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Summary. Diffraction gratings are often used in optical metrology. When an electromagnetic wave is incident on a grating, the periodicity of the grating causes a multiplicity of diffraction orders. In many metrology applications one needs to know the diffraction efficiency of these orders. Since the period of a grating is often of the same order of magnitude as the wavelength, it is needed to solve Maxwell's equations rigorously in order to obtain these diffraction efficiencies. Two of those methods are the rigorous coupled-wave analysis (RCWA) and the C method.
In this paper a comparison is made between RCWA and the C method with respect to accuracy and speed. Restrictions are made to one-interface problems, which means that only two media are involved separated by one interface, and only gratings are considered with a periodicity in only one direction.

Key words: diffraction gratings, C method, RCWA

1 Introduction

When the grating's period is of the same order of magnitude as the wavelength, rigorous methods are required to solve Maxwell's equations. At the time Jean Chandezon introduced his method [1, 2], another method called rigorous coupled-wave analysis (RCWA), was already widely used [3, 4]. The main question remains when one should use RCWA or the C method. Although both methods have a completely different approach for solving the grating problem, it is widely known, that solving eigenvalue problems is the most computationally expensive operation in both methods. That is why this paper concentrates on the computations of the eigenvalue problems to select a criterion for the usage of a certain method. Therefore, the differences between the methods will be discussed and, as an example, a sinusoidal grating is used to illustrate the criterion.

2 Mathematical problem

An infinitely long, one-dimensional grating with only one interface is shown in Figure 1. One-dimensional implies that the grating is periodic, say with period Λ, in the x-direction and constant in the y-direction. The fact that the grating is assumed to be infinitely long, allows a restriction to only one period. The domain exists of two media, denoted by Ω_1 (usually air) and Ω_2 (dielectric or metal). The boundaries are denoted by Γ_m for $m = 1, ..., 5$.

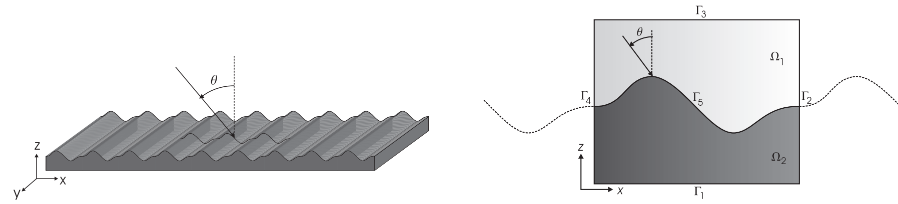

Fig. 1. Left: three dimensional representation of the diffraction grating; **right**: the domain of interest.

The media are assumed to be linear with respect to the electromagnetic fields, homogeneous, isotropic, time-invariant, dispersion-free, source-free and non-magnetic. The electromagnetic fields are assumed to be time-harmonic, which implies that the initialization phase is neglected. The incident field is either TE or TM polarized. All these assumptions reduce the local Maxwell equations to a generalized Helmholtz equation [2].

$$\nabla^2 F(x,z) + k^2 n^2(x,z) F(x,z) = 0, \tag{1}$$

where F is either the electric field E_y for TE polarized light or the magnetic field H_y for the TM case. The parameter $n = \sqrt{\varepsilon(x,z)\mu_0}$ is the refractive index and $k = \omega\sqrt{\varepsilon_0\mu_0}$ is the wave number.

On boundaries Γ_1 and Γ_3, the outgoing wave condition holds, which means that the fields have to be finite for $z \to \pm\infty$. The restriction to only one period gives a pseudo-periodic boundary condition at Γ_2 and Γ_4 by invoking the Floquet-Bloch theorem.

$$F(x,z) = F(x+\Lambda, z)\exp(i\sin\theta), \quad 0 \le x < \Lambda, \quad -\infty < z < \infty. \tag{2}$$

The last boundary is Γ_5 and on this interface, the tangential components of the electromagnetic fields are continuous.

3 Solution methods

From general grating theory it is known that above and below the grating grooves, the Rayleigh expansion holds as a solution of the field:

$$F(x,z) = \sum_{m=-\infty}^{\infty} A_m \exp(ik_{xm}x + ik_{zm}z), \tag{3}$$

where the A_m are the reflection coefficients in the upper halfspace or the transmission coefficients in the lower halfspace and k_{xm} and k_{zm} are known coefficients. This Rayleigh expansion is a direct consequence of the outgoing wave condition, the pseudo-periodic boundary condition and the Helmholtz equation that holds in the upper and lower halfspace. The reason the Rayleigh expansion does not hold inside the grating grooves is that the complex permittivity is not a constant, but a function of x and z. This leads to an eigenvalue problem in both methods. The details of the methods are discussed separately.

- **RCWA**
  By eliminating the z-dependency of the complex permittivity, it is possible to write the solution inside the grooves as a Fourier expansion, since only a dependency on the periodic coordinate x is present. The way RCWA accomplishes this, is by slicing up the grating domain such that inside each slice, the permittivity only depends on x. At the boundaries between two slices, the tangential components of the electromagnetic fields are continuous. In this way, the unknown reflection and transmission coefficients of the upper and lower halfspace can be connected to each other and determined. However, introducing the Fourier expansion in the Helmholtz equation gives an eigenvalue problem of size $2N + 1$ for both TE and TM polarization for every slice.

- **C method**
  The C method uses a completely different approach. The method uses the idea that if the grating interface were flat, the Rayleigh expansions would be valid for the entire domain, except at the interface. The C method ensures the grating interface to be flat by introducing a new coordinate system. A restriction of the method is that the interface can be described by a function of x, i.e. $z = a(x)$. There are parametric descriptions, but that is only for stability purposes. The coordinate transformation is given by

  $$u = x, \quad v = y, \quad w = z - a(x). \tag{4}$$

  The periodicity is preserved in the coordinate u and the grating interface is now described by a flat line given by $w = 0$. However, in the generalized Rayleigh expansion, a new unknown turns up. By substituting this expansion into the transformed Helmholtz equation, an eigenvalue system has to be solved for each **medium**, but since TE and TM polarization cannot be separated this time, the size is $4N + 2$.

Figure 2 points out how the two methods handle the mathematical model obtained in section 2. The main differences between the C method and RCWA are:

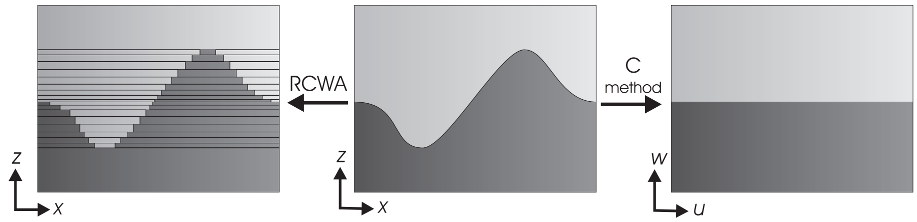

Fig. 2. Schematic representation of the way the RCWA and C method remove the z dependency.

- There is one eigenvalue problem per **layer** of size $2N + 1$ for RCWA vs. one per **medium** of size $4N + 2$ for the C method.
- RCWA solves one eigenvalue system for each polarization state, while the C method solves one eigenvalue system for both TE and TM polarization simultaneously.
- RCWA approximates the grating interface, while the C method does not.
- RCWA can handle all types of diffraction gratings, including overhanging gratings, while the C method is restricted to interfaces which can be described by a function of the periodicity coordinate.

A general eigenvalue system of size $p \times p$ takes $O(p^3)$ flops. For the C method only two eigenvalue systems have to be solved of twice the size of the eigenvalue systems obtained with RCWA, but when RCWA uses q layers it also has q eigenvalue systems. Altogether, this implies that RCWA may have 8 times more layers than the number of media for the C method to have an equal number of computations.

4 Results

To show the results, test case 2 from [2] has been used. It concerns a sinusoidal grating with a period which is equal to twice the wavelength. The refractive index of the upper medium is 1 (air), while the one of the lower medium is 1.5 (dielectric). The amplitude of the sine equals the size of the wavelength.

Figure 3 shows the results of RCWA for several values of N and several numbers of layers q. It can be seen that it is not the number of harmonics N that determines the diffraction efficiency mostly, but the number of layers q. To have the relative difference between RCWA and the C method below 1 %, RCWA already needs 15 to 20 layers, while for 0.1 % 50 to 80 layers are necessary. It should be noticed that the layer thickness has been chosen equidistant.

To conclude, this paper shows that the number of layers needed to approximate the grating to obtain an accurate (defined by user) result, is the most important criterium and not the number of harmonics. Secondly, for general

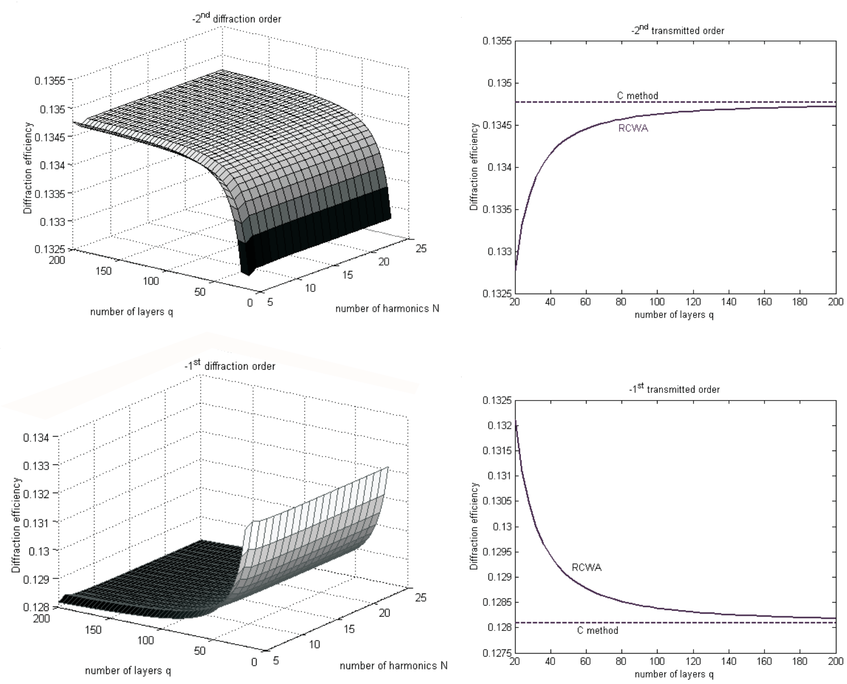

Fig. 3. Diffraction efficiencies of the -2$^{\text{nd}}$ and -1$^{\text{th}}$ diffraction order as a function of the number of layers and the number of harmonics (*left*) and if $N = 14$ a comparison with the C method.

grating profiles the C method will obtain the answer with less computational efforts if RCWA uses more than 10 layers to approximate the grating profile.

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