Prospects and Limits of the Rayleigh Fourier Approach for Diffraction Modelling in Scatterometry and Lithography

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ABSTRACT

With ever shrinking feature sizes in semiconductor and photonics industry, the demand and the challenges for optical modelling in terms of accuracy has increased dramatically over the last decade. Rigorous modal diffraction methods such as the RCWA, the Differential method or the C-method provide sufficient accuracy, however, they are rather costly particularly for 3D patterns.

In this paper, we are suggesting an approach which is based on the so-called Rayleigh hypothesis. The basic idea of this method is to extend the expansion of the electromagnetic field components into Rayleigh modes inside the grating grooves as opposed to the RCWA where the expansion within the slices is done in so-called Bragg modes. Therefore, the Rayleigh-Fourier method does not need a diagonalization for the decoupling of the modes. It requires only the formation of an interface transition matrix, the elements of which can be computed analytically. As a consequence, it is very fast both for 2D as well as for 3D.

Here, we discuss the details of the method and show how it can be combined with other modal methods into one framework. The application limits are discussed in terms of the corrugation depth of the grating, the shape of the grating profile, the pitch and the refraction index contrast. Surprisingly, the method can be applied far beyond the Rayleigh limit in a sort of semi-convergent regime when implemented and utilized carefully. Due to its speed, the method might be an appropriate choice for real time regression particularly for only slightly corrugated multilayer stacks.

Keywords: Optical Scatterometry, Lithography Simulation, Grating Diffraction

1. Introduction

During the last decade, several rigorous methods have been developed and matured for the accurate computation of the diffraction response of gratings. Here, the focus was mainly on modal methods where the field components are developed in Fourier series. The most universal modal method is the RCWA [1,2] where a given profile is decomposed in thin slices. Then, the diffraction problem for each slice is solved by means of a Fourier transformation the refraction index distribution within the slices in horizontal direction and coupling the electromagnetic fields in vertical direction by applying the boundary conditions. Alternatively, the boundary conditions can also be applied in horizontal direction resulting in the so-called classical modal method [3]. Furthermore, the slicing can be replaced by a numerical integration in vertical direction which is utilized in the D-method [4]. Eventually, one can introduce a new curvi-linear coordinate system which follows the interface between two materials or the surface of the grating. This is realized in the Chandezon or Coordinate transformation method (C-method) [5,6]. Last but not least, different methods can be applied layer wise to take advantage of the individual strengths of the method and effectively adapt it to the corresponding layer. An example is given in [6] where the RCWA and C-method are combined in a hybrid C-RCWA.

All this methods rely on the scattering matrix coupling [7] of the fields in vertical direction to insure a stable convergence and to avoid ill-posedness of the necessary matrix inversions. The individual methods exhibit advantages and disadvantages. For example, the RCWA shows convergence problems for high contrast materials and small sidewall angles in TM polarization. On the other hand, the C-method cannot deal with vertical or overhanging profiles. However, all the methods have in common that the resulting differential equation system usually requires the solution of an Eigen system. And it is a well known matter of fact that Eigen solvers scale with the third power of the matrix size in terms of computation costs. Therefore, there is a strong desire for methods that are faster but still accurate enough.

In practical applications, the interfaces to be modelled are often only slightly corrugated. Examples are defects in EUV masks or diffracting laser mirrors. In this paper, we show that the Rayleigh-Fourier method is an ideal substitute for only slightly corrugated gratings. Moreover, it is shown by means of numerical experiments that this is true even far beyond the validity of the Rayleigh criterion.

The paper is organised as follows. In chapter 2, the theory of the Rayleigh-Fourier method is outlined. This is followed by section 3 which contains all the numerical experiments to explore the validity range of the method for different conditions, e.g., corrugation depth, pitch and refraction index for a single interface. In addition, multiple interfaces are discussed. A brief summary concludes the paper in section 4.

2. Theory

The Rayleigh method is based on the so-called Rayleigh hypothesis. It states that the Rayleigh expansion which is usually only valid outside the grating region (region a in figure 1) can be extented into the grating (region b). According to the fundamentals of light scattering theory [8], this can be done as long as:

$$h \cdot \cos\vartheta < \frac{\lambda}{8} \tag{1}$$

holds where h is the grating height, θ is the angle of incidence and λ is the wavelength. This would mean that the grating height has to be below 62 nm when illuminating with 500 nm wavelength under normal incidence. Moreover, the criterion neither takes the profile into account nor worries about the correlation length or pitch for a periodic pattern, respectively.

In general, there are three different methods based on the Rayleigh hypothesis – the point matching or collocation method, the Rayleigh Fourier (RF) method and the Least Square Approximation Method (LSAM) [9,10,11]. In all these methods, the fields on both sides of the interface are matched to each other in a specific way. Unfortunately, all the methods presented in the literature cannot easily deal with multilayer stacks since the matrices are build in a way to match the boundary conditions on the interface. For the same reason, the RF cannot easily combined with other diffraction methods such as the RCWA.

Therefore, we derive a technique based on the Rayleigh Fourier approach where the propagation across an interface separating two different materials can be done by a single matrix which can easily included in the scattering matrix algorithm. The basic principle of the Rayleigh-Fourier method consists in the development of the electromagnetic fields into Fourier modes and the matching of these modes at the interface. To this end, a local coordinate system is introduced on the interface in order to enable the direct application of the boundary conditions of the tangential fields. The corresponding theory is discussed in detail in [12]. Here, only a short summary is given.

The situation is depicted in figure 1.

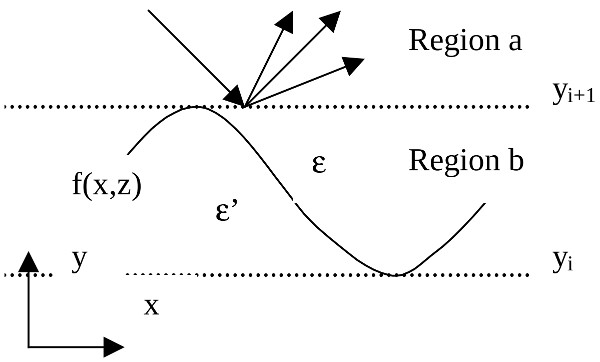

Fig. 1: Grating setup and coordinate system

We assume that the interface is given by the function f = f(x,z). Then, a local coordinate system along the interface is introduced by means of:

$$\begin{gathered}\vec{n} = \vec{e_y} - grad_{\parallel} f(x,z) \\ \vec{t_1} = \vec{e_y} \times \vec{n} \\ \vec{t_2} = \vec{n} \times \vec{t_1}\end{gathered} \tag{2}$$

First, the fields are propagated from the ±waves in the homogeneous area to the tangential fields at the interface by means of:

$$\begin{pmatrix} E_{t_1} \\ H_{t_2} \\ H_{t_1} \\ E_{t_2} \end{pmatrix}_{f(x,z)} = \int d\vec{\beta} \cdot e^{i\vec{\beta}\cdot\vec{r}_{\|}} \cdot D \cdot \Gamma \cdot T \cdot \begin{pmatrix} e_+ \\ e_- \\ h_+ \\ h_- \end{pmatrix}_{y_i} \tag{3}$$

Here, T is a propagation matrix that propagates the field from the reference plane y_i to the interface f(x,z). Furthermore, Γ is a matrix that transforms the ± waves into the tangential fields and D is a rotation matrix that transforms the global tangential fields into the local tangential fields as defined by (2). Moreover, β is given by the Bloch theorem: $\beta = \beta_0 + m\lambda/\text{pitch}$ (for 1D grating) and $r_{\|}$ is a vector in the xz-plane ($=e_x$ for 1D).

The same procedure can be done when approaching from the other side of the interface. By a formal inversion one can write:

$$\begin{pmatrix} e_+ \\ e_- \\ h_+ \\ h_- \end{pmatrix}_{y_{i+1}} = \left(\frac{1}{2\pi}\right)^2 \int d\vec{r}_{\|} \cdot e^{-i\vec{\beta}\cdot\vec{r}_{\|}} \cdot T^{-1} \cdot \Gamma^{-1} \cdot D^{-1} \cdot \begin{pmatrix} E_{t_1} \\ H_{t_2} \\ H_{t_1} \\ E_{t_2} \end{pmatrix}_{f(x,z)} \tag{4}$$

Merging (3) and (4) together into one expression results in an expression that connects the ± waves on either side of the interface:

$$\begin{pmatrix} e_+ \\ e_- \\ h_+ \\ h_- \end{pmatrix}_{y_{i+1}} = \int d\vec{\beta} \cdot J^{\varepsilon',\varepsilon}_{\vec{\beta}',\vec{\beta}} \cdot \begin{pmatrix} e_+ \\ e_- \\ h_+ \\ h_- \end{pmatrix}_{y_i} \tag{5}$$

with:

$$J^{\varepsilon',\varepsilon}_{\vec{\beta}',\vec{\beta}} = \left(\frac{1}{2\pi}\right)^2 \int d\vec{r}_{\|} \cdot e^{-i\vec{\beta}\cdot\vec{r}_{\|}} \cdot T^{-1} \cdot \Gamma^{-1} \cdot D^{-1} \cdot D \cdot \Gamma \cdot T \cdot e^{-i\vec{\beta}'\cdot\vec{r}_{\|}} \tag{6}$$

Finally, the transition is realized by means of the J-matrix. Basically, the J-matrix consists of four submatrices that describe the polarisation coupling cases, i.e., TE→TE, TM→TM, TE→TM and TM→TE.

Beside a prefactor, the elements of the J-matrix are given by the diffraction integral:

$$X^{\hat{\alpha}}_{\hat{\vec{\beta}}} = \frac{\varepsilon - \varepsilon'}{(2\pi)^2 \cdot \hat{\alpha}} \int dr_{\|} e^{i\vec{\beta}\vec{r}_{\|} + i\hat{\alpha} f(x,z)} \tag{7}$$

The hats for α and β mean that it is formed by the sum or difference of the α and β on either side of the interface (for detail see [12]). The α itself is given by the dispersion relation $\alpha = \sqrt{\varepsilon - \beta^2}$.

The diffraction integral has an analytical solution for sinusoidal and piecewise linear profiles. Therefore, the population of the J-matrix can be done very fast as compared to the Eigen solve of the most other rigorous methods.

Finally, the coupling of the Rayleigh-Fourier method with the RCWA is straightforward having the J matrix available. Assuming for example an interface which is calculated with the C-method and which is embedded between two RCWA-slices (1 and 2). Then, the ±waves on the front and back side of this interface can be connected by applying the boundary conditions via:

$$\begin{pmatrix} s_+ \\ s_- \end{pmatrix}_f = \Gamma_f^{-1} \cdot \Gamma_1 \cdot T_1 \cdot \Gamma_1^{-1} \cdot J \cdot \Gamma_2 \cdot T_2 \cdot \Gamma_2^{-1} \cdot \Gamma_b \cdot \begin{pmatrix} s_+ \\ s_- \end{pmatrix}_b \tag{8}$$

Of course, the waves have to be sorted for cause- and response waves, and the various matrices have to be coupled in a recurrent way following the rules of the s-matrix coupling.

3. Numerical Results

In this section, the validity range of the Rayleigh Fourier implementation shall be investigated. First, gratings made from purely dielectric materials shall be regarded. The refraction index is 1.5. Because these gratings are losless, the analysis can be based on the energy criterion, i.e., the deviation of the sum of all propagating diffraction orders from one. In this paper, only sinusoidal profiles are considered. Furthermore, we look at two different grating periods – a small period in the range of the light wavelength and a larger one (12x lambda).

The results for the single sinusoidal grating are shown in figure 2. The order truncation is ±5, ±10 and ±20, the grating pitch is 0.5 microns and 5 microns, respectively. The wavelength is 0.4 microns and the light incidence is normal.

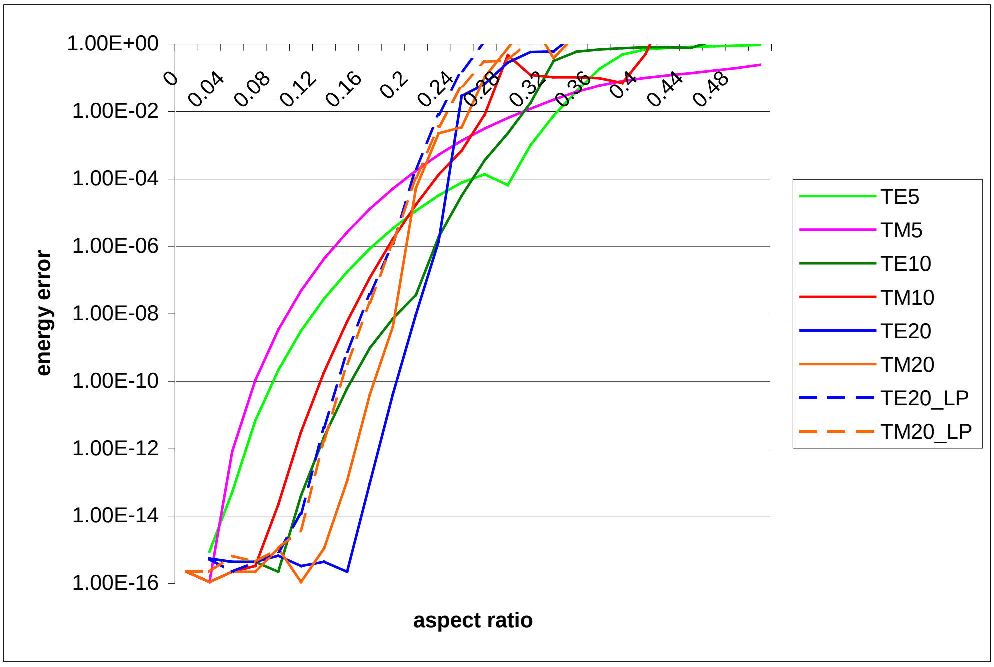

Figure 2: Energy error for a sinusoidal dielectric grating. Both polarisations (TE and TM) are shown for different number of diffraction orders (±5, ±10 and ±20) and the grating pitch is 0.5 µm and 5 µm (marked by _LP). The incident light is normal and has a wavelength of 0.4 µm.

Obviously, the convergence increases with higher order number as expected. Moreover, TE shows slightly better convergence than TM. And the convergence behaviour is slightly worse for the large period grating. However, the error is still in the range of 10^{-5} for an aspect ratio of 0.2. And this means the grating depth is 1 micron for a grating pitch of 5 microns. Related to the wavelength this gives a ratio of 2.5 ! This value is a multiple of the Rayleigh criterion of 0.125. In conclusion, it turns out that the aspect ratio plays a more essential role than the grating depth to wavelength ratio in terms of the convergence range of the Rayleigh Fourier method.

The next numerical example is a sinusoidal grating made from Silicon. The complex refraction index is n = 5.57 + j0.387 at 400 nm wavelength. Since the energy criterion cannot be applied anymore in this case, the results are compared with the RCWA (23 slices and 46 slices, respectively) and the C-method. A relative error is calculated as err = (RF-RCWA)/RCWA. The results are shown in figure 3.

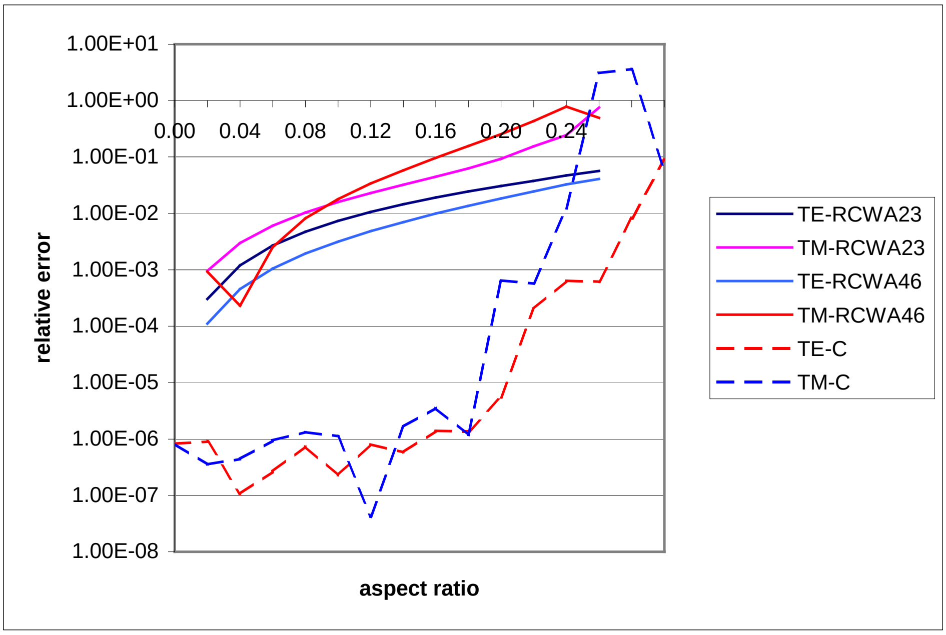

Figure 3: Relative error for a sinusoidal dielectric grating. The reference is the RCWA with 23 slices, RCWA with 46 slices and C-method. Both polarisations (TE and TM) are shown. The incident light is normal and has a wavelength of 0.4 µm.

It becomes evident that the Rayleigh-Fourier results correlate much better with the results from the C-method. The relative error is below 10^{-6} for an aspect ratio up to almost 0.2. This corresponds to a grating depth to wavelength ratio of 0.25 which is still the double of the Rayleigh criterion. The worse correlation of the RF-results with those obtained from the RCWA is due to the known issues of the RCWA itself caused by the slicing and the incorrect application of the Fourier factorization for profiles that deviate from binary [13].

In the third numerical example, a quick look shall be thrown on the application of the Rayleigh-Fourier method for multilayer systems. Here, a sinusoidal grating is considered which is coated with another material resulting in a multilayer grating with two parallel sinusoidal interfaces. Again, a purely dielectric grating is regarded with a substrate index of 1.8 and a layer index of 1.5.

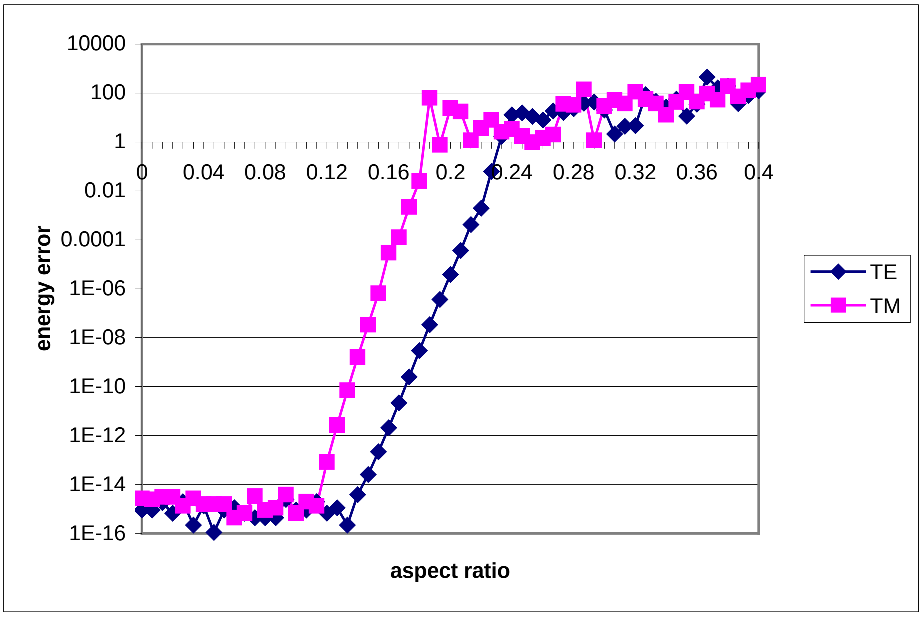

Figure 3: Energy error for a coated sinusoidal dielectric grating ($n_{substrate}$ = 1.8, $n_{coating}$ = 1.5) versus the aspect ratio (grating depth to pitch). The coating layer thickness is equal to the corrugation depth. The grating pitch is 0.5 µm. The incident light is normal and has a wavelength of 0.4 µm.

Again, the convergence is quite good for apect ratios below 0.2 for TE-polarisation and slightly worse 0.18 for TM-polarisation.

4. Conclusion and Outlook

The paper has shown how to implement the Rayleigh-Fourier method in a scattering matrix algorithm. In this way it can be combined with the RCWA and the C-method into a hybrid frame. Then, slightly corrugated interfaces can be very rapidly solved with the Rayleigh-Fourier whereas interfaces that do not have slope angles well below 90 degrees can be solved with the C-method. All other interfaces including overhanging profiles as well as volume scatterers can be treated by means of the RCWA.

Moreover, it was shown by means of numerical tests that the Rayleigh-Fourier method remains valid beyond the Rayleigh criterion, particularly for gratings with large pitch. It turned out that the aspect ratio, i.e., grating depth to pitch is much more essential as a validity criterion than the depth to wavelength ratio. These results hold more or less for both dielectric gratings as well as gratings made from Silicon.

Further work should focus on other surface profiles such as triangular and binary profiles. Besides, it is planned to combine the Rayleigh-Fourier method with the RCWA in order to model multilayer gratings. Also, the extension of the method to 3D should be taken into consideration if the previous tests can be accomplished successfully.

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