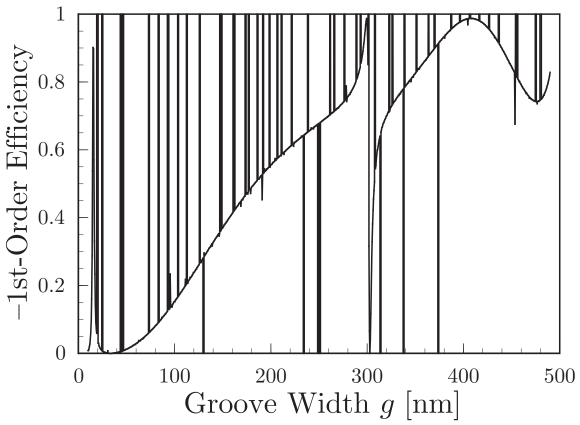

Fig. 4: Same as in Fig. 2, but computed by the RCWM with SMPA for $N = 100$ and $M = 100$.

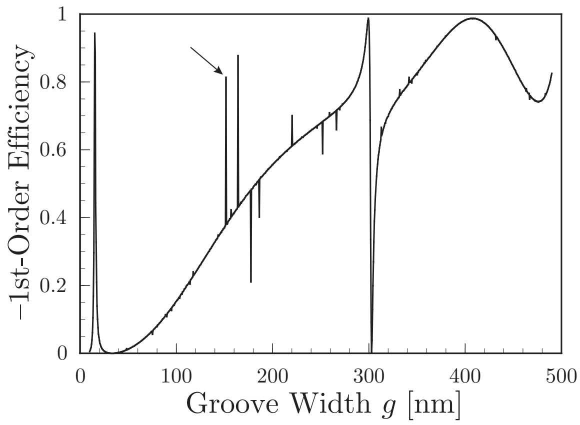

Fig. 5: Same as in Fig. 2, but computed by the DM-IMS with SMPA for $N = 100$, $M = 100$, and $\Delta y = h/100$.

artifacts is less than that in Fig. 2 though those amplitudes are much larger. This fact means that one reason of the numerical artifacts in Fig. 2 is simply due to the small truncation order but there exist other difficulties lying behind.

As written before, the RCWM solves the CDES as an eigenvalue problem. But there is another method that solves the CDES and obtains the transmission matrix of each layer with the help of numerical integration algorithms. In the narrow sense, this numerical integral approach is called the differential method (DM). This approach usually uses an explicit integration scheme to solve the CDES. However, the explicit integration schemes tend to be less stable for larger truncation order, and it has been known that the DM with the implicit integration scheme provides much more stable numerical computation [8]. The −1st-order diffraction efficiencies of the same grating as Fig. 2 are computed by the DM based on the implicit midpoint scheme (DM-IMS) with the help of SMPA and plotted in Fig. 5. The parameters for numerical computation are chosen as $N = 100$, $M = 100$, and the step thickness $\Delta y = h/100$ for the IMS. Clearly, the DM-IMS is much more stable than the RCWM though there still remain a small number of numerical artifacts.

3 Extrapolation Approach

Hosono and Yamaguchi [9] applied the homogeneous multilayer approximation method to a lossless plasma slab in which permittivity is continuous and has both positive and negative values, and pointed out a difficulty due to numerical stability. They estimated the transmission and the reflection coefficients using the extrapolation technique with assuming loss terms. This problem is recently studied by Yamasaki *et al.* [10,11] using the Fourier series expansion method, and validated also the extrapolation technique. The grating under consideration is lossless, and the permittivity inside the groove region has both positive and negative values though it is given by discontinuous function of x. Of course, the differential theory of gratings has to introduce truncation for practical computation, and then the permittivity distribution is approximated by a truncated Fourier series giving a continuous function. Consequently, the origin of the numerical instability is thought to be same as the difficulty of lossless plasma slab.

Here, the extrapolation technique is applied to estimate the efficiencies of lossless gratings. Assuming the real part of refractive index $\Re(n_s)$, the grating becomes lossy. The efficiencies calculated by the DM-IMS with SMPA for $M = 100$, $\Delta y = h/100$, and various truncation orders N are plotted as a function of $\Re(n_s)$ in Fig. 6. The parameters are same as Fig. 2 but the groove width is fixed to $g = 151.6$ nm that gives a large artifact as pointed by arrow in Fig. 5. Some unphysical behaviors are observed for $\Re(n_s) < 0.2$, but reasonable results are obtained in the other range. The efficiencies of lossless grating are estimated by the quadratic extrapolation

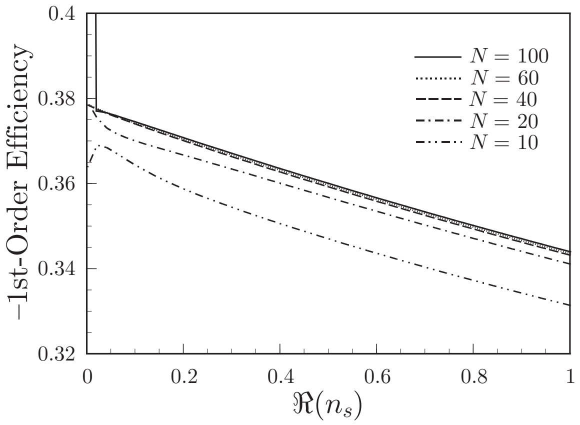

Fig. 6: Efficiency of the grating with $g = 151.6\,\mathrm{nm}$ as function of $\Re(n_s)$. The results are computed by the DM-IMS with SMPA with $M = 100$, $\Delta y = h/100$, and various N.

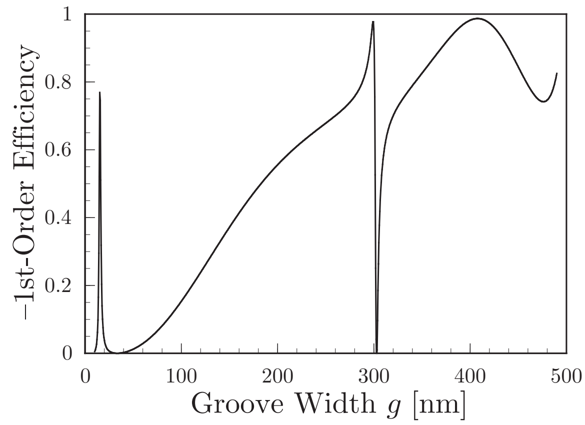

Fig. 7: Same as in Fig. 5, but estimated by quadratic extrapolation with assuming lossy substrate of $\Re(n_s) = 0.2, 0.25, 0.3$.

and plotted in Fig. 7. The efficiencies are calculated at $\Re(n_s) = 0.2, 0.25, 0.3$ by the DM-IMS with SMPA with $N = 100$, $M = 100$, and $\Delta y = h/100$. The results show great improvements in numerical stability and numerical artifacts appeared in Fig. 5 are completely suppressed and good agreement with those of the rigorous modal method given in Fig. 3(b) of Ref. [3].

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