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TECHNISCHE OPTIK
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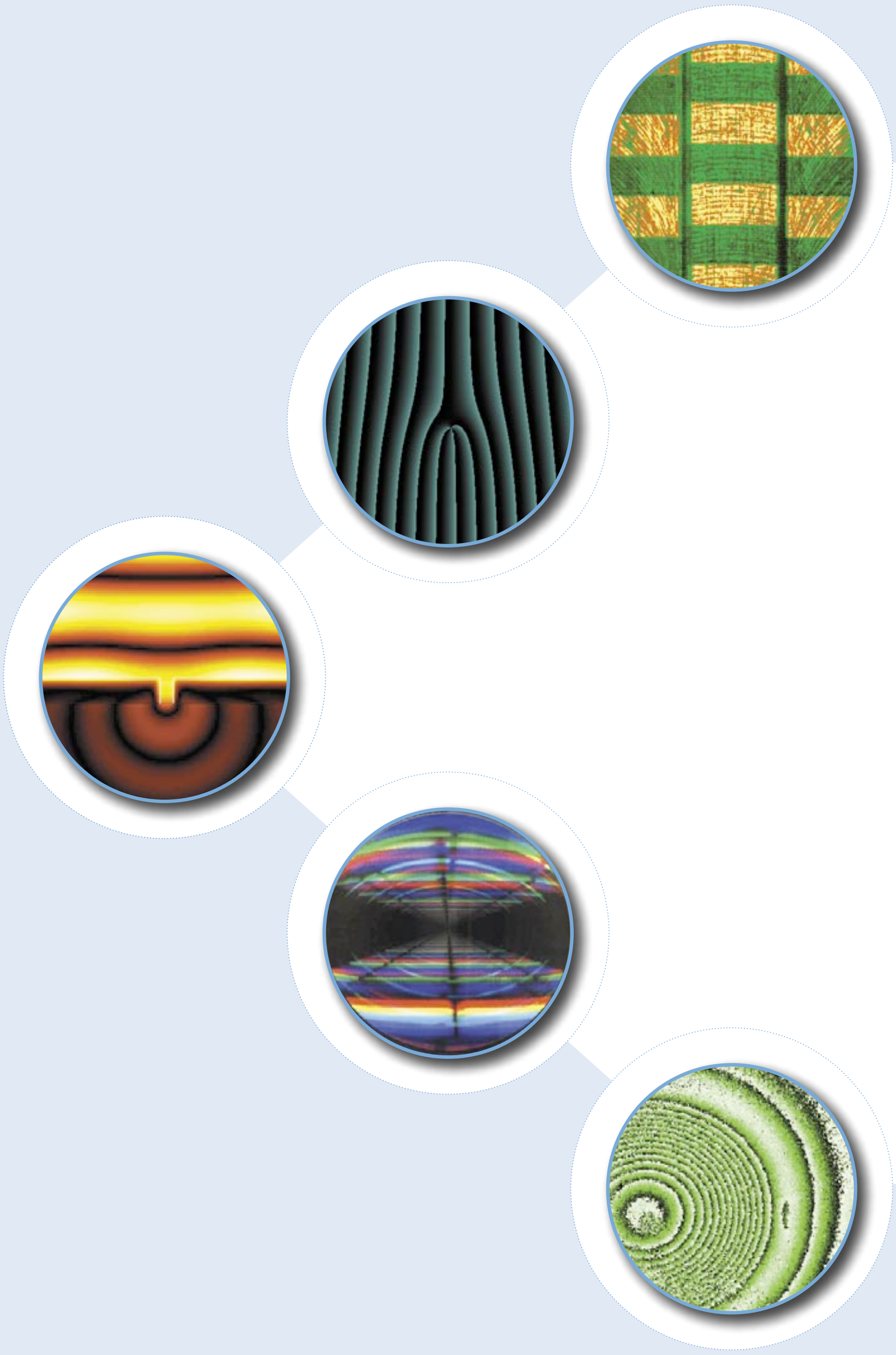


Universität Stuttgart

High Resolution Metrology and Simulation

Simulation of diffraction at large structures using the fieldstitching method

Scatterometry from arbitrarily shaped 3-D structures:
Comparison between experiment and simulation
Supported by: BMBF FKZ 01M3154D and 01M3131540
Project: "Abbild Part 1 / 2"

Tensor-tomography: Reconstructing a cube of fused silica using projections from three directions

MICROSIM – ITO's Rigorous 3D-Maxwell Solver

New developments in our simulation tool MicroSim:
Convergence improvement for RCWA for crossed grating structures using normal vector fields

Simulation of diffraction at large structures using the fieldstitching method

S. Rafler, T. Schuster, N. Kerwien, W. Osten

A part of the Landesstiftung project “Rigorose numerische Simulation in Optik-Design und hochauflösender Messtechnik (RISOM)” was the investigation of simulation methods for large structures such as diffractive optical elements. As this is not possible in a single rigorous computation when using a method such as the RCWA, due to the size of the simulation area, we have implemented the field-stitching method of Layet and Taghizadeh. This method allows the simulation area to be split in sections that can be computed separately on a desktop PC.

A large aperture, such as the DOE depicted in Fig. 1, is divided into equally spaced sub-apertures. These sub-apertures overlap on the left and right edge. They are treated as local gratings in the following rigorous calculation. The overlap is necessary to minimize the error coming from the "wrong" continuation at the edges of the local grating periods. The bigger the overlap, the smaller the error. We have verified a 10λ distance to yield converged results in all cases. We have computed the nearfields of the sub-apertures (with overlap) with our tool MicroSim to show that they do not deviate significantly from the nearfields of the whole structure computed without field-stitching.

The obtained diffraction orders of the local calculations are taken as Rayleigh coefficients at the top (or the bottom) of the local structure. The field expressed in these Fourier-coefficients is equated with the field at top of the whole structure. Then the Rayleigh coefficients and subsequently the diffraction orders of the whole DOE can be obtained.

For the test structure depicted in Fig. 1, which consists of randomly spaced areas of random refractive indices, the amplitude and phase errors have been investigated. The results can be seen in Figs. 2 and 3.

The field-stitching method offers the possibility of combining faster (e.g. scalar) methods to simulate areas of a structure showing feature sizes well above the considered wavelength with rigorous calculations of areas of the structure showing subwavelength features. It is, however, only useful if the overlap of 10λ can be taken into account. So the aperture size should be 100λ or greater.

Also, 2-D Fieldstitching has been investigated. Unfortunately the 10λ overlap zone rules this approach out for practical use at the moment.

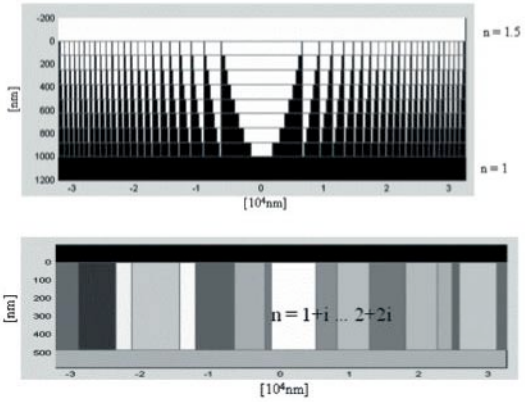


Fig. 1: Structures used for test purposes (modeled with MicroSim)

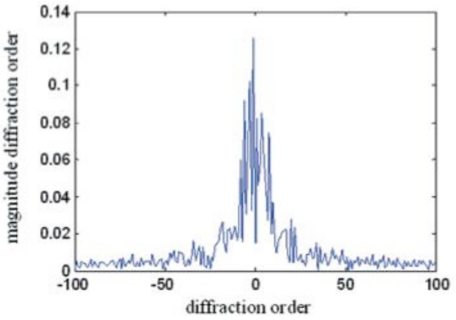


Fig. 2: Diffraction amplitudes for random test structure (computed with MicroSim)

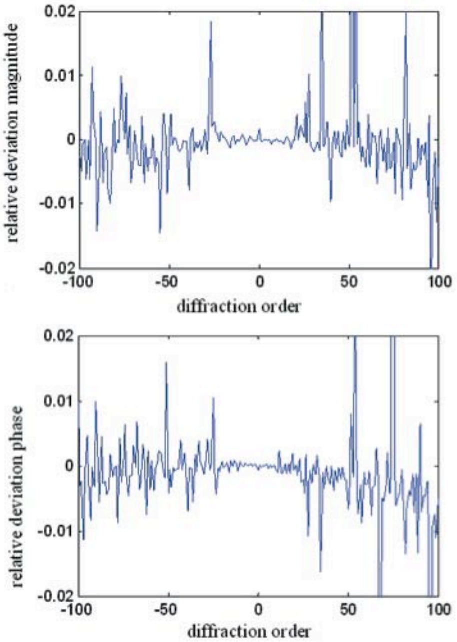


Fig. 3: Errors in the amplitude and phase of the field-stitching calculation compared with the full aperture calculation

Scatterometry from arbitrarily shaped 3-D structures: Comparison between experiment and simulation

T. Schuster, S. Rafler, N. Kerwien, W. Osten

In two consecutive BMBF projects Abbild 1 and Abbild 2 ITO has been a partner and subcontractor of Qimonda, formerly Infineon Technologies. The subject of the work at ITO is the investigation of scatterometry for CD metrology in simulation and experiment.

As was reported in the annual report 2003 / 2004, in the beginning of the project the main focus was on simulation. ITO's simulation tool MicroSim, which comprises an RCWA module, was extended for scatterometry for this project. The accuracy of the simulation results depends on the various input parameters was investigated. A study of sidewall roughness and linewidth fluctuations was carried out and presented on CLEO Europe in Munich [1].

More recently, the RCWA routines have been extended to arbitrary 3-D structures with the aim of matching simulated scatterometric signals with measured ones. Both tasks, the implementation as well as the comparison between simulation and experiment, will be reported below.

As scatterometry is already well established for 2-D structures (line gratings), it was desirable to extend MicroSim to arbitrarily shaped 3-D structures. Fig. 1 depicts the new structure types using a top down view onto an elementary cell. The cell is continued periodically in both directions of the drawing plane. Three structure types can be processed using analytical Fourier series expansion: a rectangle, an ellipse and even a polygon. For totally arbitrary structures, the grating type 'cavity' was introduced, which makes use of the Fast Fourier Transform. The aspect ratio of the elementary cell is arbitrary as well as the number of Fourier modes accepted in the two directions of periodic continuation. Layer stacks of such structures open up virtually endless possibilities for defining structures.

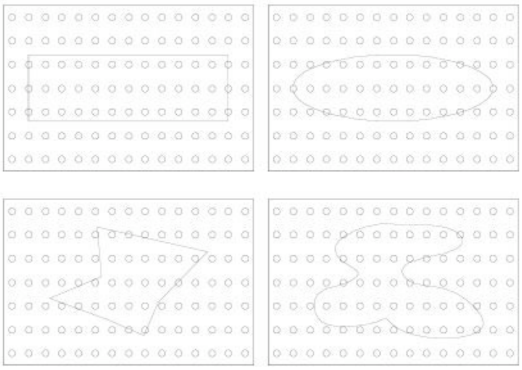


Fig. 1: New structure types in MicroSim.

The new possibilities in MicroSim have been applied to asymmetric nanostructures from Qimonda. A good qualitative agreement between simulation and measurement could be observed, c.f. Fig. 2. The results were presented on the DGaO Jahrestagung 2006 in Weingarten [2]. For a quantitative matching of the spectra an improved modelling is required. One main subject of the present work consists in improving the modelling of structures for RCWA simulations on the basis of SEM images. Apart from that, novel measurement configurations like a ϕ-scan are investigated. This means, that a sample with asymmetric structures is rotated during ellipsometric measurements around its axis. First results will be presented on the "Optical Metrology" SPIE conference in Munich in June [3].

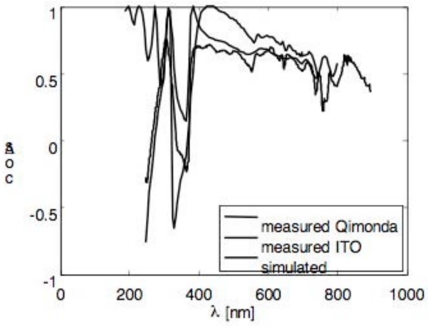


Fig. 2: Comparison simulation and measurement

Supported by: BMBF FKZ 01M3154D and 01M3131540
Project:"Abbild Part 1 / 2"

References:

[1] Schuster, T.; Kerwien, N.; Osten, W.; Reinig, P.; Moert, M.; Hingst, T.; Mantz, U. "Effect of linewidth fluctuations and sidewall roughness in scatterometry", Talk on "Conference on Lasers and Electro-Optics" (CLEO Europe), Munich June 12-17 2005.

[2] Schuster, T.; Kauffmann, J.; Kerwien, N.; Tiziani, H.J.; Osten, W.; Reinig, P. "Scatterometrie an Kreuzgitterstrukturen", Proc. DGaO 2006, Weingarten.

[3] Schuster, T.; Rafler, S.; Osten, W.; Reinig, P.; Hingst, T. "Scatterometry from crossed grating structures in different configurations", Proc. SPIE 6617, 2007.

Tensor-tomography: Reconstructing a cube of fused silica using projections from three directions

J. Kauffmann, H.J. Tiziani, W. Osten

Transparent bulk components show anisotropic inhomogeneities of their refractive index. These components can be for example glass blanks for high precision optics or polymer melts for rheological studies. Fig. 1 shows a model of such a spatial distribution of the refractive index ellipsoids.

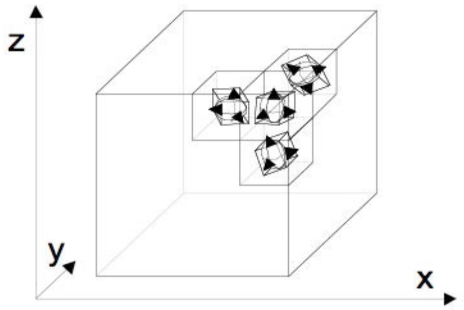


Fig. 1: Model of the spatial distribution of the refractive index ellipsoids.

Optical tensor tomography reconstructs 3D tensor fields of transparent bulk components from Jones matrix measurements taken from different projection directions. The 3D tensor fields are the anisotropic refractive index ellipsoid variation.

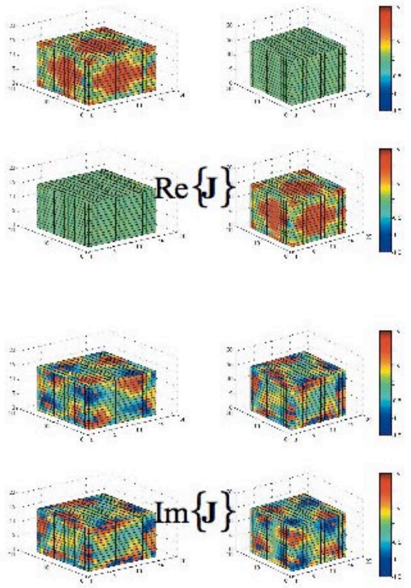


Fig. 2: Jones matrix of a cube measured from three projection directions.

A measurement of a fused silica cube (18cm x 18cm x 18cm) is shown in Fig. 2. Just three projections from the sides of the cube were used, with 15 x 15 measuring points. The Jones transition matrices were measured with a commercial Jones polarimeter at Carl Zeiss SMT AG. Reconstruction using a 17x17x17 cell model is shown in Fig. 3.

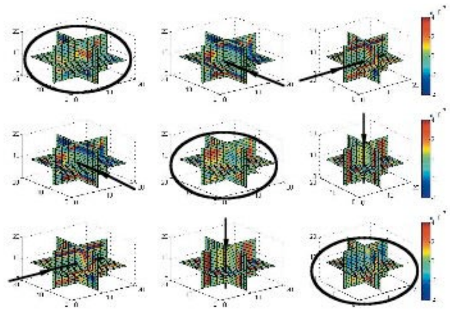


Fig. 3: Reconstruction using a 17x17x17 cell model

The diagonal tensor elements can be resolved in depth. However due to the tensor projection the off diagonal elements cannot be resolved in depth with just three projections. Also on the cubes the effect of corner clamping and gravitation effects on birefringence can be seen. The consistency of the reconstruction was tested by simulating a measurement with the reconstructed anisotropic inhomogeneity. Comparing that to the actually measured values results in a correlation of better then 0.95.

The contributions from Michael Totzeck, Birgit Enkisch, Ralf Müller and Daniel Krähmer and the financial support by the Photonics BW are gratefully acknowledged.

References:

[1] Kauffmann, J.; Kerwien, N.; Tiziani, H.J.; Osten, W. "3D anisotropy reconstruction: an iterative tensorial tomographic algorithm" Proceeding of the ICO, 615-616, 2004 Tokyo

[2] Kauffmann, J.; Kerwien, N.; Tiziani, H.J.; Osten, W. "Tomographic methods to characterize three-dimensional refractive index inhomogeneities" ASPE 2005 Summer Topical Meeting, Middletown, USA

MICROSIM – ITO's Rigorous 3D-Maxwell Solver

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

MICROSIM is a software package for the full numerical simulation of Maxwell equations, without physical approximation in the diffraction problem domain. In addition to its simulation features, the calculation and visualization of the corresponding near-fields and microscopic far-field images are also possible. The applications of MICROSIM range from rigorous treatment of scatterometry and diffractometry, e.g. for semiconductor industry, to near-field calculations and systematic investigations of microscopic imaging techniques.

MICROSIM is completely implemented in Matlab. This allows us to combine the necessary flexibility required for a research environment with a user-friedly graphical interface. Due to MICROSIM's modular structure, extensions and adoptions of the simulation kernel to different project related demands can be performed quickly and easily.

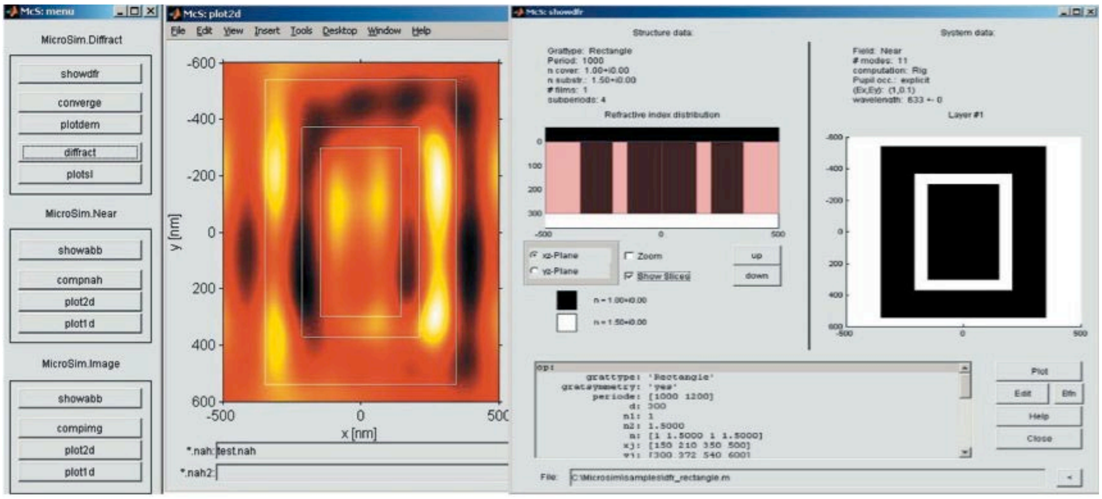
The diffraction spectrum computed with the program module *Diffract* is the basis for the calculation of the corresponding near and far-fields. It provides complete information on the grating in the pupil-plane of an imaging system. *Diffract* is based on rigorous coupled wave analysis (RCWA), in combination with the enhanced-transmittance-matrix approach. This provides the coupling of different grating layers. The parameters for the structure, illumination and computation are defined in a Matlab-file and can be visualized and changed in a GUI. The whole operation of the program can be done via this interface (Fig. 1) or with batch-files for systematic variations of parameters in overnight-computations.

MICROSIM provides different classes of gratings in 2D and 3D. The implemented 2D structure types consist of line-gratings with multiple layers, where in each layer the refraction index is piecewise constant but otherwise arbitrary.

In the 3D case different cross-sections are implemented. These include circles, squares, ellipses and rectangles with different grating-periods in the x- and y-directions, as well as structures within any given user defined boundary in the framework of RCWA.

In order to compute near- or far-fields for arbitrary illumination conditions, the diffraction spectrum has to be calculated for a group of different plane waves which are defined by a set of polarisation-states, wavelengths and angles of incidence. When the complete rigorous diffraction spectrum in the pupil-plane becomes accessible, different microscopic imaging techniques can be simulated by appropriate filtering in the pupil-plane. These include bright field microscopy under full consideration of polarisation dependent aberrations and apodisations, dark-field imaging, Zernike phase contrast, interference microscopy and different types of polarisation microscopy.

The computation of the near-fields in particular offers a deep insight into the interaction of the light with the structure and thus also into the optical image formation by the consideration of evanescent field components. These modes carry the complete high resolution information of the structure. Because of their exponentially short range they don't contribute to the far field, so they don't become directly apparent in the microscopic far-field image.



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*.nah2:

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Period: 1000
n cover: 1.00+i0.00
n substr.: 1.50+i0.00
films: 1
subperiods: 4

Field: Near
modes: 11
computation: Rig
Pupil occ.: explicit
(Ex,Ey): (1,0.1)
wavelength: 633 +- 0

● xz-Plane
○ yz-Plane
☐ Zoom
☑ Show Slices

■ n = 1.00+i0.00
□ n = 1.50+i0.00

```
op:
        grattype: 'Rectangle'
    gratsymmetry: 'yes'
         periode: [1000 1200]
               d: 300
              n1: 1
              n2: 1.5000
               n: [1 1.5000 1 1.5000]
              xj: [150 210 350 500]
              yj: [300 372 540 600]
```

File: C:\Microsim\samples\dfr_rectangle.m

Fig. 1: typical Screenshot of the MICROSIM graphical user interface

New developments in our simulation tool MicroSim:

Convergence improvement for RCWA for crossed grating structures using normal vector fields

T. Schuster, J. Ruoff (Carl Zeiss SMT), N. Kerwien, S. Rafler, W. Osten

MicroSim is a versatile simulation package for computing grating diffraction and high NA microscopic images [1]. The mainly applied method in the diffraction module is rigorous coupled wave analysis (RCWA). MicroSim was developed in the late 1990's at ITO and since then has been under constant development.

Recently an improvement of the convergence of RCWA for crossed grating structures was proposed by ITO and Carl Zeiss [2]. RCWA is based on a Fourier series expansion. In order to save computation time as few Fourier coefficients (modes) as necessary to obtain a sufficiently accurate result are retained. The complexity of RCWA applied to crossed gratings with the truncation order n is $O(n^6)$; thus it is a great benefit to reduce the number of required Fourier modes for crossed grating structures.

The proposed improvement is based on the reformulation of the differential method of Popov and Nevière. The key point in this formulation is to find a normal vector (NV) field which is orthogonal to the material boundary and which contains the local orientation of the material boundary. This information has to be transferred to Fourier space, in order to correctly form the product $D=\varepsilon \cdot E$ as a convolution in Fourier space. To this end the NV has to be continued throughout the complete elementary cell. This continuation, however, is not unique and different continuations can lead to different convergence behavior. The theoretical details of this procedure are omitted here for the sake of brevity, but can be found in [2].

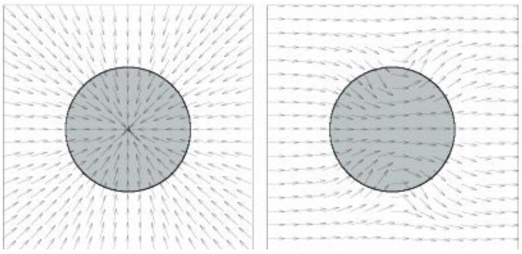

Fig. 1: Possible NV field for a circle

For various example structures we set up different types of NV fields. Fig. 1 shows two possible fields for an array of circles, each of the shown square cells is continued periodically in both directions of the plane to form a grating structure. The NV field on the left hand side (named "radial") shows discontinuities at the cell boundaries, which should be avoided using Fourier series expansion. The field on the right hand side (named "electrostatic"), however, shows two point singularities on the material boundary, i.e. two points where field is not normal to the boundary.

It can be seen that setting up an ideal NV field is impossible. Nevertheless, the convergence of the proposed formulation of the RCWA using either of the two NV fields is better than the formulations known from the literature. The convergence curves are depicted in Fig. 2. The previous formulations are denoted by "Li" and "Moharam". For details please see [2].

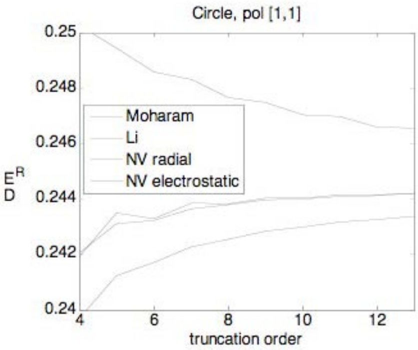

Fig. 2: Convergence curves for an array of circular cavities

References:

[1] Totzeck, M. "Numerical simulation of high-NA quantitative polarization microscopy and corresponding near-fields", Optik 112 No. 9, 399-406, 2001

[2] Schuster, T.; Ruoff, J.; Kerwien, N.; Rafler, S.; Osten, W.; "Normal vector method for convergence improvement using the RCWA for crossed gratings", S. Opt. Soc. Am. A 24 No. 9, 2880 - 2890, 2007.

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