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In-process characterization of sub-wavelength structures

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Abstract
The production of large area, periodically patterned surfaces with sub-wavelength structures depends on reliable in-process inspection to ensure that the topographical requirements are constantly met. The measurement of these surfaces is challenging because of the small structural length and the short available measuring period. Visible light diffraction-based methods, non-contact, with very short measuring time, are in this respect an appropriate diagnostic tool. This paper presents a high accuracy large scale mapping of the period and surface profile modulation depth of a sub-wavelength grid using laser light in the low visible wavelength range. Rigorous simulations of light scattering on sinusoidal gratings assisted to design the optical setup and the evaluation algorithms for the profile modulation depth. The measured values of the surface feature size coincide well with reference results of AFM measurements. The observed sensitivity of the method for local variations of the spatial surface properties proofs that the measuring principle is suitable for the setup of an efficient in-process measurement method.

Keywords: Light diffraction, optical diagnostics, periodic structures, in-process measurement

1. Introduction

Large area nanostructured surfaces and films have a broad spectrum of applications in the industry, science and life, with optical or physical functionalities such as light management or specific contact properties. The constant compliance with the topographical requirements is essential for the industrial production. Present manufacturing processes usually rely on offline surface measuring techniques as AFM or SEM for quality inspection. Laser light scattering measurements provide surface information fast, integrally and non-contact offering a high potential for in-process applications. Scattered light distributions are particularly suited for rapidly recognizing defects since they include the surface topography data [1]. In the particular case of periodically patterned surfaces visible light diffraction-based methods are an appropriate diagnostic tool. However designing the measuring method is challenging due to the short structural length and needs simulative assistance [2].

2. Discrete dipole approximation algorithm

The discrete dipole approximation (DDA) algorithm was introduced to calculate light scattering by non-spherical dielectric grains [3]. It is a flexible technique to simulate scattering and absorption of electromagnetic radiation by objects of arbitrary geometry. The method is based on the approximation of the target object by a similarly shaped collection of individual polarisable point dipoles. The DDA formulation turns exactly into the integral form of Maxwell's equations for light scattering computation when assuming infinitesimal distances between the dipoles. Each dipole is characterized by an oscillating polarization that depends not only on the interaction with the incident field, but also on the interaction of the dipoles among themselves, giving rise to a system of complex linear equations for the whole ensemble. The solution of this system delivers the set of polarization vectors which enables to calculate the scattered field. Both the theory of DDA and its numerical expression underlie permanent further development [4].

The practical application of the method, due to the interaction matrix dimensions, relies on efficient numerical algorithms such as the open source code Amsterdam DDA (ADDA) [5], which is used for this work. Depending on the parameters of the scattering problem, for example target size, shape, orientation or refraction index, the simulations can be very demanding in terms of the hardware and computational time. Since ADDA delivers comprehensive 4π scattering information it represents a powerful tool to determine the relevant features of the scattering pattern and the suitable parameters of a measuring method.

Figure 1. Model of a 2 µm x 4 µm sinusoidal grating with a 180 nm height.

3. Light scattering simulation results

For the DDA light scattering simulations a model of the nanostructured surface (Fig. 1) was extracted from reference AFM measurements and discretised into a regularly spaced dipole model. To describe the scattering problem in an appropriate manner a 10 nm dipole-dipole distance was chosen. Structures with a 204 nm grating constant and different grating heights, ranging from 60 nm to 310 nm, on a 120 nm thick substrate were generated. A uniform average refraction index of 1.5 was assumed.

For 405 nm laser light the first-order diffraction maximum is accessible for very large incidence angles with respect to the surface normal at very large diffraction angles, near the incident beam. An 86° incidence for the simulated scattering pattern leads to well defined broad diffraction peaks separated by less than 20° on the reflection and the transmission side of the surface plane and far enough on each side of the incident beam. Their summed integral intensity as a function of the grating height h is depicted in Fig. 2. A sigmoid function of the form $I = a/(1 + q\cdot e^{-bh})^{1/v}$, where a, q, b and v are fitting parameters, reflects the expected asymptotic tendency of the diffracted intensity to a maximum and was therefore chosen for fitting (Fig. 2, insert). Background intensity values at $h = 0$ can be reached for $v < 1$. The parameter q is related to $I(0)$ and b is the growth rate. An upper limit for the variation of a, the upper asymptote, was arbitrarily set to 10% of the total scattered intensity.

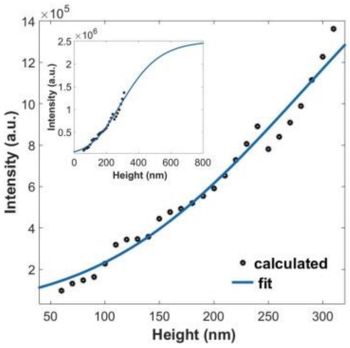

Figure 2. Summed integral intensity for the first-order diffraction maxima (reflection and transmission side) and the fitting curve. Insert: The asymptotic course of the fitting function.

The results predict a high sensitivity of the diffracted intensity for grating heights between 150 nm and about 400 nm (Fig. 2, insert). Scanning a large area grating should accurately detect local changes of the surface profile modulation depth with a spatial resolution determined mainly by the laser beam dimensions at the surface and the scan spatial frequency.

4. Diffraction measurements

A 40 cm broad grating (cut at 50 cm length) with both height and period of about 200 nm imprinted on a transparent foil in a roll-to-roll procedure was vertically fixed, parallel to a 2-axis scanning setup. A laser system and a camera were solidly connected to the scanning stage. Collimated 405 nm laser light illuminated the surface at an 86° incidence angle slightly out of the scattering plane allowing for both of the diffraction maxima to be simultaneously observed on a screen placed on the stage directly under the laser beam. The camera directed on the screen recorded the position and intensity of the two maxima during the 25 cm × 23 cm scan. The scan step was in both the horizontal (x) and vertical (y) direction 1 cm. The upper margin of the grating was located at y = 23 cm.

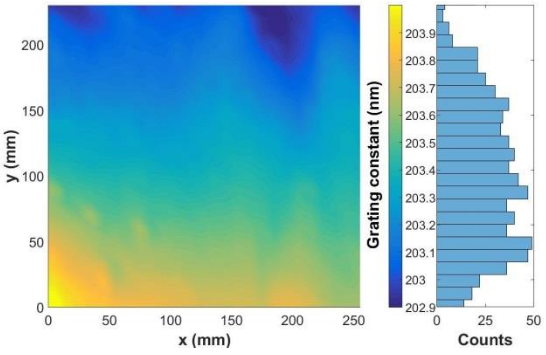

Figure 3. Mapping of the grating constant and the correspondent histogram.

The mapping of the grating constant (Fig. 3), calculated from the locally resolved variation of the diffraction angle, reveals a continuous slight increase towards the middle of the foil. This is illustrated by the histogram on the right side of Fig. 3 and could be explained by the production procedure. A maximum uncertainty of 0.1 nm for the grating constant was calculated considering the foil's undulation and the uncertainty in determining the diffraction maxima position. The results show a good qualitative agreement with AFM measurements performed on another section of the foil.

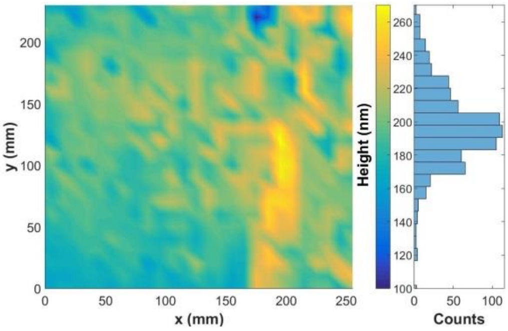

Figure 4. Mapping of the calculated grating height and the corresponding histogram.

Figure 4 depicts a mapping of the grating height as calculated from the locally resolved summed integral intensity of the diffraction maxima using the calibration function determined by simulations. The width and position of the maximum of the height distribution showed by the histogram in Fig. 4 agrees with the reference measurements too.

4. Conclusions

It was shown that simulations of light scattering on sub-wavelength sinusoidal gratings can assist to design an accurate evaluation algorithm for the profile modulation depth, avoiding the expensive and time consuming process of reference sample manufacturing and measurement. Large area mapping of the grating constant and height, in good agreement with AFM measurements, revealed the high sensitivity of the visible light diffraction-based method. The ability to quickly detect small variations of the spatial surface properties proofs that the measuring principle is suitable for the setup of an efficient in-process measurement method. Future work includes the simulation of more structures to refine the fitting curve, the measurement of calibration samples and an uncertainty assessment, finding other effects for lower dimensionality or differently patterned surfaces.

5. Acknowledgements

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