The fast solver to calculate the scattered fields from nano-periodic structures based on integral equations

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***Abstract*—Nano-periodic metallic grating structures are novel components that have several extraordinary optical transmission phenomena, such as surface plasmon polariton (SPP). In this work, we proposed a new efficient method based on the modified Neumann-to-Dirichlet (NtD) map to calculate the scattered fields from the nano-periodic metallic grating structures. In each sud-domain from the periodic metallic gratings, we construct the modified NtD map operators by boudary integral equations. The new operators avoid the numerical instability of the condition numbers from the challenging metallic materials with complex refractive index. Numerical result demonstrates that the new method achieves high accuracy for metallic diffraction gratings and indicates the phenomenon of surface plasmon polariton.**

***Index Terms*—integral equation method, modified Neumann-to-Dirichlet map, surface plasmon polariton**

I. Introduction

Diffraction gratings are a class of optical components with certain regular surface patterns. In recent years, metallic gratings have attracted much attention due to their extraordinary optical transmission. Absorption anomalies could happen on the interface between a metallic and a dielectric medium due to surface plasmon polariton (SPP) excitations. It is an intrinsical excitation whose electromagnetic field decays exponentially with distance from the surface. Our work aims to find a simple, efficient and accurate numerical method to investigate the propagation behavior of waves through metallic gratings.

Several computational algorithms have been developed to predict the behavior of the nano-periodic structures in recent years. In our previous works [1], [2], the Neumann-to-Dirichlet (NtD) map method was developed for scattering problems from the periodic dielectric gratings. Though this method works well for the dielectric gratings, the operator will break down during the simulation of the metallic gratings due to the complex index of refraction. To avoid the numerical instability issue, we construct a stable operator to replace the overflowing one. Instead of deriving the boundary integral equations for the propagation constants [3], we make full use of the quasi-periodic condition to reduce high computational complexity and adopt the operator marching method to analyze the multilayered structures. Numerical result demonstrates that the proposed method achieves high accuracy for the scattered fields from metallic grating structures.

II. The Modified NtD Map Method

The nano-periodic metallic grating structures we considered here is shown in Fig. 1. Since the material of the grating is metal, $\varepsilon^{(2)}$ is a complex parameter here. The groove depth is h, while the duty cycle is a/d.

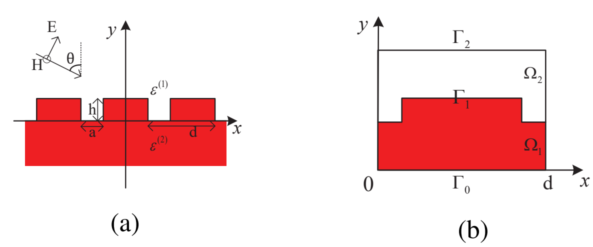


Fig. 1. A typical metallic grating structure. (a) The diffraction configuration; (b) Division of the domain for one period.

As is discussed in our previous works [1], [2], we adopted the operator marching method to analyze multilayered periodic structures. Then we use the interface conditions to solve the wave transition, and calculate the Neumann-to-Dirichlet map $\mathcal{V}$ with boundary integral equations to solve the wave propagation. To discretize the boundary integral equation, we use the Nyström method with a graded mesh. In the traditional Nyström method, we separate the logarithmic parts from the integral operators $\mathcal{S}, \mathcal{K}$ as follows:

$$S = S_1 \ln\left(4\sin^2 \frac{t-\tau}{2}\right) + S_2, \tag{1}$$

$$K = K_1 \ln\left(4\sin^2 \frac{t-\tau}{2}\right) + K_2, \tag{2}$$

where

$$S = \frac{i\sigma}{2} H_0^{(1)}(k_0 n r), \quad S_1 = -\frac{\sigma}{2\pi} J_0(k_0 n r), \tag{3}$$

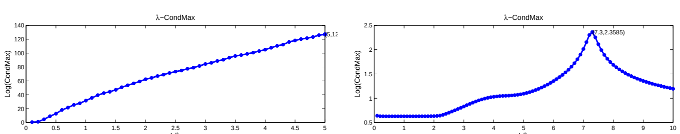
$$K = -\frac{ik_0 n\zeta}{2r} H_1^{(1)}(k_0 n r), K_1 = \frac{k_0 n \zeta}{2\pi r} J_1(k_0 n r). \tag{4}$$

However, this splitting method is not good if the diffraction grating is composed of metal material.

The refractive index of the metal material $n = \sqrt{\eta}/k_0$ here is a complex parameter. Thus we can separate the imaginary part and assume it as in_l where n_l is a real number. Since k_0 and r are real numbers, parts of the Bessel functions in the expressions of $S_1,\ K_1$ (3, 4) could be rewritten as

$$J_\nu(ik_0 n_l r) = i^\nu I_\nu(k_0 n_l r), \quad \nu = 1, 2, \tag{5}$$

where $I_\nu(x)$ is a real function and grows exponentially when the argument x becomes large. Thus, the terms S_1 and K_1 are oscillating around zero with amplitudes increasing when r becomes large. It's expensive for computing the NtD map $\mathcal{V}$ and the overflow may happen when n_l goes large. Assume the permittivity of the medium in Fig. 1 is $\varepsilon = (0.1 + 5.0i)^2$, then the condition number of the NtD operator is shown in Fig. 2 (a). We can see that the condition number of the NtD operator from the metallic layer blows up with increasing L/λ, which implies that the traditional NtD map method is unsuitable to deal with the metallic gratings.



(a) (b)

Fig. 2. Maximal condition numbers of the NtD operators (a) The traditional one; (b) The modified one.

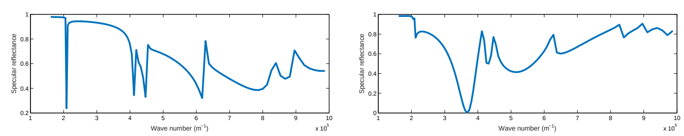
To avoid the numerical instability when the Nyström method is applied for the metallic grating, we truncate the remainder of the series expansion of $J_\nu(z)e^{iz}$ and then multiply it by e^{-iz} to introduce a new operator $\hat{J}_\nu(z, M)$ to replace $J_\nu(z)$. The operator can be written down as follows:

$$\hat{J}_\nu(z, M) = e^{-iz} z^\nu \sum_{k=0}^{M-\nu} \sum_{m=0}^{[\frac{k}{2}]} \frac{(iz)^k}{m!(m+\nu)!(k-2m)!2^{2m+\nu}}. \tag{6}$$

Obviously, $J_\nu(z) - \hat{J}_\nu(z, M) = O(z^{L+1})$. What's more, $\hat{J}_\nu(z, M)$ has a very similar behavior as $J_\nu(z)$ as $z \to 0$ and decays exponentially as $|z|$ becomes large. To evaluate the new modified NtD operator, we compute the condition numbers again, and the results are shown in Fig. 2 (b). We could see that the new modified NtD operator is much mroe stable than the traditional one from the comparison.

III. Numerical Examples

To valiate the proposed numerical method, we conduct an example from [4], whose schematic picture is the same as Fig. 1. The width and period of the grooves are $a = 0.5\mu m, d = 3.5\mu m$, and the incident angle is $\theta = 21°$. Here we compute two cases with the depths $h = 0.2\mu m$ and $h = 0.4\mu m$ for comparison. The material of the grating is gold, which changes the diffraction efficiency as the wave number varies. We compute the specular reflectance as a function of the wave number (k) of the incident wave. The results are shown in Fig. 3. The reflecticity minima in the figure correspond to SPP excitations, which located at $k = 2.1 \times 10^5 m^{-1}$, $k = 4.2\times10^5 m^{-1}$, $k = 4.5\times10^5 m^{-1}$, and $k = 6.3\times10^5 m^{-1}$ in Fig. 3 (a). However, with increasing depth, the resonances are broadened due to radiation dampling, and the reflectance minima start to change. Thus in Fig. 3 (b), the excited modes have a hybrid character, combination of SPPs with waveguide modes localized at the grooves. Our generated results agree well with results in [4].



(a) (b)

Fig. 3. Calculated specular reflectance of the gold grating with the incident wave number varies. (a) $h = 0.2\mu m$; (b) $h = 0.4\mu m$.

IV. Conclusion

Periodic metallic grating structures have several special electromagnetic properties, such as surface plasmon polariton (SPP), which are important in the modern nano-optics applications. In this work, we proposed the new modified Neumann-to-Dirichlet (NtD) map based on the boundary integral equation method to calculate the scattered fields from the metallic gratings. The modified NtD map operator avoids the blow up problem from the metallic gratings, and thus is stable for those with complex refractive index. Numerical result indicates the efficiency of the proposed method on simulation of the electromagnetic scattered fields from the metallic grating structures.

References

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