A scatterometry inverse problem in optical mask metrology

R Model 1,6, A Rathsfeld 2, H Gross3, M Wurm3, B Bodermann3
1Physikalisch-Technische Bundesanstalt, Institute Berlin, Abbestrasse 2-12, 10587 Berlin, Germany
2Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstrasse 39, 10117 Berlin, Germany
3Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany
E-mail: regine.model@ptb.de

Abstract. We discuss the solution of the inverse problem in scatterometry i.e. the determination of periodic surface structures from light diffraction patterns. With decreasing details of lithography masks, increasing demands on metrology techniques arise. By scatterometry as a non-imaging indirect optical method critical dimensions (CD) like side-wall angles, heights, top and bottom widths are determined. The numerical simulation of diffraction is based on the finite element solution of the Helmholtz equation. The inverse problem seeks to reconstruct the grating geometry from measured diffraction patterns. The inverse operator maps efficiencies of diffracted plane wave modes to the grating parameters. We employ a Newton type iterative method to solve the resulting minimum problem. The reconstruction quality surely depends on the angles of incidence, on the wave lengths and/or the number of propagating scattered wave modes and will be discussed by numerical examples.

1. Introduction
Scatterometry is an optical technique based on the analysis of electromagnetic radiation scattered by a periodically structured sample. This non-imaging method is typically used in semiconductor fabrication metrology to meet the challenges of the submicron technology. The evaluation of photomasks and wafers in lithography is an important application in this field. Besides the three standard methods currently used, atomic force microscopy (AFM), scanning electron microscopy (SEM), and optical microscopy [1-3], scatterometry advantageously is a non-destructive, non diffraction-limited, and fast optical tool with access to all geometric parameters of the periodic structure [4-8].

The principle mode of operation is the following: An incident monochromatic laser beam interacts with some periodic surface (grating) and the light is scattered into the full hemisphere above and below the sample. However, the main part of the scattered wave is split into sharp diffraction orders of reflected and/or transmitted plane wave modes. The measured diffraction patterns contain information about the profile geometry and the optical properties of the grating. The highly nonlinear relation between the measurement data and the sample characteristics requires an efficient iterative algorithm applicable to a variety of different combinations of possible measurement sets and parameters to be reconstructed. A priori knowledge on these structure parameters, e.g. on their size itself or on the interval of variation, reduces the complexity of the problem. On the other hand, the measurement data is a small subset of the diffraction efficiency pattern, depending on the properties of the incoming wave (wavelength, angle of incidence, polarization).
The mathematical model of scatterometry is based on the time-harmonic Maxwell’s equations [9,10]. In case of grating structures periodic in one direction and homogenous in another direction, the model reduces to a boundary value problem for the Helmholtz equation. Generally, different methods to solve this forward problem are known. As examples we mention the rigorous coupled wave analysis [11,12] and the finite element method (FEM) [13-15]. Because of its reliability and flexibility we prefer the FEM accepting longer computing time in some applications. The algorithm for the inverse problem is based on the minimization of an objective functional, usually a least squares sum or a weighted least squares sum, in more general cases it contains linear terms, too [16,17].

In the present paper, the measurement configuration as well as the geometric parameters characterizing the structure of the probes are described first. Note that throughout the whole paper examples of EUV (ultra violet) masks are considered exclusively. Next, the mathematical formulation of the scattering problem is given completed by some instructive forward calculations under varying parameters. Section 4 discusses the inverse algorithm and presents profile reconstruction results. The paper concludes with some reflections concerning the practical application and further research.

2. Measurement configuration and grating structure

The objects under investigation in scatterometry are (nano-) structured optical gratings. Ideally, an optical grating is a special surface structure of an infinite plate consisting of different non-magnetic materials with periodic permeability $\mu_0$ and dielectric constant $\varepsilon$. The coordinate system is chosen as shown in Figure 1, the material distribution is supposed to be periodic with period $d$ (pitch) in $x$-direction and to be homogeneous parallel in $z$-direction. In other words, grooves in $z$-direction are generated. Consequently, $\varepsilon$ is invariant with respect to $z$, and the $y$-axis is perpendicular to the plate.

In the case of in-planar diffraction the plane of incidence formed by the incident beam and the $y$-axis is perpendicular to the direction of the grooves. Assume, we have a beam incident under the angle of $\theta$. Then the directions of the reflected diffraction modes are given by the grating equation

$$\sin \theta + \sin \theta_n = \frac{n \lambda}{d}$$

where $\theta_n$ are the angles of the reflected diffraction orders and $\lambda$ is the wave length. The numbers $n = 0, \pm 1, \pm 2, \ldots$ denotes the orders of the diffraction modes. Notice, the $\theta_n$ only depend on the wavelength and pitch but not on the profile structure. The last, however, is decisive for the magnitude of the efficiencies.

We distinguish the two polarization states of a monochromatic light source: the transverse electric (TE or p-polarized) if the incident E-field is parallel to the grooves of the grating and the transverse magnetic (TM or s-polarized) if the E-field is perpendicular to the grooves. Measurements may be performed in different configurations. First, the angular configuration, where the wavelength $\lambda$ is held constant and where the angle of incidence $\theta$ varies, and second, the spectral configuration, where $\theta$ is constant and where $\lambda$ varies.

The geometrical features of main interest are the width of the absorbing structure, the top CD, furthermore the bottom CD and the sidewall angle (see Fig. 1) where CD stands for “critical dimension” and is a small dimension in the range of nanometers.

Figure 2 shows a cross section profile of our test example under investigation. The grating profile is described by a set of parameters. In case of the EUV-mask we have 27 parameters including the optical indices of the materials. Some of them are illustrated in Fig. 2 by $p_i$, $i$ varying. The geometrical
properties, we are interested in for this investigation, are the bottom CD (p₂p₃), the height (p₆), and the top CD (p₇p₈) of the TaN layer [5].

The main component of such EUV-masks is the multilayer beneath the structured area, covering the whole mask. This multilayer (ML) system acts as an interference mirror (Bragg mirror) at the design wavelength and its use is necessary, because no single material offers a sufficiently high reflectivity in the EUV range. The multilayer is manufactured with a certain error, which usually varies over the whole mask. Hence, the imperfection of each layer as well as the imperfection in the structured area (characterized by the actual quantities to be measured) affect the measurement. In the DUV range (deep ultraviolet) the sensitivity w.r.t. ML deviations has been found to be marginal in comparison to EUV scatterometry [5]. In accordance with scatterometric measurements at the new hybrid ellipsometric DUV scatterometer of the PTB [18] for the numerical study a wavelength \( \lambda = 193 \text{nm} \) was chosen. In this way we can separate the influence of the ML from that of the structure.

3. Mathematical modelling and forward simulation

The functional relation between the input (the incoming wave) and the output (diffraction efficiencies, phase shifts) can be described by a mathematical model based on Maxwell’s equations. It depends on the one hand on the parameters of the incoming wave, the wavelength \( \lambda \) and the angle of incidence \( \theta \in (-\pi/2, \pi/2) \), and on the other hand on the mask parameters, i.e. the refraction indices and the geometric parameters of the grating. The coordinate system is chosen as shown in Figure 2 for the example of an EUV mask.

For simplicity, the upper cover material is assumed to be vacuum and the incident wave is normalised to have a unit amplitude. Unlike the generalized (conical) case, we consider in-planar diffraction with incident wave directions restricted to the \( x-y \) plane resulting in reflected and transmitted plane wave modes in the \( x-y \) plane, too. Then, the incident light can be described as a superposition of TE or s-polarised and TM or p-polarised light. The transverse component of the respective fields can be determined from the two-dimensional Helmholtz equation

\[
\Delta u(x, y) + k^2 u(x, y) = 0 \tag{1}
\]

with the piecewise constant wave number function \( k = k(x, y) = \omega \sqrt{\mu_0 \varepsilon(x, y)} \) and angular frequency \( \omega \) of the incident light wave. On material interfaces the solution \( u \) and its normal derivative \( \partial_n u \) for TE polarisation respectively the solution \( u \) and product \( k^{-1} \partial_n u \) for TM polarisation have to cross the interface continuously. In the infinite regions the usual outgoing wave conditions are required. Therefore, the domain \( \Omega \) in the cross section plane for the FEM solution of (1) can be reduced to a rectangle with the \( x \) - coordinate varying between zero and the period \( d \) and with two artificial boundaries \( \Gamma^\pm = \{ y = \pm d \} \) (cf. Figure. 2) located in the first lower coating (\( \Gamma^- \)) and in the surrounding vacuum (\( \Gamma^+ \)), respectively. For (1), a boundary value problem on \( \Omega \) is to be solved with quasi-periodic boundary condition \( u(0, y) = u(d, y) \exp(-\text{i}kd) \) on the lateral boundary part and with non-local boundary conditions on \( \Gamma^\pm \). Furthermore, starting with the TE polarisation, at the horizontal boundaries the
component $u = E_z$ admits a Rayleigh expansion of the form

$$E_z(x,b^+) = \sum_{n=-\infty}^{\infty} A_n^+ \exp(+i\beta_n^+ y) \exp(i\alpha_n x) + A_0^{inc} \exp(-i\beta_0^+ y) \exp(i\alpha)$$

(2)

$$E_z(x,b^-) = \sum_{n=-\infty}^{\infty} A_n^- \exp(-i\beta_n^- y) \exp(i\alpha_n x)$$

(3)

with $k^\pm = k(x,b^\pm)$, $\alpha_n = k^+ \sin \theta + \frac{2\pi}{d} n$, $\beta_n^\pm = \sqrt{(k^\pm)^2 - (\alpha_n)^2}$, and $A_0^{inc} = 1$

The important Rayleigh coefficients $A_n^\pm$ are those with $n$ for which $\beta_n^\pm$ is a real number. Indeed, they describe magnitude and phase shift of the propagating plane waves. More precisely, the modulus $|A_n^\pm|$ is the amplitude of the $n$th reflected respectively transmitted wave mode and $\arg\left(A_n^\pm / A_0^{inc}\right)$ the phase shift. The coefficients $A_n^\pm$ for imaginary or complex $\beta_n^\pm$ lead to evanescent waves, only. The optical efficiencies of the grating are the quantities to be measured and determined by

$$e_n^\pm = \beta_n^\pm |A_n^\pm|^2 / \beta_0^+ |A_0^{inc}|^2.$$  

(4)

Note, that the efficiency of a transmitted or reflected mode is nothing else but the portion of energy transferred from the incoming light to this mode. The case of TM polarization is analogously.

For the numerical analysis of DUV scatterometry on EUV masks we use the software package DIPOG [17] which solves direct problems for optical gratings and inverse diffraction problems. For the boundary value problem of the elliptic differential equation (1), the finite element method was implemented which allows simulating the diffraction by gratings with arbitrary geometry. However, if the ratio period $d$ over wavelength $\lambda$ is large, better results are achieved with a generalized FEM (GFEM) with different trial space of approximation functions, for details see [17]. The coefficients of the Rayleigh expansion $A_n^\pm$ are computed from the FEM solution of the Helmholtz equation (1). Then, the efficiencies are obtained from equation (4).

Before starting the inverse problem we investigate the sensitivity of the diffraction efficiencies (cf. equation (4)) with respect to structure variations. First, we simulate reflectometric measurements: We calculate the scatterograms for s- and p-polarised incoming light independence of the angle of incidence $\theta$. Here, we tune $\theta$ from 3° to 81° (normal to grazing) in 1° steps. The results for the reflected modes are shown in Figure 3. The propagating orders incoming light in dependence of the angle of incidence are found to be between -8 and +4. It starts for $\theta = 3°$ with diffraction orders from -4 till +4.
and ends for $\theta = 81^\circ$ with orders from -8 till 0. The efficiency of the $0^{th}$ order starts for $\theta = 3^\circ$ at a value of 0.394, ends for $\theta = 81^\circ$ at 0.589, and passes a minimum of 0.193 at 57°. Also $\Psi_0'(\theta)$ has a minimum here. This means 57° is the Brewster angle of this structure. The $1^{st}$ diffraction order reaches a maximum at 0.155 for $\theta = 42^\circ$, and the $-1^{st}$ order a maximum of the same value for $\theta = 63^\circ$. In the $0^{th}$ order discontinuities in the derivative w.r.t. the angle can also be observed. These are the Rayleigh anomalies, which appear at the angles of incidence where higher orders just become evanescent. A similar situation has been found for the reflected diffraction patterns under TM-polarisation, but the surface looks slightly smoother. In this case, the minimum of the $0^{th}$ diffraction order is reached at an angle smaller than that for TE polarisation, namely at $\theta = 51^\circ$ with a minimal efficiency of 0.217. Since the ML stack has a high absorbance and is relatively thick, practically no light gets through it. Therefore we got no propagating modes in transmission.

In the next step we investigated the sensitivity of the scatterometric measurands w.r.t. the variation of geometrical dimensions of special interest, as example w.r.t. the side wall angle (SWA). The variation of the SWA is realized by a change of the bottom CD moving the x-coordinates of the left ($p_3$) and right ($p_2$) edge of the SiO$_2$ layer (see Figure 2). In the nomenclature of the DIPOG variables, this means $p_2$ and $p_{16}$ alter in the same manner between 0.57333 and 0.59333. The variables $p_3$ and $p_{17}$ alter symmetrically to $p_2$ and $p_{16}$. So we generate symmetrically a side wall angle between 81.3° and 98.7° on both sides of the structure. The results are depicted in Figure 4. For the simulation the angle of incidence of 6° was chosen. The trends of the measurable values, the efficiencies, do not show any oscillations in the direction of the parameter variation. The same is valid for the other parameters. This is a necessary requirement for the uniqueness of the solution of the inverse problem.

4. Reconstruction of the grating profile

The inverse problem consists in the calculation of an optical grating, whose diffraction patterns approximate the measurement data the best. In general, the measurements of the diffraction efficiency patterns, the phase shifts, the total energy, the reflected and transmitted energy for different angles of incidence, wavelengths, polarisation states and directions (transmission and reflection) are possible. For example, in the present paper we choose the efficiency patterns of a single wavelength (193 nm) and TE polarisation in reflection for different angles of incidence. On the other hand, the mask parameters chosen for identification are a subset of all profile parameters. Here, the bottom CD, the top CD and height of TaN are selected as an example for a test of the DUV scatterometry. The best approximation is found minimizing a nonlinear objective functional in simple cases a least squares or a weighted least squares problem. In certain cases linear terms may be helpful and are optionally incorporated in the objective functional, too. All five optimization algorithms available in DIPOG [17] start with an initial value and operate iteratively. Four are gradient based local optimizers [19], and one is a stochastic global optimizer of simulated annealing [20]. Unfortunately, as many inverse problems the inverse scatterometry may be ill-posed, that means, at least one of the following conditions is violated: existence, uniqueness or stability of the solution. Often the most serious difficulty in scatterometry consists in the existence of several local minima of the objective function. Nevertheless, there are a lot of supporting techniques to catch the correct solution as regularization...
methods [21,22], a convenient selection of measurement data [6], a proper scaling and number of
parameters, proper weights within the objective function [7], a limitation of the feasible parameter
region. In the presented example, a regularization according Tikhonov with the Hansens L-curve
method do not improve the result.

We use the simulated diffraction patterns for all significant diffraction orders under 27 angles of
incidence between 3° and 81° as test measurement data. However, we use a finer FEM-grid than for
the reconstruction. In this way, we have a highly accurate data set at our disposal.

As assumption we postulate the structure to be symmetric. In this way, for example, the DIPOG
parameter $p_4$ is dependent on $p_2$ and $p_6$ on $p_7$ etc. (see figure 2). Furthermore, the side wall angles of
the SiO$_2$ layer and of the Ta layer (anti-reflection coating) are fixed to 90° and to 82.6°, respectively.
The geometrical properties which we are interested in are the bottom CD, the height and the top CD of
the TaN layer. In this way, the SWA of the TaN layer is determined simultaneously. In the DIPOG
nomenclature, searching the interesting quantities amounts in searching for $p_2$, $p_6$ and $p_7$.

The least squares sum describes the deviations between the measurement data and the efficiencies
of the determined grating structure. For the uniqueness of the solution of the inverse problem the
minimum of the objective function in the feasible region of the parameters should be unique. For
details see [19]. For a two-dimensional parameter set DIPOG generates a graphic visualization of the
objective function and the gradient field. In this way any two-dimensional section of the graph of the
objective function and the gradient field can be displayed.

In our case of a three-dimensional optimization problem, we choose the three pairs of two parameters
($p_2$, $p_6$), ($p_2$, $p_7$), ($p_6$, $p_7$) and fix in each case the remaining third parameter. A feasible region of
(0.57333, 0.59333) for both $p_2$ and $p_7$ corresponds to a variation of the bottom CD and top CD of TaN
in the range 140nm ±16.8nm. For the height of the TaN layer $p_6$, a feasible region in the range 54.9nm
±10nm is chosen. Thus the variation of the SWA of the TaN layer results in a range 90° ± 20.5°.
Altogether, we choose advisedly broad ranges for the parameter set to be identified within the grating
reconstruction.

![Isoline plot of the objective functional and its gradient field](image1)

![Surface plot](image2)

Fig. 5. Objective functional depending on a) $p_2$ and $p_6$ and c) $p_2$ and $p_7$ for all angles. b) and d)
show the respective surface plot

Figure 5a shows the isoline plot of the objective functional and its gradient field for the parameter
pair ($p_2$, $p_6$) standing for the bottom CD and the height of the TaN layer, Figure 5b the corresponding
surface plot in logarithmic scale. We observe that the minimum is unique. However, there exists a flat region in the plane. Nevertheless the chance for convergence in this case is quite good. Amazingly, the situation for \((p_2, p_7)\) in Figures 5c and 5d turns out to be even better. The result for \((p_6, p_7)\) lies in between. A single minimum and a fast convergence as consequence of the steep gradients can be predicted. The results of the inverse solutions for the parameters \(p_2, p_6\) and \(p_7\) are in excellent agreement with the nominal values. Nevertheless, Figure 5 only shows two-dimensional sections across a – here – three-dimensional volume (three free parameters). A better guaranty for a successful identification of the geometric grating parameters is possible if the optimization algorithm is started several times with different initial conditions. Actually, we have chosen the initial values all at the boundary of the feasible region. The minimization of the objective function has been executed by a Newton type method with SQP iteration. In all cases, we have found a perfect match of the three parameters reconstructed from the efficiency patterns of 27 angles of incidence. This results suggests the question, how many measurements are at least necessary for a unique and accurate identification of the three parameters under test? A series of 27 reconstructions using only the scatterogram obtained with a single angle of incidence as input data, showed that, for each angle \(\theta \leq 57^\circ\) the reconstruction works successfully. For \(\theta > 57^\circ\) the reconstruction failed. Remember that \(\theta = 57^\circ\) is the Brewster angle, and the efficiency of \(0^\text{th}\) order reflected mode has its minimum here. As an example, Figure 6 shows the objective functional for \(\theta = 6^\circ\). It illustrates the well-posedness of the two-dimensional problem for \(p_2\) and \(p_7\). The situation of the two other pairs of parameters is similar. The treatment of measurement uncertainty may follow the investigations \[23,24\].

5. Conclusions
The forward problem for the hybrid ellipsometric scatterometer is formulated by the Helmholtz equation with special boundary conditions and solved by a generalized FEM technique. The inverse problem, the reconstruction of the grating structure by means of efficiency pattern, is a highly nonlinear operator solved by a Newton type optimization technique. In the DUV range, the sensitivity of the data set w.r.t. the profile parameters of the grating enables sufficient for a successful reconstruction tested by an EUV mask and a wavelength of 193nm. The angle of incidence has to be smaller or equal to the Brewster angle of 57\(^\circ\). If this condition is fulfilled, then the efficiency pattern of a single angle is sufficient for the reconstruction of the several geometric mask parameters. In case of realistic measurement data, the situation could be changed and data for more angles might be needed. Compared to EUV scatterometry, the influence of multilayer deviations in DUV scatterometry is marginal. In this way, the determination of the absorber structure can be separated from that of the multilayer. Note that, sometimes, the determination of the multilayer stack is difficult.

The next tasks will be the application of the inverse method to real data combined with some statements to the measurement uncertainty. Generally, a great problem is the nonexistence of a “golden standard” for reliable measurements of grating profiles, the currently used methods (AFM, SEM, optical microscopy) may give differing results.

References
[1] Bodermann B and Bosse H 2007, An approach to validation of rigorous modelling in optical CD
microscopy by comparison of measurement results with independent methods, Proc. SPIE 6617, 66170Y-1–66170Y10

[2] Dersch U, Korn A, Engelmann C, Frase C G, Haessler-Grohne W, Bosse H, Letzkus F and. Butschke J 2005, Impact of EUV mask pattern profile shape on CD measured by CD-SEM, Proc. SPIE 5752 , 632-645

[3] Cho S, Yedur S, Kwon M and Tabet M 2006, CD and profile metrology of EUV masks using scatterometry based optical digital profilometry, Proc. SPIE 6349, 634921

[4] Wurm M, Bodermann B, Model R and Groß H 2007, Numerical analysis of DUV scatterometry on EUV masks, Proc. SPIE 6617, 661716-1 – 661716-12

[5] Groß H, Model R, Bär M, Wurm M, Bodermann B and Rathsfeld A 2006, Mathematical modelling of indirect measurements in scatterometry, Measurement 39, 782-794

[6] Groß H, Rathsfeld A, Scholze F, Bär M and Dersch U 2007, Optimal sets of measurement data for profile reconstruction in scatterometry, Proc. SPIE 6617, 66171B-1–66171B-12

[7] Groß H and Rathsfeld A 2008, Sensitivity analysis for indirect measurement in scatterometry and the reconstruction of periodic grating structures, Waves in Random and Complex Media, 18:1, 129—149

[8] Pomplun J, Burger S, Schmidt F, Zschiedrich L, Scholze F, Laubis C and Dersch U 2006, Rigorous FEM simulation of EUV masks: influence of shape and material parameters, Proc. SPIE 6349, 63493D

[9] Bao G and Dobson D C 1998, Modeling and optimal design of diffractive optical structures, Surveys on Mathematics for Industry 8, 37-62

[10] Petit R (ed.) 1980 Electromagnetic theory of gratings (Berlin: Springer)

[11] Lalanne P and Morris G M 1996, Highly improved convergence of the coupled-wave method for TM-polarization, JOSA A 13, 770-784

[12] Li L 1997, New formulation of the Fourier modal method for crossed surface-relief gratings, JOSA A 14, pp. 2758-2767

[13] Bao G 1995, Finite element approximation of time harmonic waves in periodic structures, SIAM J. Numer. Anal., 32, 1155-1169

[14] Elschner J, Hinder R and Schmidt G 2002, Finite element solution of conical diffraction problems, Advances in Comp. Math 16, 139-156

[15] Urbach H P 1991, Convergence of the Galerkin method for two-dimensional electromagnetic problems, SIAM J. Numer. Anal. 28, 697—710

[16] Elschner J and Schmidt G 1998, Numerical solution of optimal design problems for binary gratings, J. Comput. Physics 146, 603-626.

[17] Elschner J, Hinder R, Rathsfeld A and Schmidt G, DIPOG Homepage, http://www.wias-berlin.de/software/DIPOG

[18] Wurm M, Bodermann B, Pilarski F 2007, Metrology capabilities and performance of the new DUV scatterometer of the PTB, Proc. SPIE 6533, 65330H-1 - 65330H-8

[19] Fleischcr R 2000, Numerical methods of optimization (Wiley&Sons)

[20] van Laarhoven P J M and Aarts E H L 1988, Simulated annealing: Theory and Applications, (Kluwer Academic Publishing Group)

[21] Colton D and Kress R 1992, Inverse Acoustic and electromagnetic scattering theory, Applied Mathematical Science 93, (Springer)

[22] Vogel C R 2002, Computational methods for inverse problems (Philadelphia: SIAM)

[23] Al-Assaad R M and Byrne D M 2007, Error analysis in inverse scatterometry. I. Modeling, J. Opt. Soc. Am. 24, 2, 330-338

[24] Groß H, Model R, Rathsfeld A, Scholze F, Wurm M, Bodermann B and Bär M 2008, Modellbildung, Bestimmung der Messunsicherheit und Validierung für diskrete inverse Probleme am Beispiel der Scatterometrie. VDI Berichte 2011, 337-346