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C Method with Adaptive Resolution (AR)

Author: J. Bischoff/ Osires Optical Engineering Ilmenau

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1. Scope

State of the art for modal diffraction methods is using an equidistant sampling along the lateral axis of a profile /1/. In general, this works well and besides it is relatively easy to implement. However, when the slope angle of the profile exceeds approximately 85 degrees it is not sampled sufficiently. This results in erroneous calculations. An appropriate mean to overcome this serious problem is the adaptive resolution method. This approach is based on an adaptive sampling rather than ignoring the profile steepness at all. It means to increase the number of sampling points in areas with strong gradients and reduce it where the profile is shallow.

The two sampling cases are opposed in fig. 1 for an example, where the orange points present the standard C-method (CCM) and the blue points present the adaptive resolution methode (C-AR). The difference becomes particularly visual near the edges. While, the points for the C-AR are dense and hardly to be resolved in the plot, a clear gap is to be observed across the edge for the standard method.

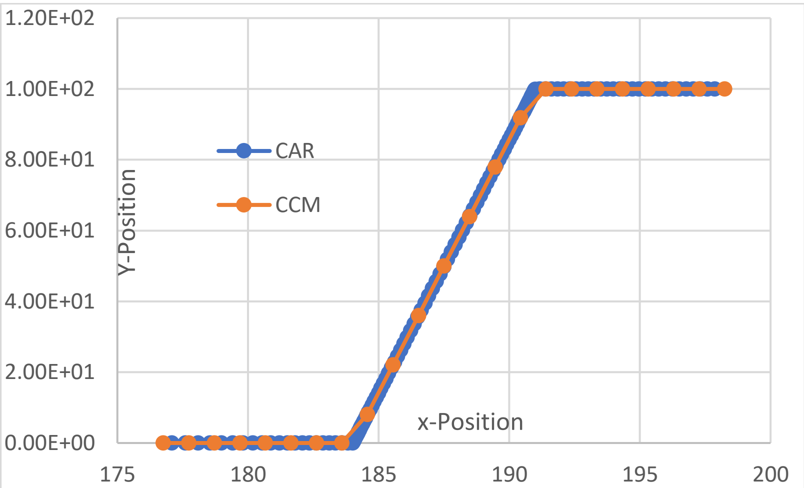

Abbildung 2: Profile sampling comparison between Standard C-Method and CM with adaptive Resolution

2. Theory and Implementation

The theory of the adaptive resolution method is given in detail in /3/. The coordinate transformation for the Standard C-Method is: x = u, y = v + p(u), z = w.

Then, the Eigen equation that can be derived from the differential equation system follows:

$$\mathbf{L}_A \begin{pmatrix} \psi_q \\ \psi'_q \end{pmatrix} = \frac{1}{r_q} \mathbf{L}_B \begin{pmatrix} \psi_q \\ \psi'_q \end{pmatrix}, \tag{1}$$

The matrices L_A und L_B arising from the profile function **p** are:

$$\mathbf{L}_A = \begin{bmatrix} -\alpha\dot{\mathbf{p}} - \dot{\mathbf{p}}\alpha & \mathbf{I} + \dot{\mathbf{p}}\dot{\mathbf{p}} \\ \mathbf{I} & \mathbf{0} \end{bmatrix},$$
$$\mathbf{L}_B = \begin{bmatrix} -\alpha\alpha + n^2\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}, \tag{2}$$

Here, ψ_q denote the Eigen vectors, r_q the Eigen values, **a** is a diagonal matrix, formed by the elements $a_m = \sin\vartheta + m\frac{\lambda}{d}$, **I** the unit matrix and $\dot{\boldsymbol{p}}$ a matrix, formed by the elements

$$\dot{p}_{mn} = \dot{p}_{m-n} = \frac{1}{d}\int_0^d \frac{dp}{du} e^{i2\pi(m-n)\frac{u}{d}} du \tag{3}$$

Further, λ represents the wavelength of light, d the grating period and p the profile function. The matrix $\dot{\boldsymbol{p}}$ is the Toeplitz-matrix of the der Fourier-transform of the profile function derivative.

In contrast to this, an additional coordinate transform of the x-coordinate becomes necessary for the AR-method yielding: x = f(u), y = v + p(f(u)), z = w. In this case, a solution with the same characteristic Eigen system (1) results but with different matrices L_A und L_B:

$$\mathbf{L}_A = \begin{bmatrix} -\alpha\dot{\mathbf{f}}^{-1}\dot{\mathbf{p}} - \dot{\mathbf{p}}\dot{\mathbf{f}}^{-1}\alpha & \dot{\mathbf{f}} + \dot{\mathbf{p}}\dot{\mathbf{f}}^{-1}\dot{\mathbf{p}} \\ \mathbf{I} & \mathbf{0} \end{bmatrix},$$

$$\mathbf{L}_B = \begin{bmatrix} -\alpha\dot{\mathbf{f}}^{-1}\alpha + n^2\dot{\mathbf{f}} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}, \tag{4}$$

$$\dot{f}_{mn} = \dot{f}_{m-n} = \frac{1}{d}\int_0^d \frac{df(u)}{du} e^{i2\pi(m-n)\frac{u}{d}} du \tag{5}$$

This transformation is elaborated in formulas (35) and (36) of /3/ in detail. This schema was extented by us to be applicable for generic piecewise linear profiles.

3. Simulations

The diffraction efficiencies have been calculated and compared for symmetric, metallic trapezoid profiles with slope angles between 60 and 90 degrees for the following methods:

- C-Method with FFT (CC)
- C-Method with discreet FT (1C)

- RCWA /2/
- C-Method with Adaptive Resolution (C-AR).

The results are shown for the zero and first diffraction order in TE- und TM-Polarisation in the following figures.

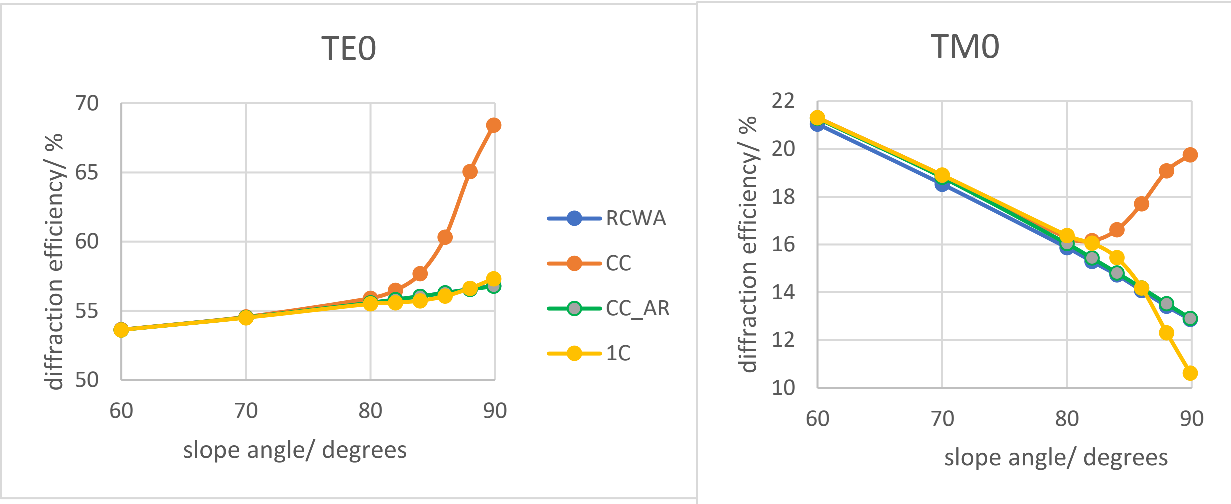

Fig 2: *Comparison of zero order diffraction efficiencies* vs. slope angle for a trapezoid profile

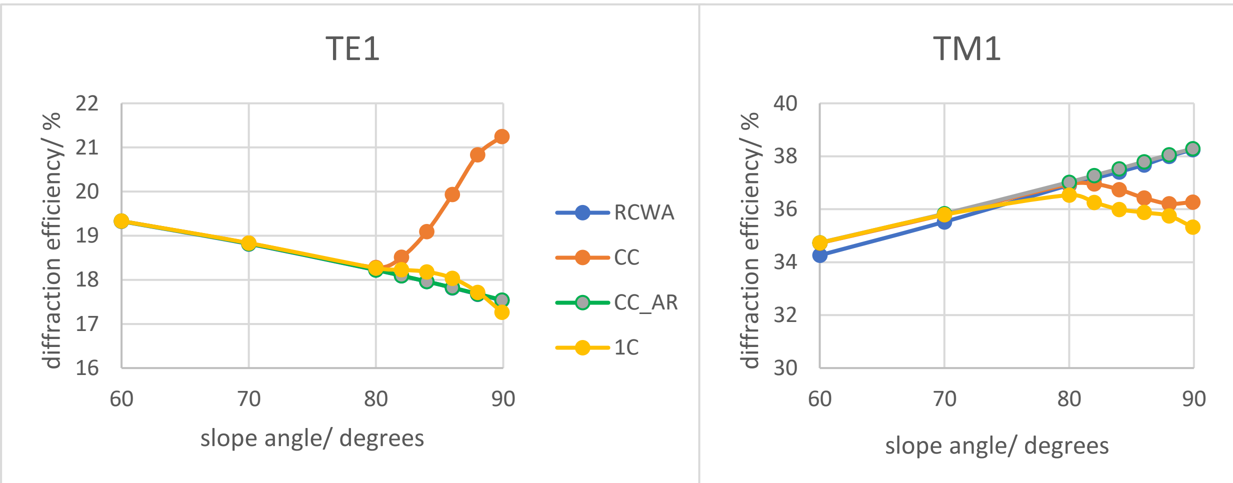

Fig 3: *Comparison of first order diffraction efficiencies* vs. slope angle for a trapezoid profile

Apparently, the results for the C-Method with adaptive resolution are almost identical to those of the reference method RCWA even for slope angles beyond 80 degrees. There are only slight differences for TM-polarisation. These result however from the known issues of RCWA for metallic materials in TM. Furthermore, it is visible that the standard-C-Method for both implementations (with FFT as well as with discreet FT) can be considered to be sufficiently accurate for slope angles up to about 80 degrees. On the other hand, there are clear differences for both implementations beyond 80 degrees. Mostly, the results for discreet FT are closer to the reference (RCWA) and C-AR, respectively.

References

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/2/ Moharam MG, Pommet DA, Grann EB. Stable implementation of the RCWA for surface-relief gratings: enhanced transmittance matrix approach. J. Opt. Soc. Am. **A 12**, 1077-1086 (1995).

/3/ G. Granet, J. Chandezon, J.-P. Plumey, „Reformulation of the coordinate transformation method through the concept of adaptive spatial resolution. Application to trapezoidal gratings," J. Opt. Soc. Am. **A 18** (9), 2102-2108 (2001).