High Resolution Metrology and Simulation

Simulation based sensitivity analysis of scatterometry measurements for future technology nodes
Supported by: BMBF (FKZ 13N9432)
Project: “Nananaßistik”

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Supported by: ASML Netherlands

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Project: “Optim”

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Simulation based sensitivity analysis of scatterometry measurements for future technology nodes

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As part of the BMBF project “Nano-analytik” we have analyzed the extendability of scatterometry towards small ground rules using a simulation based approach. Within the last years, scatterometry has evolved into one of the most important methods for CD metrology used actually in semiconductor industry. As the size of semiconductor structures keeps decreasing with up-coming technology nodes, searching for optimized measurement configurations to exploit maximum sensitivity gets more important. These optimized configurations can be accessed with a simulation based approach using our software package MICROSIM [1] to solve the Maxwell equations with help of the RCWA method.

The first task was to verify the agreement of simulation and measurement of a given structure. Therefore we started with simple line-gratings with different pitch periods, produced with e-beam lithography at Qimonda (Dresden). These structures were measured with an industrial scatterometry tool at Qimonda and the same measurement was modelled and simulated with MICROSIM later. As shown in fig. 1 there is a very good agreement of simulation and measurement for these structures.

The next step comprises the analysis of the sensitivity to different structure parameters as structure-height, CD, pitch, sidewall angle and different roundings by varying the measurement configuration as wavelength and incident angle. Fig 2 shows such a sensitivity plot for the CD parameter of a structure. This sensitivity analysis was also performed for different structure sizes correlating with actual and future technology nodes [2]. Performing such sensitivity analysis makes it possible to predict optimized measurement configurations, possibilities and demands on future industrial scatterometry tools. Further investigations on more complex structures and towards smaller structure size are the next tasks in the project and are work in progress.

Fig. 1: Comparison of a measurement and the corresponding simulation with MICROSIM of a line grating structure.

Fig. 2: Sensitivity of resist line-grating (CD 48 nm) to the structure height in dependence of the wavelength and the incident angle.

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Approximative field stitching algorithm for simulating line edge roughness (LER) in scatterometry

T. Schuster, S. Rafler, V. Ferreras Paz, K. Frenner, W. Osten

Optical scatterometry relies on simulations of light diffraction using rigorous algorithms such as Rigorous Coupled Wave Analysis (RCWA). Up to now, most simulation models neglected any imperfections of the periodic continuation. Since line edge roughness (LER) is presently becoming more crucial in semiconductor technology, one must no longer ignore this perturbation of the periodic continuation. Instead, one has to investigate the influence of light scattering which can arise from LER on the different variants of scatterometry in order to still obtain reliable results.

Recently ITO presented an approach to deal with such imperfections. A well known field stitching algorithm by Layet and Taghizadeh [1] was adopted. Whereas these authors comprised an overlap region in the simulation of single patches to be stitched together in order to be fully rigorous, we skip this overlap and thus introduce Kirchhoff-boundaries, i.e. the fields at these virtual lateral boundaries feature unphysical leaps which is the key point of Kirchhoff’s diffraction theory.

The idea of applying Kirchhoff’s approximation to present dense line structures with, e.g., 50 nm CD and 100 nm pitch appears incomprehensible at first glance bearing typical interaction lengths of 5–10 wavelengths in mind. However, Kirchhoff’s approximation can be applied whenever the influence of the unphysical leaps is small. This is the case when structures are sufficiently large such that the overall portion of the erroneous nearfield is small, but also, if the leaps themselves are small compared to the absolute values of the fields. Considering LER a small perturbation of a perfect periodic structure is hence a good justification for applying Kirchhoff’s approximation. Of course, the approximation is better the smaller the LER amplitude and depending on the acceptable error a threshold for its validity can be defined.

The range of validity of the proposed method was investigated. The method proved to be applicable to the problem if the LER amplitudes are sufficiently small. Figure 1 shows an example nearfield for the case of a relatively large LER amplitude of 4 nm peak to peak and a wavelength of 400 nm. The illumination is a single plane wave with almost grazing incidence. The leaps in the field amplitude are small but clearly recognizable. Figure 2 shows the field amplitude of the 0th diffraction order of the resulting farfield for the stitched and unstitched case. The peak to peak depth of the LER is gradually increased in order to study the error of the stitched field amplitude as a function of a small perturbation of the periodic continuation. As can be seen the errors keep acceptable for roughness depths of a few nanometers. A more detailed review of these activities is given in [2].

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Recent extension of our simulation tool ITO-Microsim:
Automated normal vector field generation

T. Schuster, P. Götz, K. Frenner, S. Rafler, W. Osten

The rigorous Maxwell solver ITO-Microsim has been under constant development for many years. Recently, the convergence of the diffraction computation using Rigorous Coupled-Wave Analysis (RCWA) has been improved for the case of 2D periodic gratings.

The achieved convergence improvement is based on Popov’s and Nevière’s reformulation of the differential method [1] which is closely related to RCWA. After a long discussion these authors recognized that prior convergence problems due to an erroneous application of convolution rules in discrete Fourier space can be overcome by decomposing the electric field in real space into a component parallel and perpendicular to each point of a material boundary and taking the information about the local orientation of the boundary over to Fourier space by a Fourier expansion of the normal vector (NV) field.

To that end a continuation of the NV field from the material boundaries toward the homogeneous regions is required. Applying this technique to the RCWA poses the additional restriction that the NV field must point only in lateral directions which inevitably introduces singularities and/or discontinuities, c.f. Fig. 1.

While in a first work [2] semi-automated algorithms with moderate computational efficiency served the purpose to demonstrate the principle of the method, the recent improvements [3] consist of a fully automated NV field generation with optimized performance. The new algorithm can cope with arbitrarily shaped geometries, unit cells with three or more different materials and even multiply connected regions.

The NV generation consists of two steps. In a first step the NVs at the material boundaries are computed by a simple gradient operation. In the second step the remaining points of a Cartesian raster are filled by an interpolation relying on inverse distance weighting. This way the discontinuities in the NV field are placed in sufficient distance to the boundaries. The numerical complexity of this interpolation can be reduced from $O(n^3)$ to $O(n^2)$ by a progressive refinement algorithm which ensures that the gain of computational speed is not wasted by additional costs for the NV field generation.

Figure 1 shows the NV field for a structure of intersecting circles obtained with the new algorithm. The corresponding convergence curves labeled “NV method without preferred direction” can be seen in Figure 2. They are compared to an alternative version of the algorithm “… with preferred direction” and previous RCWA formulations which feature poorer convergence. For details please refer to [3].

**References:**


Design of Optical Metamaterials with respect to near-farfield-transformation

S. Maisch, K. Frenner, W. Osten

After the theoretical prediction of V. Veselago[1] in 1976, materials with simultaneous negative magnetic permeability $\mu < 0$ and electric permittivity $\varepsilon < 0$ being able to transmit electromagnetic waves without exponential damping, J. Pendry [2] showed these systems bending light in the “wrong direction”, namely showing a negative index of refraction $n < 0$.

These materials gained attention because they can be used for sub-\(\lambda\) resolution imaging and invisibility cloaking.

The main problem was and remains the fact that metamaterials have to consist of internal features smaller than the wavelength used, but for applications in the optical range still larger than typical molecular structures or lattice constants. While being relatively simple to be built for the microwave range by a spatial arrangement of electrical resonators of millimetre size, at optical and infrared frequencies, the resonator size is in the nanometre range requesting the most advanced nano fabrication tools for their construction.

We performed a careful evaluation of layered metamaterials of resonant gold and silver structures in dielectric resin by RCWA (rigorous coupled wave analysis) simulation of their effect on the phase and amplitude of the transmitted light and calculating an effective index of refraction of these materials. These results are used in a closed-loop process to geometrically optimize nano patterned metamaterials.

Fig. 1 shows a four-layered resonant structure (split ring resonator, SRR) used as one example and manufactured by the 4th Physics Institute, among other radically different structures as a starting point for the optimization of the negative magnetic response by variation of the geometric parameters. RCWA is capable of simulating the optical properties of these structures including the effects of mutual coupling of the resonators.

![Fig. 1: Four-layered resonant gold nano structure and its geometric parameters.](image1)

In fig 2 the simulated transmission and reflection spectra of the SRR are shown. Fig. 3 shows the retrieved index of refraction for a different meander nanostructure exhibiting a strongly negative resonance.

![Fig. 2: RCWA-simulated transmission (T) and reflection (R) spectra (left), and index of refraction (right) of the structure in fig. 1, in s- and p-polarization.](image2)

![Fig. 3: Retrieved real part $n$ of the refractive index for a meander nanostructure. Just above a wavelength of 500 nm the index of refraction exhibits strongly negative behaviour.](image3)

These materials are suited for the design of Pendry’s superlens, capable of imaging the near-field. Further research is about magnifying super lenses using geometric shape functions and a near-field to far-field transformer. Both RCWA and differential method analysis were performed on magnifying superlens designs.

These investigations showed meander shaped nanostructures being well suited for manufacturing negative index materials. Their optical properties may be tuned similar to the SRRs, while being less demanding in the nano patterning process, allowing metamaterials at visible wavelengths instead of near IR.

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Defect detection on Wafers: Simulation and Measurement

S. Rafler, T. Schuster, K. Frenner, W. Osten

In the BMBF project “Nano Analyik” the ITO works on with its industry partner Qimonda within the subtopic „Defectoscopy“. The goal in this subtopic is the derivation of methods for the prediction of defect signal strengths for certain configurations of inspection tools.

The inspection system in our case is a microscope with high NA objectives, monochromatic Köhler illumination and pupil filters. The image is generated on a CCD camera. Such a microscope is available in the ITO clean room and we can get samples from the inspection systems at Qimonda.

Since the defects are of nanometer size (Fig. 1) they are not resolved, although UV illumination can be used. Nonetheless one can see dark or light spots where the defect is in the surrounding field without defects (Fig. 2). The contrast of this defect signal to the surrounding pattern noise is the value which is crucial for the successful detection of the defect. One can enhance the contrast, i.e. the signal to noise ratio, by varying optical system parameters.

To be able to get ahead of the current node in the development of even smaller technologies, one seeks to simulate the defect detection. This is done at the ITO with the program package Microsim which was developed at the institute and is based on the Rigorous Coupled Wave Analysis. The advantage of this method is that once the diffraction orders of the structure of interest have been computed, the far field image can be generated in short time. In the course of this an arbitrary set of diffraction orders can be left out to model different pupil filters.

The defect types of interest require the time consuming simulation of two-dimensionally periodic gratings. In the project several methods to shorten this time have been implemented [1]. Symmetries of structure and illumination are used and for orthogonal polarizations only one computation has to be carried out. Furthermore the computation has been parallelized so it can run on several computers at once.

Littrow angles play a special role in the discretization of the illumination pupil [2]. First they allow the optimal approximation to the theoretically infinite densely sampled pupil (Fig. 3) and second they allow to use information from the normal incidence computation to be used for the oblique incidence angles which saves most of the computation time. In the course of the project we must now bring simulation and measurement together more closely by modeling the structures in a more complex way and by testing a whole range of parameters.

Fig. 1: SEM picture of an "open" type defect.

Fig. 2: Simulated defect type "open" as seen in an optical microscope.

Fig. 3: Convergence of the signal to noise ratio with respect to the pupil discretization step.

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