XXI IMEKO World Congress “Measurement in Research and Industry”
August 30 − September 4, 2015, Prague, Czech Republic

IMPACT OF STOCHASTIC LINE EDGE ROUGHNESS PATTERNS ON SCATTEROMETRY

Hermann Gross, *Sebastian Heidenreich*, *Markus Bär*

Physikalisch-Techn. Bundesanstalt, Braunschweig and Berlin, Germany, hermann.gross@ptb.de

Abstract – We present a fast non-rigorous method for the analysis of stochastic line edge roughness (LER) with amplitudes in the range of a few nanometers, based on a 2D Fourier transform method. LER has an significant impact on the light diffraction patterns measured by scatterometry. Scatterometry is a fast, non-destructive optical method used in wafer metrology to determine the geometry parameters of periodic surface structures from scattered light intensities.

Keywords: scatterometry, critical dimensions (CDs), line edge roughness (LER), Fourier optics

1. INTRODUCTION

Non-imaging metrology methods like scatterometry are in contrast to optical microscopy non-diffraction limited and grant access to the geometrical parameters of periodic structures like structure width (CD), period (pitch), sidewall angle or height of trapezoidal bridges (lines) [1], [2]. Scatterometry is an indirect optical method. From scattered relative light intensities, i.e., the measured efficiencies, the geometrical parameters of irradiated surface profiles and their uncertainties are reconstructed. The evaluation of structure dimensions on photo masks and wafers in lithography [3], [4] is an important application. In the semiconductor industry both the feature sizes and the required limit of measurement uncertainty decrease continuously and shorter wavelengths like extreme ultraviolet (EUV) at 13.5 nm will be applied.

A comparison of the reconstructed surface profiles using EUV-scatterometry and the results obtained using atomic force and electron microscopy [5] has revealed that scatterometry can underestimate the sidewall angle, an important feature of the EUV-mask, by several degrees. Imperfect modeling is supposed to be one of the main reasons for this result [6], [7], [8]. In particular, to get more reliable simulations and reconstructions, effects like line edge roughness (LER) and further model based impacts have to be taken into account (cf. [9], [10], [11], [12] for the details). Torcal-Mila et al. [13], and also Kato and Scholze [8] have suggested approximative analytical expressions for the impact of line edge roughness on the scattered efficiencies. They have applied Fraunhofer’s diffraction method on gratings with randomly disturbed periodicity, i.e., the Fourier transform of the reflectivity function of perturbed binary gratings were investigated. They found damping of the mean efficiencies with increasing diffraction orders, which was confirmed by rigorous FEM simulations for a real EUV mask [9]. In these FEM investigations, large computational domains containing many line-space structures with stochastically chosen widths were used. Hence, these results were still obtained for a simplified model of rough line edges, i.e., without modeling the line edges as a stochastic process with a prescribed auto-correlation function analogously to what is often done in the metrology of rough geometries. There are several publications [14], [15], [16], where the modeling of line edge roughness as a stochastic process starts with an exponentially decaying autocorrelation function for the position of an edge point along the line. The standard deviation σ of the roughness amplitude, the linear correlation length ξ, and the roughness exponent α are characterizing the autocorrelation. Randomized line edge profiles are generated by calculating the associated power spectrum density (PSD) function belonging to the autocorrelation function, then disturbing it by a random complex phase term and subsequently applying inverse Fourier transform.

The objective of the present paper is to demonstrate that the LER-induced attenuation of the mean efficiencies for higher diffraction orders is supported by a stochastic model of line edge roughness combined with a fast approximative calculation of the relative light intensities in the far field. The LER simulation uses a 2D binary aperture plane with many slits whose boundary lines are rough. Different roughness patterns are realized by different values of the standard deviation σ of the roughness amplitude, the correlation length ξ and the roughness exponent α. To avoid time consuming rigorous numerical calculations, the light intensity is approximately computed by a fast 2D-Fourier transform of the light distribution of the binary aperture plane applying the Fraunhofer approximation.

2. ROUGH APERTURES

In order to examine the impact of LER on the measured efficiencies in dependence on different roughness patterns, we open with the creation of randomly perturbed 2D binary line-space structures. The line edge positions are controlled by an exponentially decaying autocorrelation function allowing a significantly more realistic modeling of line edge roughness. We represent 2D-binary line-space gratings by square arrays of strip shaped slits, i.e., square apertures composed of many slits. In order to create rough boundary lines for the slits, we use an autocorrelation function to describe the variations along the edges. Considering lines $\{(x(y), y) : y \in R\}$ along y-direction with random variables $x(y)$, we assume a constant mean value $\langle x(y)\rangle = x_0$ and that the correlation depends on the distance $r = |y_1 - y_2|$ only, i.e., $x(y_1,y_2) = x(r)$. Furthermore, we assume the exponentially decaying autocorrelation function

$$x(r) = \sigma^2 e^{-(r/\xi)^{2\alpha}} \qquad (1)$$

where σ is the standard deviation of the edge positions, ξ is the linear correlation length along the line, and α is called roughness exponent. Recent publications, e.g. Mack and Bergner et al. [14], [15], [16], are starting with such an exponentially decaying function for modeling a stochastic process which ends up in randomized line edges or surfaces. The investigations here are addressing the 1D case of randomly rough lines. Randomized line edge profiles $x(y)$ are generated by calculating the associated power spectrum density function PSD(r^{-1}) that belongs to the autocorrelation function $x(r)$ in a first step. Then we apply to the calculated PSD a random complex exponential phase term, being uniformly distributed in the range of [0, 2π]. Subsequently, the inverse Fourier transform of that disturbed PSD provides a rough line edge $x(y)$ along y-direction. The edges of the aperture slits are created by repeating this process independently from each other. Fig. 1 gives an example of a whole aperture created with σ = 3 nm, ξ = 10 nm and α = 0.5. To get a sufficient resolution, the pixel size (stepsize of discretization for the Fourier transform) is 0.1 nm in both directions of the 2D apertures broadening upon a total range of 1µm × 1µm. The investigated rough apertures are typically composed of four periodically arranged slits, i.e., the corresponding grating period is 250 nm and the mean width of the rough slits is 125 nm (cf. Fig. 1). Typical values of α are in the range of 0.3 – 1.5. We choose several slits per apertures to improve the spatial averaging of the irradiance pattern associated with the randomized aperture.

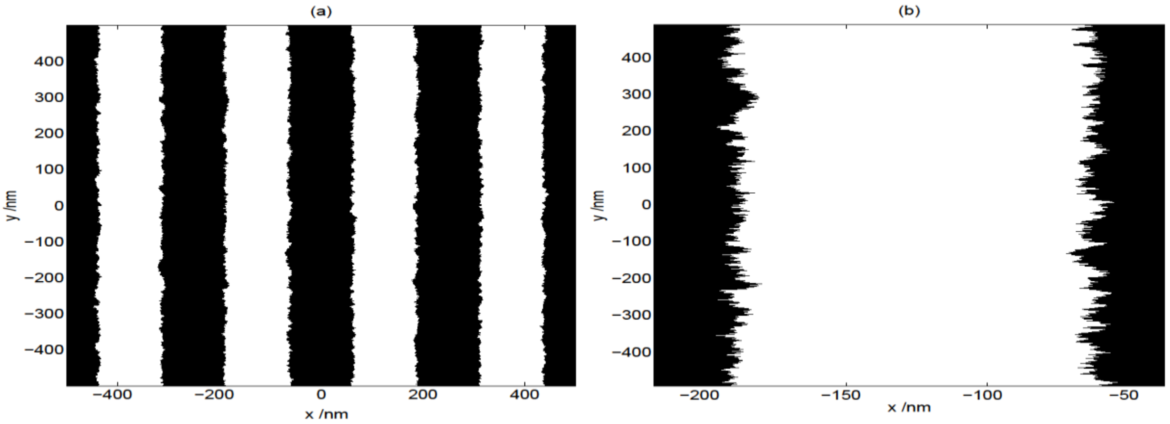

Fig. 1. (a) Example of a rough aperture; size 1.0 x 1.0 µm^2; resolution 0.1 nm (10^4 x 10^4 grid points); four slits per aperture, i.e., 125 nm width of the slits; 250 nm period; all edges non-correlated; used PSD with σ=3nm, α=0.5 and ξ=10nm. (b) Zoomed area of the same aperture.

3. FRAUNHOFER APPROXIMATION

Fourier optics is well known for being a cornerstone in the analysis of imaging, diffraction, coherence and propagation through random media [17]. The mathematical description of the propagation of an optical field from one location, for example a diffractive aperture, to another is one of its most essential tasks. In general the propagation behavior of electro-magnetic waves in matter is based on Maxwell's equations, where the electric field E and the magnetic field H are coupled. However, assuming a linear and isotropic dielectric medium, where additionally the material properties are invariant in one direction, both fields are decoupled and scalar diffraction equations can be applied.

Under these ideal conditions a monochromatic plane wave with wavenumber k and orthogonal incidence on a diffractive aperture is considered. Its propagating radiation in a parallel observation plane far away from the aperture can be elegantly expressed as the Fourier transform of the field distribution in the source plane applying the Fraunhofer approximation. A detailled derivation of the corresponding formula for calculating the light distribution in the observation plane is given in [18]. We apply this Fraunhofer expression with a wavelength λ of 13.5 nm and a distance of 1 m from the aperture plane to calculate the irradiance pattern of the rough apertures and of the corresponding unperturbed non-rough aperture.

4. NORMALIZED IRRADIANCE PATTERN OF ROUGH APERTURES

The key for analyzing the impact of roughness is to compare the mean light intensities calculated for ensembles of rough apertures to that of the unperturbed non-rough aperture. Any systematic impact on the mean efficiencies should then be identified obviously. In previous investigations that made use of computationally expensive FEM simulations [9], this strategy has already been applied successfully.

An example for the relative deviations of light intensities in dependence on the diffraction orders for several ensembles of rough apertures are depicted in Fig. 2. The shown cases differ from each other by an increasing standard deviation σ of the autocorrelation function (cf. Eq. (1)) from 2 nm to 5 nm used to generate the rough edges of the apertures. The roughness exponent α was fixed to 1.0 and the correlation length ξ was set to 10 nm. Each ensemble has eleven samples of rough apertures whose relative deviations are depicted as circle symbols. Their mean values are marked by diamond symbols. The bridge to slit ratio was 1:1, i.e., both parameters have a nominal value of 125 nm. Only the orders with intensities significantly greater than zero are considered.

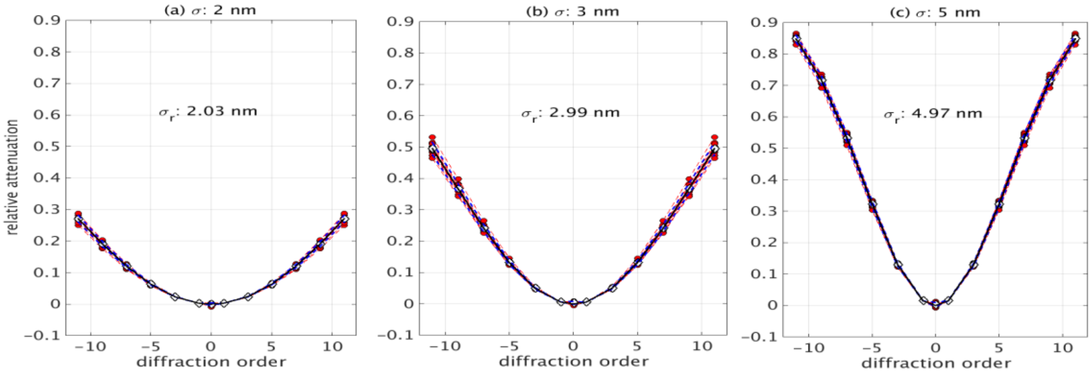

Fig. 2. Rel. deviations from efficiencies of the unperturbed structure depicted as circles; diamond symbols represent the mean deviations of all samples & solid line the exponential approximation; (a) - (c) for three different σ = (2, 3, 5) nm; α = 1 and ξ = 10 nm for all three examples.

A systematic nonlinear decrease of the mean efficiencies for higher diffraction orders along with slightly increasing variances is observed. This is established for different degrees of roughness expressed by the different σ values for three ensembles. Only a few ten samples for each ensemble are necessary to reveal a stable bias of the mean efficiencies. Consequenty, we conclude that the revealed attenuation of the mean perturbed light intensities of diffraction order j can be modeled by

$$\langle f_{j,pert} \rangle = e^{-\left(\frac{2\pi j}{d}\right)^2 \sigma_r^2} f_{j,ref} \qquad (2)$$

Here $f_{j,ref}$ denotes the light intensities of the unperturbed aperture at diffraction order j and d is the period of the bridge-slit structure. σ_r depicts that value for the standard deviation of the roughness amplitude which represents the best-fit result for the mean normalized deviations (cf. [18] for more details).

We have examined many different ensembles of rough apertures representing variant roughness patterns characterized by different values of σ, ξ, and α. Only a slight increase within a range of maximal 5% were found for the determined σ_r compared to the imposed standard deviation σ of the associated rough ensemble. Fig. 3 summarizes these findings for many different ensembles up to a correlation length of 150 nm and for two different values of α = 1.0 and α = 0.5. Further ensembles of roughness patterns with larger correlation lengths up to 1000 nm have been investigated by extending the computational grid from a size of 1.0 x 1.0 µm^2 to 3.36 x 3.36 µm^2. Furthermore the impact of the roughness exponent α has been investigated in more detail and the results will be published soon.

5. CONCLUSIONS

We have proposed a 2D-Fourier transform method as a simple and efficient algorithm to complement previous investigations on the systematic impact of line edge roughness on light diffraction patterns of periodic line-space structures. In particular, this has been done in the EUV regime, where the light diffraction pattern is characterized by many significant wave modes with higher diffraction orders. The irradiance of illuminated rough apertures far away from the source plane is numerically calculated very efficiently as the 2D-Fourier transform of the light distribution in the aperture plane and then compared to those of the unperturbed, ’non-rough’ aperture. Rough random boundaries are generated for the aperture slits by PSD functions ensuring realistic line edge profiles comparable to those of 3D atomic force microscopy (AFM) measurements along the sidewalls of the absorber lines (cf. [18]). A few samples (e.g. ten) are sufficient to determine a stable estimate for the bias of the mean values at different diffraction orders. Compared to the diffraction pattern of the unperturbed aperture, the mean efficiencies of the rough apertures show a systematic exponential decrease for higher diffraction orders. The standard deviation of the edge fluctuations σ_r and the diffraction order j govern the revealed exponential damping factor according to (2).

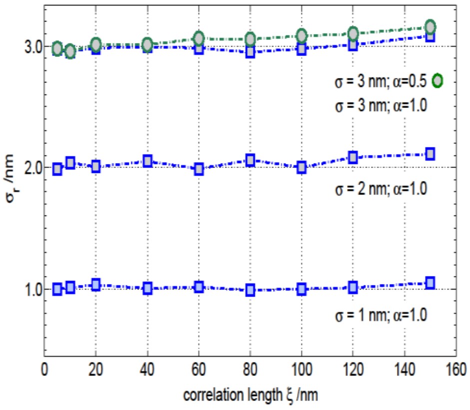

Fig. 3. Reconstructed values of σ_r for ensembles of rough apertures (2D-binary gratings) generated with different values for the standard deviations σ, the correlation lengths ξ and the roughness exponents α.

ACKNOWLEDGMENTS

Results are part of project IND 17 within the European Metrology Research Programme (EMRP).

REFERENCES

[1] B.K. Minhas, S.A. Coulombe, S. Sohail, H. Naqvi, and J.R. McNeil. Ellipsometric scatterometry for metrology of sub-0.1μm-linewidth structures. Appl.Optics, 37:5112–5115, 1998.

[2] H.T. Huang and F.L. Terry Jr. Spectroscopic ellipsometry and reflectometry from gratings (scatterometry) for critical dimension measurement and in situ, real-time process monitoring. Thin Solid Films, 455:828–836, 2004.

[3] C.J. Raymond, M.R. Murnane, S. Sohail, H. Naqvi, and J.R. McNeil. Metrology of subwavelength photoresist gratings using optical scatterometry. J. Vac. Sci. Technol., B, 13(4):1484–1495, 1995.

[4] C.J. Raymond, M.R. Murnane, S.L. Prins, S. Sohail, H. Naqvi, J.R. McNeil, and J.W. Hosch. Multiparameter grating metrology using optical scatterometry. J. Vac. Sci. Technol., B, 15(2):361–368, 1997.

[5] M.Wurm. ¨Uber die dimensionelle Charakterisierung von Gitterstrukturen auf Fotomasken mit einem neuartigen DUV-Scatterometer. PhD thesis, Friedrich-Schiller-Universit¨at Jena, 2008.

[6] H. Gross, A. Rathsfeld, F. Scholze, and M. Bär. Profile reconstruction in extreme ultraviolet (EUV) scatterometry: modeling and uncertainty estimates. Meas. Sci. Technol., 20:105102, 2009.

[7] H. Patrick, T. Germer, R. Silver, and B. Bunday. Developing an uncertainty analysis for optical scatterometry. Proc. SPIE, 7272:72720T, 2009.

[8] A. Kato and F. Scholze. Effect of line roughness on the diffraction intensities in angular resolved scatterometry. Appl. Opt., 49(31):6102–6110, 2010.

[9] H. Gross, M-A. Henn, S. Heidenreich, A. Rathsfeld, and M. Bär. Modeling of line roughness and its impact on the diffraction intensities and the reconstructed critical dimensions in scatterometry. Appl. Optics, 51:7384–7394, 2012.

[10] M.-A. Henn, H. Gross, F. Scholze, M. Wurm, C. Elster, and M. Bär. A maximum likelihood approach to the inverse problem of scatterometry. Optics Express, 20, No. 12:12771–12786, 2012.

[11] M-A. Henn, S. Heidenreich, H. Gross, A. Rathsfeld, F. Scholze, and M. Bär. Improved grating reconstruction by determination of line roughness in extreme ultraviolet scatterometry. Optics Letters, 37 (24):5229–, 2012.

[12] M-A. Henn, H. Gross, S. Heidenreich, F. Scholze, C. Elster, and M. Bär. Improved reconstruction of Critical Dimensions in Extreme Ultraviolet Scatterometry by Modeling Systematic Errors. Meas. Sci. Technol., 25:044003 (9pp), 2014.

[13] F.J. Torcal-Milla, L.M. Sanchez-Brea, and E. Bernabeu. Diffraction of gratings with rough edges. Optics Express, 16:19757–19769, 2008.

[14] B.C. Bergner, T.A. Germer, and T.J. Suleski. Effective medium approximations for modeling optical reflectance from gratings with rough edges. J. Opt. Soc. Am. A, 27:1083–1090, 2010.

[15] C.A. Mack. Analytic form for the power spectral density in one, two, and three dimensions. J. Micro/Nanolith. MEMS MOEMS, 10(4):040501–, 2011.

[16] C.A. Mack. Generating random rough edges, surfaces, and volumes. Appl. Optics, 52:1472–1480, 2013.

[17] J.W. Goodman. Introduction to Fourier Optics. Roberts & Company, Greenwood Village, 2005.

[18] H. Gross, S. Heidenreich, M.-A. Henn, G. Dai, F. Scholze, and M. Bär. Modelling line edge roughness in periodic line-space structures by Fourier optics to improve scatterometry. J. Europ. Opt. Soc. Rap. Public.,9:14003,2014.