Investigation of Polarization State of Diffraction Orders
Grating structures are widely used for various optical applications, such as spectrometers, near-eye display systems, pulse shaping etc. The fast physical optics software VirtualLab Fusion provides versatile and handy tools for the rigorous analysis of arbitrary grating structures by applying the Fourier modal method (FMM, also known as RCWA). For this purpose, complex 1D- or 2D-periodic structures can be configured using either interfaces and/or modulated media, which allows for a very flexible configuration of any kind of grating profile. In this use case, the investigation of the polarization state of diffracted orders is discussed in detail.
Task Description

ideal plane wave
- 633nm central wavelength
- φ: vary between 0°-90°
- θ: 45°

grating
- 250nm period
- only zeroth reflection order
- structure:
  a) binary grating (ideal case)
  b) binary grating with sloped walls (compared to measurement)

task:
- Calculate efficiency and Rayleigh coefficients as a function of φ.
The efficiency of a diffraction order \((n)\) represents how much of the impinging power is diffracted into this particular order. It is calculated from the complex-valued Rayleigh coefficients, which comprise the full information of the (vectorial) electromagnetic field, per diffraction order. The Rayleigh coefficients themselves are the results of the rigorous analysis of the eigenvalue problem of the grating by FMM.

If the Rayleigh coefficients are given in the TE/TM coordinate system (CS), the efficiency can be calculated by

\[
\eta = \frac{n_{\text{out}}}{A^2 n_{\text{in}} \cos \vartheta_{\text{in}}} \cos \vartheta_{\text{out}} \left[ |R_{n}^{\text{TE}}|^2 + |R_{n}^{\text{TM}}|^2 \right],
\]

where \(n_{\text{in}}/n_{\text{out}}\) are the refractive indices of the superstrate and substrate and \(\vartheta_{\text{in}}/\vartheta_{\text{out}}\) the incidence and diffraction angles of the analyzed order. Furthermore, \(A\) represents the amplitude of the impinging wave.

If the Rayleigh coefficients are given along \(x\), \(y\) and \(z\), the following equation has to be applied:

\[
\eta = \frac{n_{\text{out}}}{A^2 n_{\text{in}} \cos \vartheta_{\text{in}}} \cos \vartheta_{\text{out}} \left[ |R_{n}^{x}|^2 + |R_{n}^{y}|^2 + |R_{n}^{z}|^2 \right].
\]

Hence, the coordinate system of the given Rayleigh coefficients has to be considered. By default, \(R_{n}^{x}, R_{n}^{y}, R_{n}^{z}\) are provided in the CS of the grating.
Grating Structure Parameters

- A grating structure with a rectangular shape is investigated.
- For the sake of simplicity, the configuration of the grating is chosen such that only the zeroth order in reflection ($R_0$) is propagating.
- The following grating parameters are chosen in accordance with the above:
  - grating period: 250nm
  - fill factor: 0.5
  - grating height: 200nm
  - material $n_1$: fused silica (from catalog)
  - material $n_2$: TiO$_2$ (from catalog)
Now, the grating is illuminated with TE-polarized light and a variation of the angle of conical incidence ($\varphi$) is applied.

As mentioned, the squared amplitudes of the Rayleigh coefficients will provide information about the polarization state of the particular order.

In order to receive the Rayleigh coefficients as a detector result, please activate the Single Order Output in the Grating Order Analyzer and choose the desired coefficients.
The Rayleigh coefficients now provide the information of the polarization state:

- In case of non-conical incidence ($\varphi = 0$), $|R^\text{TE}_0|^2$ is 1 (V/m)$^2$, whereas $|R^\text{TM}_0|^2$ is 0. This means the diffracted light is TE-polarized, entirely.

- For $\varphi = 22^\circ$ there is a minimum of $|R^\text{TE}_0|^2$ yielding a value of 0.33 (V/m)$^2$ and a maximum of $|R^\text{TM}_0|^2$ with 0.67 (V/m)$^2$. In this case, 67% of the light is TM polarized.

- For $\varphi > 50^\circ$ the coefficients are almost constant, and thus the polarization as well.
Further Example about Grating by Passilily et al.

- In the work by Passilily et al. the polarization state of light diffracted at a subwavelength grating was investigated and optimized in order to receive a high conversion between different states.
- Thus, they compared simulated results with measurement data of a fabricated sample.
Grating Structure Parameters

• In the cited work, two different fabricated grating structures were investigated.

• Some deviation from the ideal binary shape of the grating caused by fabrication is to be expected and can indeed be observed: under-etching in the substrate and side walls that are not perfectly parallel.

• Due to missing details about the fabricated structure, we have simplified it for the simulation in VirtualLab.

• Nevertheless, should the data be available, the complex shape of the grating could be analyzed in detail.
Grating #1 – Parameters

- The sidewalls are assumed to exhibit a linear slope.
- The under-etched part in the substrate is neglected.
- In order to realize the trapezoidal shape of the grating ridges, the Slanted Grating Medium was applied.
  - grating period: 250 nm
  - grating height: 660 nm
  - fill factor: 0.75 (bottom)
  - angles of sidewalls: ±6°
  - $n_1$: 1.46
  - $n_2$: 2.08
In comparison, both figures exhibit a very good match, especially the course of the graph. There are some small deviations, caused by the simplification of the grating structure in the simulation compared to the reference. The simplifications were necessary due to the lack of data about the actual, more complex, grating structure.
Grating #2 – Parameters

- The grating is assumed to have a rectangular shape.
- The under-etched part in the substrate is neglected.
- A rectangular grating is sufficient to present such kind of grating structure.
  - grating period: 250nm
  - grating height: 490nm
  - fill factor: 0.5
  - $n_1$: 1.46
  - $n_2$: 2.08
Grating #2 – Results

• In comparison, both figures show again a very good match, especially in terms of the course of the graph.
• There are some small deviations, caused by the simplification of the grating structure in the simulation compared to the reference. The simplifications were necessary due to the lack of data about the actual, more complex, grating structure.

Passilly et al. (2008)
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