Simulating Grating Diffraction Using the Normal Vector Method

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This work presents a way to calculate normal vector (NV) fields as they are needed by the NV method, a special variant of the rigorous coupled-wave analysis (RCWA). Beforehand, a short review of the NV method is given. Finally an example of the convergence improvement of the NV method against other RCWA formulations is shown.

1 Introduction

For the numerical simulation of grating diffraction the rigorous coupled-wave analysis (RCWA) is a commonly used method. After its recognized publication in 1995 by Moharam and Gaylord [1] it turned out that its results for metallic gratings in TM polarization suffered from slow convergence due to numerical problems. While empirical solutions came from Lalanne as well as from Guizal and Granet, Li finally gave a theoretical explanation, introducing his factorization rules [2]. Since then different approaches were pursued in order to apply these rules to *crossed* gratings in order to improve convergence [3]. One of the most recent improvements for crossed gratings was presented by Schuster *et al.* [4]. They adopted the idea of the Fast Fourier Factorization by Nevière and Popov [5] and developed a *normal vector (NV) method* which is an optimized solution for the correct application of Li's factorizations rules to crossed gratings.

2 Background

Fig. 1 shows the geometry of the diffraction problem which is to be solved by the RCWA.

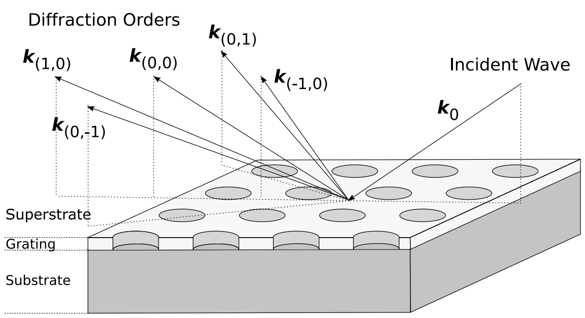

Fig. 1 *Geometry of the diffraction problem*

Using Maxwell's Equations to solve this problem the product

$$\boldsymbol{D} = \epsilon_0 \epsilon \boldsymbol{E} \quad (1)$$

must be calculated. However, the RCWA uses the Fourier expansion to transform the system of PDEs to a system of ODEs; hence, the product in Eq. (1) transforms to a convolution.

At material boundaries the normal component of Eq. (1) – in contrast to the tangential component – is a product of *complementary discontinuous* functions ϵ and $E_\perp$, as is generally known from electrodynamics. In truncated Fourier space as it is used in numerical calculations this product cannot be calculated by the usual convolution

$$[D_\perp] = \epsilon_0 [\![\epsilon]\!] [E_\perp], \quad (2)$$

as it leads to unnecessary oscillations in the dielectric displacement $D_\perp$ as shown in Fig. 2.

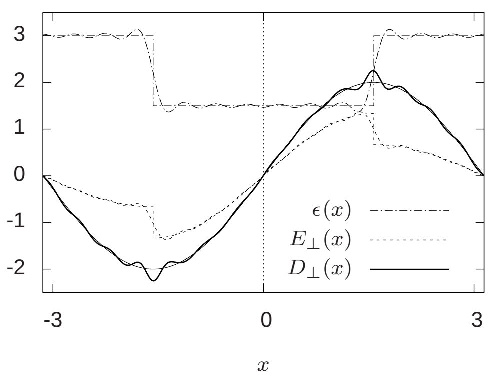

Fig. 2 *Visualization of the problems caused by truncated Fourier series.*

In Eq. 2 single brackets refer to vectors containing all Fourier coefficients of the specified function. $[\![\epsilon]\!]$ is the Toeplitz matrix of the Fourier coefficients of ϵ.

Li showed [2] that an *inverse rule* must be used instead:

$$[D_\perp] = \epsilon_0 \left[\!\!\left[\frac{1}{\epsilon}\right]\!\!\right]^{-1} [E_\perp], \quad (3)$$

Consequently the normal and tangential components must be treated differently. To separate both components at every point of the structure a projection of the electric field onto a continuous vector field is done. This vector field must be normal at the boundaries.

3 Generating the normal vector field

A bitmap serves as description for the grating structure. Different materials are indicated by different color indices. Then generating the NV field is done in two steps:

1. Calculating the gradient of the bitmap, which can now be interpreted as a potential, yields the NV on the boundaries.

2. Interpolating between these already calculated boundary vectors yields the remaining vectors in a continuous way. The interpolation used is an inverse distance weighting:

$$\boldsymbol{N}^*(\boldsymbol{x}) = \sum_{i=1}^{n_b} \frac{\boldsymbol{N}_i}{|\boldsymbol{x} - \boldsymbol{x}_i|^2} \tag{4}$$

normalized by

$$\boldsymbol{N}(\boldsymbol{x}) = \frac{\boldsymbol{N}^*(\boldsymbol{x})}{|\boldsymbol{N}^*(\boldsymbol{x})|}.$$

$\boldsymbol{N}_i$ denotes the boundary vectors, $\boldsymbol{x}_i$ their positions and n_b their count.

The shown interpolation is too slow to gain an advantage of the NV method against other methods. Therefore it is implemented in a progressive way. A progressive refinement algorithm makes sure that the considered number of boundary vectors in Eq. 4 becomes smaller with every iteration. This is possible, because the influence of distant vectors is negligible. Fig. 3 illustrates how the algorithm works.

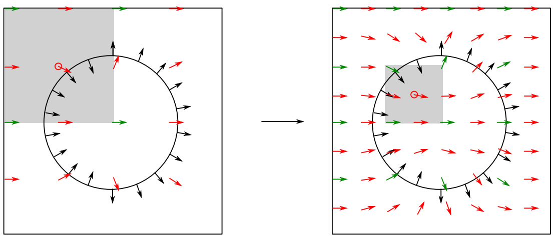

Fig. 3 *Progressive refinement algorithm for a circular structure. The third and forth iterations are shown.*

4 Results

Fig. 4 shows an example NV field created with the described algorithm. In this case the NVs calculated by the gradient were given a preferred direction to the right. This is a degree of freedom given by the definition of NVs.

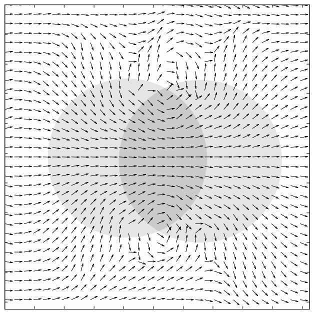

Fig. 4 *NV field of a structure with two intersecting circles.*

Fig. 5 shows the NV method's convergence improvement compared to Li's zigzag method [3] and to the original formulation by Moharam and Gaylord [1].

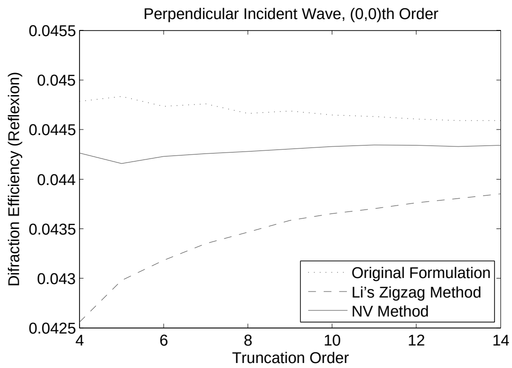

Fig. 5 *Convergences of different methods.*

5 Conclusion

With the shown NV field generation algorithm the NV method with its excellent convergence is a very attractive alternative to Li's zigzag method for crossed gratings.

References

[1] M. G. Moharam, T. K. Gaylord, E. B. Grann, and D. A. Pommet, "Formulation for stable and efficient implementation of the rigorous coupled-wave analysis of binary gratings," J. Opt. Soc. Am. A **12**, 1068–1076 (1995).

[2] L. Li, "Use of Fourier series in the analysis of discontinuous periodic structures," J. Opt. Soc. Am. A **13**, 1870–1876 (1996).

[3] L. Li, "New formulation of the Fourier modal method for crossed surface-relief gratings," J. Opt. Soc. Am. A **14**, 2758–2767 (1997).

[4] T. Schuster, J. Ruoff, N. Kerwien, S. Rafler, and W. Osten, "Normal vector method for convergence improvement using the RCWA for crossed gratings," J. Opt. Soc. Am. A **24**, 2880–2890 (2007).

[5] M. Nevière and E. Popov, *Light Propagation in Periodic Media – Differential Theory and Design* (Marcel Dekker, Inc., New York, 2003).