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Optical methods for measuring the feature size of optical diffraction gratings with nano-meter accuracy and implementation of suitable feedback control loops.

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Abstract. Surface relief diffraction gratings offer a high flexibility in their design and thus allow to synchronize their optical performance with the specific requirements of the underlying application. However, the accuracy and the specific control of the manufacturing processes are of vital importance. In this contribution, we present optical methods relying on white-light ellipsometry and how they can be exploited for the measurement of the critical dimensions of manufactured surface relief grating structures. We will furthermore present suitable processes (relying on atomic layer deposition) and how they are used in a feedback loop to control the grating's feature sizes on the nanometer scale.

1 Introduction

Modern applications in high-performance spectroscopy or chirped pulse amplification require diffraction gratings (used as dispersive elements) meeting challenging performances in terms of, e.g., diffraction efficiency, bandwidth, spectral dispersion, and stray light. Binary surface relief gratings are well suited to do that job especially when taking into account more complex descendants, e.g., backfilled gratings achieved by atomic layer deposition (ALD) [1,2,3]. Typically, such gratings exhibit periods slightly lower than the wavelength and the lateral feature size scales down to the 100nm region. Aspect ratios might achieve values up to 1:15. The grating geometry, i.e., groove width and depth, must be manufactured and controlled with very high accuracy on dimensions down to few nanometers.
Electron Beam Lithography (EBL) has been shown to be a versatile method, which allows manufacturing of patterns with very high resolution and accuracy. Reactive dry etching processes allow to transfer the exposed lithographic pattern into the underlying substrate [4].
When approaching the limits of the manufacturing processes, the real grating geometry shows inevitable deviations from the ideal structure, i.e., in general non-trivial shape deformations of the trenches. It is thus of crucial importance to be able to accurately characterize such deformations and to feed this information into a control loop to achieve diffraction gratings with unprecedented optical performance.
Here we present an indirect optical characterization method relying on white-light ellipsometry and how it can be exploited for the measurement of shape deformations of manufactured surface relief grating structures. Second, we outline how ALD can be applied to tune the grating's critical dimensions, thus allowing to push the grating's performance to its maximum.

2 White light ellipsometry and shape retrieval

Our measurement setup relies on a commercial white light ellipsometer SE850 from Sentech (typically used for the characterization of thin optical films and stacks).

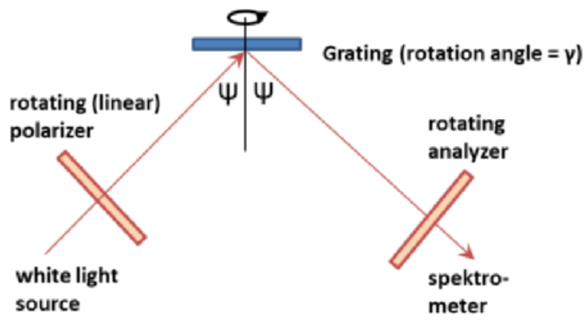

Fig. 1. Scheme of the basic measurement setup.

The basic measurement scheme is depicted in Fig. 1. The grating sample (mounted on a rotation stage) is illuminated with a collimated beam and the specular order in reflection is analysed. Additionally, rotating polarizers/analysers in the input and reflected beam path allow for dedicated selection of linear polarization states. Essentially, the setup allows for the detection of Stokes vector components S1 and S2 of the reflected beam for any arbitrary configuration. Using the rotation angle α of

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the input polarizer, the incident angle Ψ, and the grating's rotation angle γ as independent parameters, a series of Stokes-vector spectra $S1(\mathbf{p}=\mathbf{p_0},\lambda,\alpha,\Psi,\gamma)$ and $S2(\mathbf{p}=\mathbf{p_0},\lambda,\alpha,\Psi,\gamma)$ can be recorded ($\mathbf{p_0}$ denotes the sum of all structural parameters, e.g. groove width, depth, etc., which describe the grating's actual micro-structure). It is important to understand that $\mathbf{p_0}$ is assumed to be unknown and its determination is exactly the aim of the outlined method.

For the structure retrieval, the S1/S2-spectra are then compared to full vectorial numerical modelling results of the very same quantities relying on (initially inaccurate) parametrization **p**. Assuming that S1/S2 are sufficiently sensitive to variations in **p**, then a least square fitting procedure between modelled and measured spectra allows to determine the grating's actual microstructure or the corresponding set of parameters, i.e., $\mathbf{p_0}$.

3 Two practical use cases

The first example focuses on a binary transmission grating which is realized via etching into a fused silica substrate. The nominal grating is designed for maximum diffraction efficiency in the -1st order at wavelengths between 545nm – 680nm and an AOI = 41°.

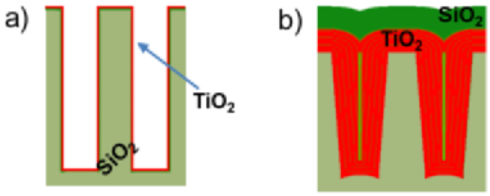

Fig. 2. a) Sketch of an ideal binary surface relief grating with conformal coating of TiO_2. b) backfilled grating with characteristic trapezoidal shape.

The associated grating profile is finished by a thin layer of titanium dioxide (TiO_2) of only 10nm to 15nm to improve performance (see Fig. 2a). The second example is a grating designed for operation at wavelengths between 745nm and 770nm with the AOI being 64°. Maximum diffraction efficiency of larger than 90% can be achieved applying a complete backfilling of the surface relief structure with TiO_2. ALD is used in both cases for deposition and the precise layer thickness intimately depends on the grating's groove width (or better: the actual trench profile) achieved in the previous dry-etching process. Hence, the knowledge of the exact dimensions of the grating's trench profile after etching is a prerequisite for the correct determination of the TiO_2 layer thickness.

Figure 3 presents a comparison of selected measured and modelled S1(λ) and S2(λ) spectra for a manufactured sample grating of the type shown in Fig. 2a prior to the application of the TiO_2 ALD coating. The modelled spectra are already the optimum solutions which provide the lowest least square error with respect to the measured spectra. Furthermore, two different shape models and thus parametrizations of the microstructure are assumed. The perfect binary shape (left column) is represented by only two parameters, namely groove depth and width. Second, a more realistic trench profile (right column) is assumed which is represented by five (instead of two) parameters.

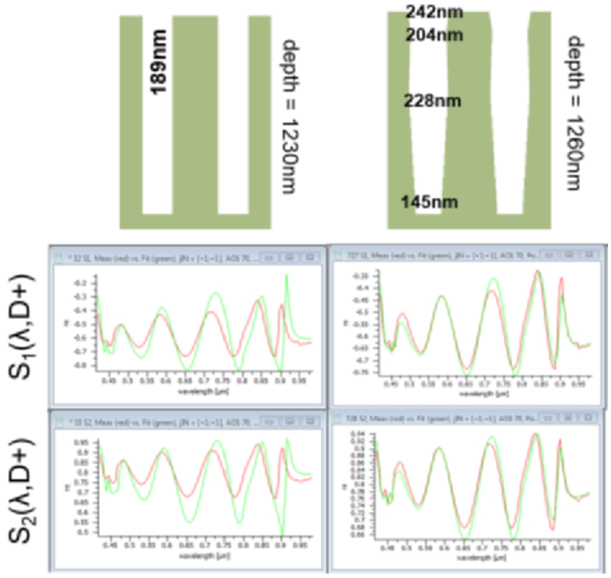

Fig. 3. Modelled (green curves) and measured (red curves) spectra of S1(λ) and S2(λ). D+ denotes diagonal linear illuminating polarization of 45°. Rotation angle is γ = 30° and incident angle Ψ = 60°. The left (right) column represents the best fit for an ideal binary (realistic) microstructure.

Comparing the accuracy of the model fitting for both profiles, it can be clearly seen, that the simple binary shape leads to considerably larger differences to the measured S1/S2 spectra. The mean square error decreases by a factor of 5 which clearly verifies the sensitivity of the method to smallest modifications on the nano-meter scale. Please note, that the left and right columns show the same values, however, on different axis scales.

The details of the second example (Fig. 2b) will be discussed in detail in the full contribution.

4 Conclusion

We have demonstrated that polarization sensitive white light reflection measurements can be used to solve the inverse scattering problem of surface relief grating structures allowing to retrieve the structural shape of the manufactured samples with high precision. Furthermore, we have used this information as a vital input to correctly adjust the precise parameters (layer thicknesses) of subsequently applied ALD coating processes.

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