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Depth sensitive Fourier-Scatterometry for the characterization of sub-100 nm periodic structures

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\textbf{Abstract} Recently Fourier-Scatterometry has become of increasing interest for quantitative wafer metrology. But also in other fields the fast and precise optical characterization of periodical gratings of sub 100 nm size is of great interest. We present the application of Fourier-Scatterometry, extended by the use of the coherent properties of white light for the characterization of sub-wavelength periodic gratings of photosensitive material structured by two-photon polymerization. First a simulation-based sensitivity comparison of Fourier-Scatterometry at one fixed wavelength, Fourier-Scatterometry using a white light light source and also additionally using a reference-branch for white-light-interference has been carried out. The investigated structures include gratings produced by two-photon polymerization of photosensitive material and typical semiconductor test gratings. The simulations were performed using the rigorous-coupled-wave-analysis included in our software package MicroSim. A sensitivity comparison between both methods is presented for the mentioned structure types. We also show our experimental implementation of the measurement setup using a white-light-laser and a modified microscope with a high-NA (NA: 0.95) objective as well as a Linnik-type reference branch for the phase sensitive measurements. First measurements for the investigation of the performance of this measurement setup are presented for comparison with the simulation results.

\textbf{Keywords} Fourier-scatterometry · white light interferometry · high resolution metrology · sensitivity analysis · two-photon-polymerization · pupil-plane scatterometry
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ABSTRACT

Recently Fourier-Scatterometry has become of increasing interest for quantitative wafer metrology. But also in other fields the fast and precise optical characterization of periodical gratings of sub 100 nm size is of great interest. We present the application of Fourier-Scatterometry, extended by the use of the coherent properties of white light for the characterization of sub-wavelength periodic gratings of photosensitive material structured by two-photon polymerization. First a simulation-based sensitivity comparison of Fourier-Scatterometry at one fixed wavelength, Fourier-Scatterometry using a white light light source and also additionally using a reference-branch for white-light-interference has been carried out. The investigated structures include gratings produced by two-photon polymerization of photosensitive material and typical semiconductor test gratings. The simulations were performed using the rigorous-coupled-wave-analysis included in our software package MicroSim. A sensitivity comparison between both methods is presented for the mentioned structure types. We also show our experimental implementation of the measurement setup using a white-light-laser and a modified microscope with a high-NA (NA: 0.95) objective as well as a Linnik-type reference branch for the phase sensitive measurements. First measurements for the investigation of the performance of this measurement setup are presented for comparison with the simulation results.

Keywords: Fourier-scatterometry, white light interferometry, high resolution metrology, sensitivity analysis, two-photon-polymerization, pupil-plane scatterometry

1. INTRODUCTION

Scatterometry is a method to analyze the diffraction spectrum from a periodic arrangement of nanostructures. It is used to reconstruct the unknown structure parameters by comparison of measured and simulated spectra. Scatterometry itself is an umbrella term for different measurement configurations such as spectroscopic ellipsometry\cite{1}, 2-\textdegree-scatterometry\cite{2}, normal incidence reflectometry\cite{3} or angular resolved Fourier-Scatterometry\cite{4}. An overview about different techniques related to scatterometry is given by Raymond\cite{5,6}.

For spectroscopic ellipsometry a fixed angle of incidence is chosen and the wavelength is varied while the ellipsometric angles (\(\Delta, \Psi\))\cite{7} or related quantities are measured at the position of 0\textsuperscript{th} diffraction order. In contrast for 2-\textdegree-scatterometry the wavelength is fixed and the incidence angle \(\Theta\) is varied measuring the diffraction efficiency of the 0\textsuperscript{th} order. These configurations can be achieved with an experimental setup as shown schematically in Figure 1.

In Fourier-Scatterometry the angular response of a sample is transformed to spatial information which can be imaged by a camera. Using a K\text{"o}hler illuminated bright-field microscope with a high-NA objective the sample is illuminated with wide incident and azimuthal angle ranges at the same time. In the imaged pupil plane each incident and azimuthal angle corresponds to one specific position in this way allowing to analyze the angular response without the need of any mechanical scanning. Having all this information available in one shot makes this method very promising for the more and more challenging task of profile metrology\cite{8}, with its often low depth sensitivity, for very small periodic structures and also Line Edge Roughness detection\cite{9,10} as used in modern semiconductor products. For that the interest in this method has grown in recent time\cite{4,11}. On the other side scanning white-light interference microscopy\cite{12} is widely used for non-contact, high-speed 3D surface metrology providing sub-nm resolution for topographic measurements.
Combining both methods, the profile-sensitive Fourier-Scatterometry and scanning white-light interference microscopy with its high topographic sensitivity by evaluating phase information is a promising approach for getting a very powerful model-based profile metrology instrument. De Groot et al. showed that imaging the pupil plane allows measuring the incident angle dependent angular response and additionally using Fourier analysis of the white-light signal even allows wavelength dependent measurements with only one measurement [13].

The measurement configuration can be seen in Figure 5.

Beside applications in metrology for semiconductor industry there are many other fields where a fast, optical non-contact method is needed for profile reconstruction of periodic nanostructures often in the regime of sub-wavelength critical structure dimension and structure period. For that we show the application of Fourier-Scatterometry and also white-light interference Fourier-Scatterometry for the profile reconstruction of line gratings of photoresist produced by two-photon-polymerization (2pp) technique at the Laser Zentrum Hannover [14,15].

2. SIMULATION

For the simulation of the scatterometric signals we use a rigorous diffraction computation based on the RCWA (rigorous coupled wave analysis). We use the software package MicroSim [16] which is under constant development at the Institut für Technische Optik (ITO). State of the art RCWA algorithms [17-19] are included. It allows simulation of diffraction from arbitrary 3D structures [20] and also implements some improved convergence behavior [21].

The modeling of our light-source is done by an illumination pupil sampled with an equidistant grid of points which are defined by their NA coordinates $N_{A_x}$ and $N_{A_y}$ with $|N_{A_x}| < 0.95$. Each point in the illumination pupil corresponds to one incident plane wave for which the diffraction spectrum is calculated with the RCWA. The calculated electric fields for each diffraction order have to be incoherently superposed in a post-processing in order to get the incoherent pupil-image. Additionally to take into account white-light the calculation has to be done also for every wavelength. Again the fields are incoherently superposed.

For the case of having a reference branch we need to model the beamsplitter and to superpose the electric field reflected by the reference mirror. This is done with help of classical Jones-Matrix calculus. Each optical element can be freely described by its corresponding Jones-Matrix. The position of the reference mirror is taken into account by a phase term depending on the position $z$ of the reference mirror. For an interferometric z-scan the object side diffraction is rigorously calculated while the reference branch and actual z-scan can be modeled fast even though precisely with Jones calculus getting a resulting pupil image for each z-position.

For being able to accurately model the experimental setup apart from being able to include the Jones Matrix description of beamsplitter and reference mirror we additionally include the spectral intensity distribution of the used white light laser and also the spectral response of the used CCD-Chip in our calculations.
3. **SENSITIVITY ANALYSIS**

We computed the pupil image for three different measurement configurations for 2pp structures on a glass substrate, on silicon, as well as for e-beam photoresist on silicon and calculated the sensitivity towards different parameters of interest.

### 3.1 Sensitivity measurands

To have some kind of measurand for the sensitivity towards a parameter of interest we use conventional uncertainty analysis as defined in the ANSI Guide to the Expression of Uncertainty in Measurement. Some explanations about the application towards scatterometry have been done by Silver et al.[22]. An actual implementation for the calculation of the 3-σ-uncertainty and the covariance matrix used to calculate the correlation between different parameters of interest can be found in Numerical Recipes in C[23].

Using that information we come to the following formulas for the calculation of the $2\sigma$-uncertainty and the covariance matrix for our application:

\[ \sigma_{jk} = \sum_{k=1}^{N} \frac{1}{\sigma_k^2} \left[ \frac{\partial I_k}{\partial x} \right] \left[ \frac{\partial I_k}{\partial y} \right] \]  \hspace{1cm} (1)  

\[ [C_{jk}] = [\sigma_{jk}]^{-1} \]  \hspace{1cm} (2)  

\[ \Delta a_k = 2 \sqrt{C_{kk}} \]  \hspace{1cm} (3)

Equation (1) is a sum for $N$ measurement points, in our case equivalent to every point in the pupil image. The variation of the parameter $f$ by $\Delta f$ gives an intensity difference of $\Delta I$. One can assume that the relationship of the measured signal difference $\Delta I$ when varying the parameter of interest $f$ by the value $\Delta f$ while keeping all the other parameters constant corresponds to the sensitivity towards this parameter. Equation (1) also requires an estimate of the standard deviation $\sigma_k$ for each data point, which corresponds to the noise in measurement. The equation (2) calculates the so called covariance matrix $[C_{jk}]$ which is the inverse of the matrix $[\sigma_{jk}]$. It gives the correlation between the parameters $f$ and $k$. The correlation coefficients can range between -1 (completely anticorrelated) and 1 (completely correlated), while a value of 0 would mean no correlation at all. Finally in equation (3) we obtain the $2\sigma$-uncertainty of a specific parameter of interest $f$.

For Fourier-Scatterometry with one fixed wavelength the sum in equation (1) is calculated for every point in the pupil image for both polarizations at the same time. For the white light interference Fourier-Scatterometry the sum is additionally taken over all the $z$ positions of the reference mirror.

The differentials used for the different parameters of interest where chosen corresponding to the values used in the work of Silver et al. in their SEMATECH funded simulation study[22]. The actual values are 0.1 nm for the critical dimension, $0.2^\circ$ for the side wall angle and 0.4 nm for the height. Additionally we also use their proposed simple noise model $\sigma_1 = 0.002 \text{ I}_{\text{max}}$ as it is a representative value for a typical commercial instrument. This value has a crucial impact on the calculated uncertainty as uncertainty is inverse proportional to it; though keeping it constant for all the simulated measurement configurations allows comparability of the uncertainty values.

### 3.2 Analyzed Structures

For the sensitivity analysis we have looked at three different types of structures. First a simple periodic line grating of photosensitive material structured by two-photon polymerization on a glass substrate, second the same structure but on a silicon substrate and third an e-beam written photoresist line-grating on a silicon substrate. The line width (CD) is 50 or 100 nm and the period (pitch) is 100 or 200 nm while the height of the photoresist is in all cases 100 nm. The side wall angle of the structures is assumed to be $87^\circ$. A schematic description of the structure can be found in Figure 2.
Figure 2. Schematic line grating of photoresist on a substrate with a mid-line-width (cd) of 100 nm, period (pitch) of 200 nm and a side wall angle (swa) of 87° with 100 nm resist height (h). The right image shows a cross section with the staircase approximation used for the RCWA simulation in MicroSim.

3.3 Pupil images

To get an idea of how a pupil image in the back focal plane of the microscope objective looks like we show in the following picture the simulated Fourier-Scatterometry pupil-images for an illumination with 410 nm and variation of the cd, height and the side wall angle. The difference in the pupil images is an indicator towards the sensitivity of this configuration.

Figure 3. Simulated Fourier-Scatterometry pupil images for a photoresist line grating on silicon illuminated with 410 nm. The cd, height and swa are varied and in the last row the intensity difference is plotted to see the sensitivity towards that parameter

3.4 Comparison of sensitivity

In the following sections we will compare the uncertainty and correlation results of Fourier-Scatterometry at 410 nm with the results of white-light interference Fourier-Scatterometry for all the three structures and the parameters cd, height and side wall angle

For the Fourier-Scatterometry pupil images we simulated an illumination of the sample with-light of a wavelength of 410 nm and calculated the $3\sigma$ –uncertainty as well as the correlation coefficients as explained in section 3.1. No reference mirror is used in this case.
We compare the values to the ones one obtains using white-light and scanning the reference mirror from -150 nm to 150 nm in 10 nm steps, as this range achieved good uncertainty values though keeping computation time reasonable. The N in the sum of Equation (1) for the calculation of the covariance matrix includes 900 pupil points multiplied by two orthogonal polarizations and 31 reference mirror positions (approx. N=55,800).

3.5 Line grating of polymerized material on glass

Table 1. 3σ –uncertainty for a line grating of polymerized material on glass illuminated at 410 nm (first value) and for white light illumination and scanning the reference mirror (second value) for dense lines with a CD of 50 nm or 100 nm.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>CD 50/ Pitch 100nm</th>
<th>CD 100/ Pitch 200nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>0.075 nm</td>
<td>0.083 nm</td>
</tr>
<tr>
<td></td>
<td>0.102 nm</td>
<td>0.153 nm</td>
</tr>
<tr>
<td>Height</td>
<td>0.277 nm</td>
<td>0.250 nm</td>
</tr>
<tr>
<td></td>
<td>0.200 nm</td>
<td>0.226 nm</td>
</tr>
<tr>
<td>SWA</td>
<td>0.177 °</td>
<td>0.139 °</td>
</tr>
<tr>
<td></td>
<td>0.284 °</td>
<td>0.250 °</td>
</tr>
</tbody>
</table>

Table 2. Covariance matrix containing the correlation coefficients for the different parameter combinations. The first value is again the Fourier-Scatterometry at 410 nm the second value the scanning white light Fourier-Scatterometry.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>CD 50/100nm</th>
<th>Height 50/100nm</th>
<th>Height 100/200nm</th>
<th>SWA 50/100nm</th>
<th>SWA 100/200nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-0.66</td>
<td>-0.66</td>
</tr>
<tr>
<td>Height</td>
<td>0.66</td>
<td>0.77</td>
<td>0.71</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>SWA</td>
<td>-0.66</td>
<td>-0.82</td>
<td>-0.77</td>
<td>-0.98</td>
<td>-0.94</td>
</tr>
</tbody>
</table>

As one can see for this type of structure the values of uncertainty and correlation are very similar or even worse for the case of white-light interference Fourier-Scatterometry. For that we looked at the same structure type but on silicon substrate instead of glass.

3.6 Line grating of polymerized material on silicon

Table 3. 3σ –uncertainty for a line grating of polymerized material on silicon illuminated at 410 nm (first value) and for white light illumination and scanning the reference mirror (second value) for dense lines with a CD of 50 nm or 100 nm.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>CD 50/ Pitch 100nm</th>
<th>CD 100/ Pitch 200nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>0.032 nm</td>
<td>0.038 nm</td>
</tr>
<tr>
<td></td>
<td>0.061 nm</td>
<td>0.074 nm</td>
</tr>
<tr>
<td>Height</td>
<td>0.164 nm</td>
<td>0.05 nm</td>
</tr>
<tr>
<td></td>
<td>0.071 nm</td>
<td>0.055 nm</td>
</tr>
<tr>
<td>SWA</td>
<td>0.162 °</td>
<td>0.138 °</td>
</tr>
<tr>
<td></td>
<td>0.122 °</td>
<td>0.287 °</td>
</tr>
</tbody>
</table>

Table 4. Covariance matrix containing the correlation coefficients for the different parameter combinations. The first value is again the Fourier-Scatterometry at 410 nm the second value the scanning white light Fourier-Scatterometry.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>CD 50/100nm</th>
<th>Height 50/100nm</th>
<th>Height 100/200nm</th>
<th>SWA 50/100nm</th>
<th>SWA 100/200nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-0.90</td>
<td>-0.66</td>
</tr>
<tr>
<td></td>
<td>-0.66</td>
<td>-0.87</td>
<td>-0.15</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Height</td>
<td>-0.90</td>
<td>-0.66</td>
<td>-0.87</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>-0.15</td>
<td>1</td>
<td>1</td>
<td>-0.98</td>
<td>-0.92</td>
</tr>
<tr>
<td>SWA</td>
<td>0.85</td>
<td>-0.21</td>
<td>0.85</td>
<td>-0.98</td>
<td>-0.92</td>
</tr>
<tr>
<td></td>
<td>-0.12</td>
<td>-0.84</td>
<td>-0.86</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameter</th>
<th>CD 100/200nm</th>
<th>Height 100/200nm</th>
<th>SWA 100/200nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>0.85</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Height</td>
<td>0.85</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>SWA</td>
<td>0.85</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>
With the silicon substrate the uncertainty especially for the height is reduced significantly by more than a factor of 3 using white light interference. Also the correlation between the different parameters especially CD with Height and SWA is strongly reduced which is important for library reconstruction.

Also one can deduce, that while the uncertainty values for the smaller structures (CD 50 / Pitch 100 nm) compared to the larger ones (CD 100 / Pitch 200 nm) stay comparable or even improve (CD and SWA), stronger parameter correlations for the smaller structures can be found.

3.7 Line grating of e-beam resist on silicon

Table 5. \( \delta \sigma \) – uncertainty for a line grating of e-beam photoresist on silicon illuminated at 410 nm (first value) and for white light illumination and scanning the reference mirror (second value) for dense lines with a CD of 50 nm or 100 nm.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>CD 50/ Pitch 100nm</th>
<th>CD 100/ Pitch 200nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>0.041 nm</td>
<td>0.037 nm</td>
</tr>
<tr>
<td>Height</td>
<td>0.199 nm</td>
<td>0.057 nm</td>
</tr>
<tr>
<td>SWA</td>
<td>0.173 °</td>
<td>0.149 °</td>
</tr>
</tbody>
</table>

Table 6. Covariance matrix containing the correlation coefficients for the different parameter combinations. The first value is again the Fourier-Scatterometry at 410 nm the second value the scanning white light Fourier-Scatterometry.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>CD 50/100nm</th>
<th>100/200nm</th>
<th>Height 50/100nm</th>
<th>100/200nm</th>
<th>SWA 50/100nm</th>
<th>100/200nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD</td>
<td>1</td>
<td>1</td>
<td>-0.89</td>
<td>-0.22</td>
<td>0.84</td>
<td>-0.48</td>
</tr>
<tr>
<td>Height</td>
<td>-0.89</td>
<td>-0.22</td>
<td>-0.83</td>
<td>-0.31</td>
<td>-0.98</td>
<td>-0.88</td>
</tr>
<tr>
<td>SWA</td>
<td>0.84</td>
<td>-0.48</td>
<td>0.82</td>
<td>0.50</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

The results for the e-beam written resist line gratings on silicon are very similar as the results for the polymerized material on silicon. Silicon or other reflective substrate seems to be crucial for good sensitivity with the white-light interference Fourier-Scatterometry especially regarding the height of the structure and the correlation between parameters.

3.8 2D Structures

Looking at 2D line gratings yield similar results, but because of highly increased computation time of RCWA simulations for 2D-periodic structures the pupil images have to be sampled less dense which allows only low resolution images of the pupils (19x19 pupil points).

3.9 Wavelet

Also traditional white-light interference evaluation by looking at the wavelet at a pupil point while scanning the reference mirror is possible. In Figure 4 the wavelet for the center pupil point for a scan from -1500 nm to 1500 nm is plotted. Using Fourier Analysis as proposed by the De Grot et al.[13] would allow to have wavelength dependent measurements for every incident direction extracted from the pupil image.
Figure 4. Intensity wavelet at the center pupil point while scanning the reference mirror

4. EXPERIMENTAL REALISATION

A schematic overview of our experimental setup can be found in Figure 5.

We use a white-light laser as our light-source, which gives us higher intensity and a more flat intensity distribution for the used wavelength range as e.g. white-light LED sources. We use a heat-protection filter to reduce the white-light spectrum to the visible range of about 400 to 800 nm as the optical elements used have better chromatic aberration corrections in this range. First we collimate the light coming out of the white-light laser fiber. The used white-light laser has an LP\textsubscript{11} mode which we have to homogenize with help of two microlens arrays to get a homogenous beam distribution [24]. We use a dispersion plate to generate a diffuse and homogenous light distribution for our Köhler illumination of the sample and at the same time to get an even light distribution in our pupil plane which we will be imaging. The light then enters a modified Leica DMR Microscope where a beamsplitter separates the light for the object and an optional mounted reference branch. The reference branch consists of a Linnik-type interferometer setup which we need to accomplish the high numerical aperture of 0.95 of our used microscope objectives (PL APO 250x / 0.95). We use the high-NA of 0.95 to achieve incident angles of up to \( \theta = \sin^{-1}(0.95) \approx 72^\circ \). The z-position of our reference mirror...
can be scanned with help of a piezo actuator. The back focal plane of the object branch and Linnik-reference branch are then imaged together with the help of a Bertrand-Lens on to a Frame-Transfer-CCD (Hamamatsu,C8000-10) to get the pupil plane images with containing our scatterometric and interferometric information.

5. MEASUREMENT

Having built the experimental setup as described in the last section we started by comparing a pupil image with our simulation.

As one can see in Figure 6 simulated and measured pupil images look similar but still some noise reduction, background substraction and calibration has to be performed until library reconstruction is possible.

6. CONCLUSION

We presented the combination of Fourier-Scatterometry and white-light interferometry and showed the application of that scatterometric method to different line grating types with a special emphasis on two-photon-polymerized material. The results show that the white light interference Fourier-Scatterometry yields higher or comparable sensitivity and less correlation between the parameters of interest in case one uses a reflective substrate as is silicon compared to Fourier-Scatterometry at a fixed wavelength and without interference. We also showed the experimental realization for such kind of measurements. The next steps are the actual parameter reconstruction of a measurement using library search methods in a pre-computed library.

7. ACKNOWLEDGEMENTS

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