Comparison of different microscope imaging models for different structure geometries on the basis of rigorous diffraction calculation

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We compared two different rigorous grating diffraction models for modelling of microscope images, the rigorous coupled wave analysis (RCWA) method and the finite elements (FEM) method. Diffraction efficiencies and the resulting microscopic (far field) images for different edge geometries are presented and advantages and disadvantages of each method are discussed.

1 Introduction

High resolution optical microscopy is still an important instrument for dimensional characterisation of micro- und nanostructures. For precise measurements of dimensional quantities a high quality modelling of the optical imaging on the basis of rigorous diffraction calculation is essential, which account both for polarisation effects and the 2D or 3D geometry of the structures.
We use two different rigorous grating diffraction models for modelling of the intensity distribution in the image plane, the rigorous coupled wave analysis (RCWA) method and the finite elements (FEM) method. We investigated the microscopic (far field) images for two different edge geometries: binary and trapezoidal gratings.
Results of this investigation for TE, TM and unpolarised illumination of the gratings are presented.

2 Test suite

Imaging parameters		
Microscope		
Transmission, Koehler illumination brightfield		
Wavelength	365 nm	
Polarisation	TE, TM, unpol.	
Condenser NA	0.6	
Objective NA	0.9	
Magnification	100	
Mask		
	Chrome	Quartz
Thickness	0.1 µm	6350 µm
N	1.843	1.460
K	-2.195	-1E-06
Calculation parameters		
Focus step size	.01 µm	
Output *x* interval	.01 µm	
Feature centred at	x = 0.00 µm	

Tab 1 *Input parameters used for the test suite*

The feature sizes to be modelled range from subwavelength to several wavelengths. They cover a matrix of linewidth and spacewidth of 101nm, 318nm, 1000nm, 3142nm and 9880nm, respectively, for a total of 25 different features. We calculated the normalised image intensity in dependence of the x coordinate for the best focus image. The latter is defined as the plane, with the largest intensity slope near the feature edge at the 50% intensity level. Finally intensity thresholds, the image intensities at the feature edge positions, are determined and compared.

3 Results for binary and trapezoidal gratings

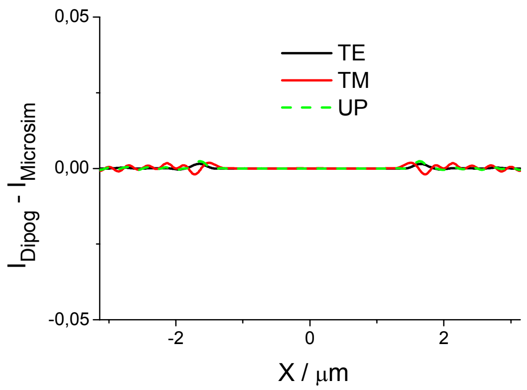

Fig. 1 *Differences between normalised image intensities calculated with FEM (Dipog [1]) and RCWA (Microsim [2]), binary grating: linewidth = spacewidth = 3142nm*

Exemplarily for one structure the intensities differences in the image plane for TE, TM and unpolarised illumination in each case for the corresponding best focal plane are depicted in Figure 1. The agreement between RCWA and FEM is excellent Maximum deviations for each polarisation are about 10^{-3}.
An overview over the results of the complete test suite for the binary gratings is given in table 2. In general there is a very good agreement between FEM and RCWA. The mean differences are typically $\leq 10^{-3}$ and the maximum differences are a few 10^{-3}. However, for the structures having the pitch values > 10µm, the maximum deviation is slightly increased to $1*10^{-2}$ and stronger residual oscillations are observed in the range of maximum transmission.

I_{FEM} - I_{RCWA}		FEM	RCWA	threshold
mean	max	threshold/%	threshold/%	difference / %
5.5E-04	1.6E-03	25.72	25.83	-0.11
1.9E-04	1.1E-03	25.80	25.75	0.05
3.9E-03	7.7E-03	25.27	25.09	0.18
1.0E-03	1.9E-03	30.26	30.28	-0.02
1.1E-03	3.7E-03	18.19	18.06	0.13
7.0E-04	4.5E-03	18.39	18.38	0.02
1.5E-03	4.0E-03	18.32	18.22	0.11
1.9E-03	4.5E-03	22.91	22.90	0.01
6.2E-04	1.1E-03	7.65	7.57	0.08
5.6E-04	2.2E-03	19.47	19.53	-0.07
3.8E-04	3.4E-03	19.32	19.30	0.02
7.4E-04	2.0E-03	19.38	19.36	0.02
1.1E-03	4.5E-03	23.15	22.99	0.16
2.9E-04	1.9E-03	7.21	7.35	-0.13
1.2E-03	4.5E-03	19.33	19.45	-0.12
2.4E-04	2.4E-03	19.37	19.39	-0.02
2.1E-04	2.0E-03	19.41	19.48	-0.07
2.4E-04	2.9E-03	22.78	22.80	-0.02
3.1E-05	7.1E-04	7.05	7.11	-0.06
1.7E-03	1.1E-02	19.35	19.26	0.08
5.5E-04	1.0E-02	19.39	20.15	-0.75
1.6E-04	3.4E-03	19.32	19.56	-0.24
1.2E-04	4.0E-03	22.88	22.57	0.31
6.1E-05	2.2E-03	7.10	7.31	-0.21

Tab 2 *Results of the model comparison for binary gratings: mean and maximum deviation between normalised intensities*

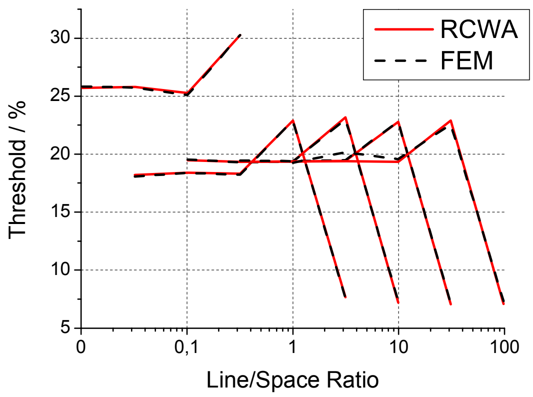

Fig. 2 *Threshold values derived for line arrays with linewidth 0.101, 0.318, 1.000, 3.142 and 9.880 µm (left to right)*

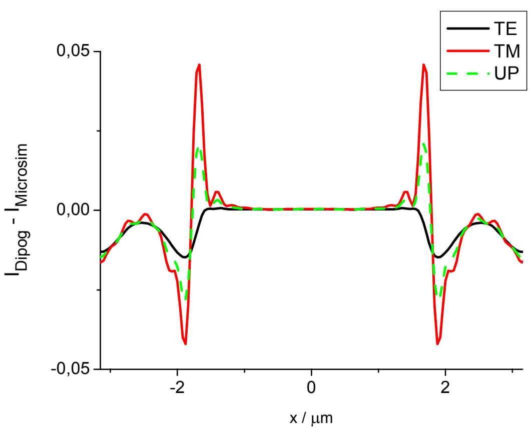

Fig. 3 *Differences between normalised image intensities calculated with FEM and RCWA methods: Trapezoid grating: edge angle 70°, line/spacewidth: 3142 nm*

The threshold values derived from the focal images differ typically over 0.1 - 0.2 % (figure 2).
Figure 3 shows a comparison of the images in the best focal plane obtained for a trapezoidal grating with a line- and spacewidth of 3142nm. For the RCWA modelling we approximated this grating using nine layers of binary gratings.
The images show significantly greater differences than for binary gratings (fig. 1). As compared to the binary grating case the deviations between FEM and RCWA are increased by a factor of 5.

4 Discussion

Our results indicate, that both methods are suitable to model the diffraction of plane waves at binary gratings and corresponding microscope images at a high level of accuracy. The observed deviations of the derived thresholds of 0.1-0.2 % yield differences of 0.5 to 1 nm for linewidth measurement.
Especially for the RCWA method with increasing periods it becomes more difficult to reach sufficient convergence. For gratings with trapezoidal grating the agreement between FEM and RCWA decreases significantly. We ascribe these differences mainly to the RCWA method, which is inherently not so well adapted to more complicated grating profiles. The trapezoid gratings are approximated by staircases of stacked binary layers. The geometrical approximation will improve with an increasing number of binary layers used. On the other hand time and memory consumption increase rapidly with an increasing number of layers. Therefore for gratings with finite edge slopes both in terms of accuracy and computation time the FEM is superior to the RCWA approach.

5 Conclusion

We have presented a comparison of two rigorous diffraction calculation programs for simulation of microscope images for binary gratings and for a trapezoidal grating. For the binary gratings an excellent agreement has been found. For gratings with a more complex edge profile the RCWA method is inferior to the FEM method.
The results obtained in the model comparison will help to reduce significantly the model induced uncertainty contribution in the uncertainty budget of our linewidth calibrations. At least for measurements of rectangular shaped structures this will enable us to reduce the uncertainty contribution due to possible modelling errors to about 1nm.

References

[1] http://www.wias-berlin.de

[2] M. Totzeck: Numerical simulation of high-NA quantitative polarization microscopy and corresponding near-fields, Optik 112, (2001), 399-406