The C-method as an Initial Value Problem: Application to Multilayer Gratings

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Abstract— We study our approach of the C-method as an initial value problem for the efficient calculation of the N-dimensional scattering matrix of a grating. We apply this method to multilayer gratings with an arbitrary number of interfaces. The interfaces can have different functional form and amplitude and can be parallel or not.

For each interface separating two homogeneous media, we consider two horizontal planes above and below the interface, and define a coordinate system such that the interface and both horizontal planes correspond to coordinate surfaces. Inside the area delimited by the two horizontal planes, the Maxwell's equations lead to an initial value problem which can be solved with initial conditions satisfying the boundary conditions. Outside this area, the fields are represented by Rayleigh expansion. The scattering matrix between two consecutive media is obtained by using continuity relations between different components of fields on the horizontal planes.

We consider a $n+1$ layer diffraction grating, thus there are n interfaces separating the layers. From the uppermost to downmost, these layers are composed of medium 1 to medium $n+1$. Each medium has a constant optical index. Thus we can calculate the scattering matrix $S_{i,i+1}$ which associate the incoming and outcoming waves from medium i and $i+1$. Then we collect all the scattering matrix of adjacent medium, $S_{i,i+1}$, $i = 1, \ldots, n$ and obtain the global matrix $S_{1,n+1}$ by combination of elementary matrices $S_{i,i+1}$, $i = 1, \ldots, n$.

The proposed method gives the efficiencies with a good accuracy. Experiments are performed on a three layer grating with interfaces described by Trigonometric functions. We also study the anomalies of coated dielectric gratings.

1. INTRODUCTION

The curvilinear coordinate method (C-method) is based on a covariant formulation of Maxwell's equations written in a coordinate system such that one of the coordinate surfaces coincide with the grating surface. It is a powerful theoretical tool for analyzing gratings [1, 2]. This method uses a new coordinate system such that the coordinates x and z are unchanged and y is replaced by $u = y - a(x)$ where $a(x)$ is the function describing the grating geometry. The new coordinate system enables us to express the problem as an eigenvalue problem which could be solved numerically. The covariant components of the electric and magnetic fields can be expanded as a linear combination of eigensolutions satisfying the outgoing wave condition. The boundary condition allows the diffraction amplitudes to be determined.

In this paper, we consider a new approach of the curvilinear coordinate method [3]. Instead of eigenproblem, this new approach translate the problem to an initial value problem which leads to the scattering matrix of a grating. We apply this method to multilayer gratings with an arbitrary number of interfaces. The interfaces can have different functional form and amplitude and can be parallel or not. For each interface separating two homogeneous media, we consider two horizontal planes above and below the interface, and define a coordinate system such that the interface and both horizontal planes correspond to coordinate surfaces. Inside the area delimited by the two horizontal planes, the Maxwell's equations lead to an initial value problem which can be solved with initial conditions satisfying the boundary conditions. Outside this area, the fields are represented by Rayleigh expansions. The scattering matrix between two consecutive media is obtained by using continuity relations between different components of fields on the horizontal planes. We consider a $n+1$ layer diffraction grating, thus there are n interfaces separating the layers. From the uppermost to downmost, these layers are composed of medium 1 to medium $n+1$. Each medium has a constant optical index. Thus we can calculate the scattering matrix $S_{i,i+2}$ which associate the incoming and outcoming waves from medium i and $i+1$. Then we collect all the scattering matrix of adjacent medium, $S_{i,i+1}$, $i = 1, \ldots, n$ and obtain the global matrix $S_{1,n+1}$ by combination of elementary matrices $S_{i,i+1}$, $i = 1, \ldots, n$.

The article is structured as follows. In Section 2, we present the Maxwell's equations under the covariant form expressed in the new coordinate system which is adapted to the grating surface and horizontal planes. In Section 3, we introduce the concept of scattering matrix and how to form the global matrix $S_{1,n+1}$ from the local matrices $S_{i,i+1}$, $1 \leq i \leq n$. In Section 4, experiments are performed on a three layer grating with interfaces described by Trigonometric functions. We also study the anomalies of coated dielectric gratings. In Section 5, results and conclusions are given.

2. THE C-METHOD AS AN INITIAL VALUE PROBLEM

We consider a $n+1$ layer diffraction grating. The interface is represented by a periodic cylindrical surface $y = a_i(x)$, $1 \leq i \leq n$. This surface separates the medium i from the medium $i+1$. In Figure 1, two representative adjacent interfaces are shown. We consider separable layered grating, meaning that there exists a horizontal line $y = y_{i+1}$ separates the interface $y = a_i(x)$ and the interface $y = a_{i+1}(x)$ for each i. The interfaces in general have different functional forms and amplitudes, but there exists a value D such that D is the period of the function or a multiple of the period. The thickness h_i is measured between the middle lines of the two boundaries. The medium between the interface $y = a_i(x)$ and the interface $y = a_{i+1}(x)$ is homogeneous with optical index ν_i, impedance Z_i and wave number k_i.

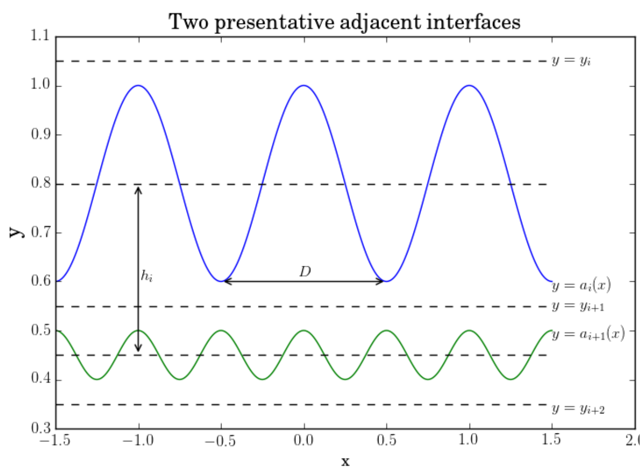

Figure 1: Notation for the description of a layered grating.

As the interfaces are separable, we can consider each interface separately and then combine to form the global matrix. For each interface $y = a_i(x)$, we consider the problem as in Figure 2.

Outside the region delimited by $y \leq y_i$ and $y \geq y_{i+1}$, under the Cartesian coordinates (x, y, z), the field is represented by a linear combination of elementary plane waves, known as Rayleigh expansion:

$$\begin{cases} F_c^{(i)}(x,y) = \sum_n \left(c_n^{(i+)} \exp(-j\alpha_n x) \exp\left(-j\beta_n^{(i)} y\right) + c_n^{(i-)} \exp(-j\alpha_n x) \exp\left(j\beta_n^{(i)} y\right)\right) \\ G_c^{(i)}(x,y) = \sum_n \frac{\beta_n^{(i)}}{k^{(j)}} \left(c_n^{(i+)} \exp(-j\alpha_n x) \exp\left(-j\beta_n^{(i)} y\right) + c_n^{(i-)} \exp(-j\alpha_n x) \exp\left(j\beta_n^{(i)} y\right)\right) \end{cases} \tag{1}$$

The subscript c denotes the Cartesian components of electromagnetic field. In $E_{//}$ polarization, $F_c^{(i)}(x,y) = E_z^{(i)}(x,y)$, $G_c^{(i)} = Z^{(i)} H_z^{(i)}(x,y)$ and in $H_{//}$ polarization, $F_c^{(i)}(x,y) = Z^{(i)} H_z^{(i)}(x,y)$, $G_c^{(i)}(x,y) = -E_x^{(i)}(x,y)$. Superscripts $(+)$ and $(-)$ denotes a plane wave moving in direction along the z-axis and inverse the z-axis, respectively. The propagation coefficients of the n-th order diffraction are presented by α_n and $\beta_n^{(i)}$ with the relation

$$\alpha_n^2 + \left(\beta_n^{(i)}\right)^2 = k_i^2 \tag{2}$$

where $\text{Im}(\beta_n^{(i)}) < 0$ and $\alpha_n = k^{(1)} \sin\theta_0 + n\frac{2\pi}{D}$. The propagation coefficient $\beta_n^{(i)}$ defines the nature of the plane wave: a propagation wave if $\beta_n^{(i)}$ is real, and an evanescent wave if $\beta_n^{(i)}$ is imaginary.

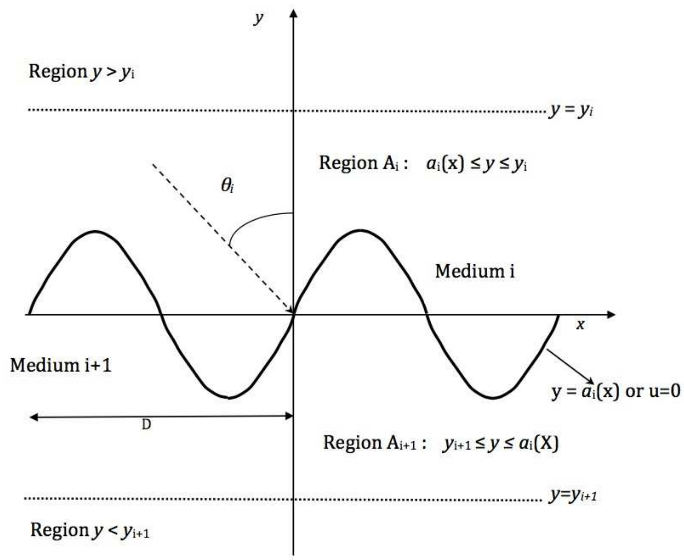

Figure 2: Notation for the description of interface $y = a_i(x)$, illuminated by a plane wave under the incidence θ_0.

We define the local scattering matrix(S-matrix) to relate the amplitudes of outgoing plane waves $(c_n^{(i+)}, c_n^{((i+1)-)})$ to those of incoming waves $(c_n^{(i-)}, c_n^{((i+1)+)})$ such that

$$\begin{pmatrix} c^{(i+)} \\ c^{((i+1)-)} \end{pmatrix} = S_{i,i+1} \begin{pmatrix} c^{(i-)} \\ c^{((i+1)+)} \end{pmatrix} \tag{3}$$

here we use $c^{(m\pm)}$ to represent a vector containing the scattering amplitudes $c_n^{(m\pm)}$, $m = i,\ i+1$.

Within the regions A_i and A_{i+1} defined by $a_i(x) \le y \le y_i$ and $y_{i+1} \le y \le a_i(x)$, we consider the non-orthogonal coordinate system defined as follows [3–5]:

$$\begin{cases} x' = x \\ u = y_m \frac{y - a_i(x)}{y_m - a_i(x)}, \quad m = i, i+1 \\ z' = z \end{cases} \tag{4}$$

The grating surface $y = a_i(x)$ coincides with the coordinate surface $u = 0$ and the horizontal plane $y = y_m$ with $u = y_m$, $m = i, i+1$. With the help of this non-orthogonal coordinate system, we manage to translate the problem to an initial value problem which can be solved numerically to obtain the local scattering matrix $S_{i,i+1}$ for all i. For more details, see [3].

We then combine the local scattering matrices to form the global scattering matrix $S_{1,n+1}$. In fact, if we have local scattering matrices $S_{p,q}$ and $S_{q,r}$ such that $p < q < r$, then we can obtain the scattering matrix $S_{p,r}$.

$$\begin{cases} \begin{pmatrix} c^{(p+)} \\ c^{(q-)} \end{pmatrix} = S_{p,q} \begin{pmatrix} c^{(p-)} \\ c^{(q+)} \end{pmatrix} = \begin{pmatrix} S_{p,q}^{(+-)} & S_{p,q}^{(++)} \\ S_{p,q}^{(--)} & S_{p,q}^{(-+)} \end{pmatrix} \begin{pmatrix} c^{(p-)} \\ c^{(q+)} \end{pmatrix} \\ \begin{pmatrix} c^{(q+)} \\ c^{(r-)} \end{pmatrix} = S_{q,r} \begin{pmatrix} c^{(q-)} \\ c^{(r+)} \end{pmatrix} = \begin{pmatrix} S_{q,r}^{(+-)} & S_{q,r}^{(++)} \\ S_{q,r}^{(--)} & S_{q,r}^{(-+)} \end{pmatrix} \begin{pmatrix} c^{(q-)} \\ c^{(r+)} \end{pmatrix} \end{cases} \tag{5}$$

Eliminating the vectors c^{q+} and c^{q-}, one glue the two scattering matrices to be one $S_{p,r}$:

$$S_{p,r} = \begin{pmatrix} S_{p,q}^{(+-)} + S_{p,q}^{(++)}(I - S_{q,r}^{(+-)} S_{p,q}^{(-+)})^{-1} S_{q,r}^{(++)} S_{p,q}^{(--)} & S_{p,q}^{(++)}(I - S_{q,r}^{(+-)} S_{p,q}^{(-+)})^{-1} S_{q,r}^{(++)} \\ S_{q,r}^{(--)}(I - S_{p,q}^{(-+)} S_{q,r}^{(+-)})^{-1} S_{p,q}^{(--)} & S_{q,r}^{(-+)} + S_{q,r}^{(--)}(I - S_{p,q}^{(-+)} S_{q,r}^{(+-)})^{-1} S_{p,q}^{(-+)} S_{q,r}^{(++)} \end{pmatrix} \tag{6}$$

So in this way, we glue $S_{1,2}$ and $S_{2,3}$ to get $S_{1,3}$, and then glue $S_{1,3}$ and $S_{3,4}$ to get $S_{1,4}$ and so on until we get the global matrix $S_{1,n+1}$. We can also explore the parallelism in this gluing operation. For example, we can in the first setp, obtain $S_{1,3}$, $S_{3,5}$, $S_{5,7}$ ... in parallel, and in the second step, obtain $S_{1,5}$, $S_{5,9}$, ... in parallel, and so on. This needs only $\mathcal{O}(\log(n))$ steps to get the global scattering matrix. Moreover, for the calculation of the local scattering matrix $S_{i,i+1}$, the proposed method in [3] leads to systems of first-order linear differential equations, the solution of which requires the choice of an iterative algorithm. The proposed method is based on numerical integrations with N independent initial vectors. The kernel of this computing process is the numerical integration. This approach is also particularly well adapted to large-scale parallel and distributed architectures. Indeed, in the context of a distributed system comprising a network of machines, each of the problems could be solved on a machine whose architecture can be single or multiple processors. The proposed new method has a significant degree of coarse grain parallelism and requires little communication. These features offer the possibility of reducing dramatically the computation time. It's an advantage compared with the conventional C-method which leads to eigenvalue problems and requires the use of global eigensolver like QR method. In order to improve the performances of the QR algorithm, we can parallelize it. Nevertheless, the exploitation of the parallelism of this algorithm is a delicate task. Indeed, in each of iteration of QR, only two rows and two columns of the matrix participate to computation imposing a parallel algorithm with a small degree of parallelism. The reduction in the computation time cannot be substantial.

3. NUMERICAL EXPERIMENTS

We perform an experiment in the article [6]. The grating considered is a sinusoidal defined by $a_1(x) = a_1 \cos(\frac{2\pi}{D}x)$, $a_2(x) = a_2 \cos(\frac{2\pi}{D}x)$. Figure 4 shows the efficiency curves under the polarization $E_{//}$, with the value of $\sin\theta_0$ varying from 0.24 to 0.38. With the same parameters as in that paper, Figure 3 is exactly the same as in the paper [6]. This can be used as a poof of the validity of our method. Moreover, we also performed more experiments to see how this figure changes when we change the amplitude of function $y = a_1(x)$ and the optical index ν_3. Figure 4 shows how it is like when $a_1 = 0.01$ and Figure 5 shows the case when $\nu_3 = 1.5$, with other parameters fixed.

In Figure 3, the parameters of the corrugated waveguide is chosen in such a way that only one mode propagate if the interface were plane. We see from Figure 3 that in the vicinity of excitation of the guided wave the efficiency changes from 0 to 1. In Figure 4, the efficiency can not reach 0, it changes from a small value close to 0 to 1. In Figure 5, the efficiency can neither reach 0 nor 1. It can be observed that when a_1 varies from 0.02 µm to 0.01 µm, the jump becomes steeper. One can also observe that the place of the jump moves towards the left direction. When we vary a_2 form 0.02 µm to 0.01 µm, no similar phenomena can be observed. In fact, the curves seem almost stay the same.

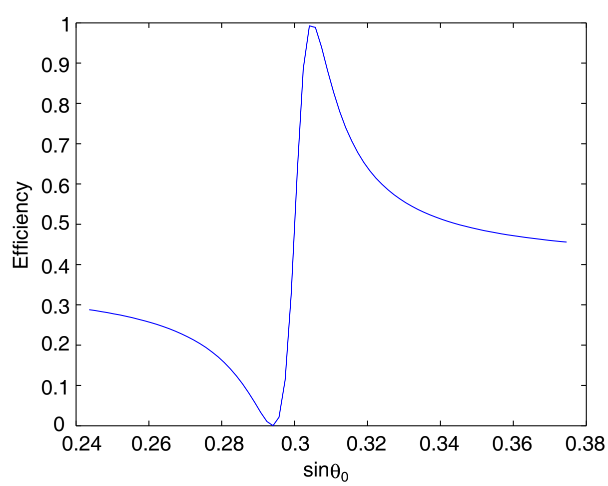

Figure 3: Diffraction efficiency of the zeroth reflected order of the sinusoidal grating. Parameters of the system are: $\nu_1 = \nu_3 = 1$, $\nu_2 = 2.3$, $h_1 = 0.19$ µm, $D = 0.37$ µm, $\lambda = 0.6328$ µm, $a_1 = a_2 = 0.02$ µm, for TE polarization.

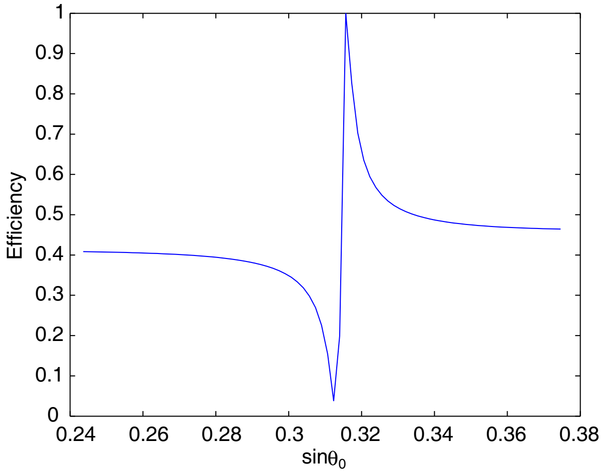

Figure 4: Diffraction efficiency of the zeroth reflected order of the sinusoidal grating. Parameters of the system are: $\nu_1 = \nu_3 = 1$, $4\nu_2 = 2.3$, $h_1 = 0.19\,\mu\text{m}$, $D = 0.37\,\mu\text{m}$, $\lambda = 0.6328\,\mu\text{m}$, $a_1 = 0.01\,\mu\text{m}$, $a_2 = 0.02\,\mu\text{m}$, for TE polarization.

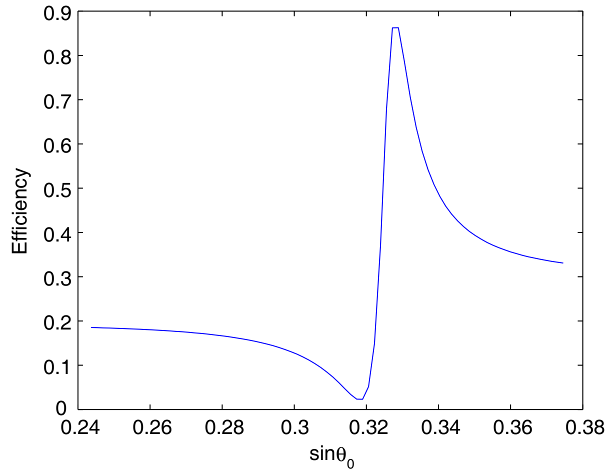

Figure 5: Diffraction efficiency of the zeroth reflected order of the sinusoidal grating. Parameters of the system are: $\nu_1 = 1$, $\nu_3 = 1.5$, $\nu_2 = 2.3$, $h_1 = 0.19\,\mu\text{m}$, $D = 0.37\,\mu\text{m}$, $\lambda = 0.6328\,\mu\text{m}$, $a_1 = a_2 = 0.02\,\mu\text{m}$, for TE polarization.

4. CONCLUSION

We studied our approach of the C-method as an initial value problem for the efficient calculation of the N-dimensional scattering matrix of a grating. We applied this method to multilayer gratings with an arbitrary number of interfaces. We have shown how to combine the local scattering matrix to obtain the global one. We have validate our method by comparison experiments results with that from published paper. The proposed method has very good accuracy as well as a natural of two level parallel property. This new version of C-method is an attractive alternative to analyze multilayered grating having parallel or non-parallel interfaces.

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