Modeling of dimensions and sensing properties of gold gratings by spectroscopic ellipsometry and finite element method

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Abstract. Gold gratings were measured by spectroscopic ellipsometry and modeled by the finite element method to investigate the capabilities of optical dimensional metrology for plasmonic diffractive structures. The gratings were prepared by electron beam lithography using parameters determined by finite element simulations for significant variations of the amplitude ratio and phase shift of the polarized reflection coefficients to achieve high sensitivity for both the measurement of the grating dimensions and the sensing capabilities. Sub-nanometer sensitivity was shown to determine the grating dimensions and the thickness of an adsorbed layer to be detected in both traditional reflection and Kretschmann-Raether (KR) configurations. The sensitivity for the refractive index of the ambient was calculated to be 10^{-5} at best, which is not significantly better than the sensitivities for plane gold layers in KR configurations. However, in diffraction-based resonant setups, the high sensitivity dips can be shifted to a larger spectral range, which is highly significant in many applications. It was also revealed that 2D models assuming a perfect geometry fit the measured ellipsometry spectra only qualitatively, leaving room for model development in the future.

1 Introduction and experimental details

Diffraction-based optical dimensional metrologies such as goniometric or Fourier scatterometry [1–3] on periodic structures have been revealed to be powerful methods due to their high accuracy, speed, and non-destructive nature. The starting point of developing traceable metrology is the instrumentation [4] and the evaluation models [5] based on accurate standard samples [6] as well as reference methods for verification [7]. In the development of reference standards, the materials based on silicon or its oxides have been used [6]; however, for a range of applications, such as sensorics, there is a need for the development of the metrology of periodic diffractive plasmonic nanostructures. This work investigates the dimensional metrology and sensing properties of gold grating structures.

Gratings with a period of 200 nm, thickness of 60 nm, and line widths (CD) of 70, 90, 110, and 130 nm were prepared on glass substrates using electron beam lithography and deposition. The dimensional parameters of the gratings were designed using calculations by the JCMsuite 6.0.10 finite element solver aiming to maximize the variation of the amplitude ratio ($\Psi = \tan^{-1}(|r_p/r_s|)$) and phase shift ($\Delta = \arg(r_p/r_s)$) of the reflection coefficients of light polarized parallel (r_p) and perpendicular (r_s) to the plane of incidence. The samples were measured by a Woollam M-2000DI ellipsometer at angles of incidence from 60° to 75°. The limit of detection was calculated using a Python interface with the JCMsuite package.

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2 Results

Figure 1 shows measured (plane of incidence perpendicular to the grating lines) and calculated Ψ and Δ spectra. The calculation assumes a perfect grating using the nominal parameters in a 2D model without fitting. Although there is slightly more than qualitative agreement, there is room for optimization. Sensitive parameters have been identified (not shown here due to the page limit) by analyzing the $f'_\Psi = \partial\Psi/\partial P$ and $f'_\Delta = \partial\Delta/\partial P$ derivatives, where P denotes the individual parameters. Knowing the standard deviation ($\sigma_{\Psi,\Delta}$) of the measured Ψ and Δ values, the limit of detection (LOD) can be estimated using $\mathrm{LOD} = \sigma_{\Psi,\Delta}/f'_{\Psi,\Delta}$, as shown in Fig. 2 for $P = n_a$, where n_a is the refractive index of the ambient. The calculation has also been made for an overlayer thickness on the surface of the grating, which also reveals sub-nanometer sensitivity.

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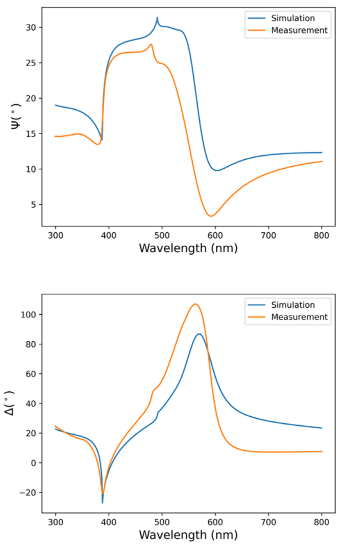

Figure 1. Ψ and Δ ellipsometry spectra calculated ("Simulation") and measured at an angle of incidence of 70° for CD = 70 nm.

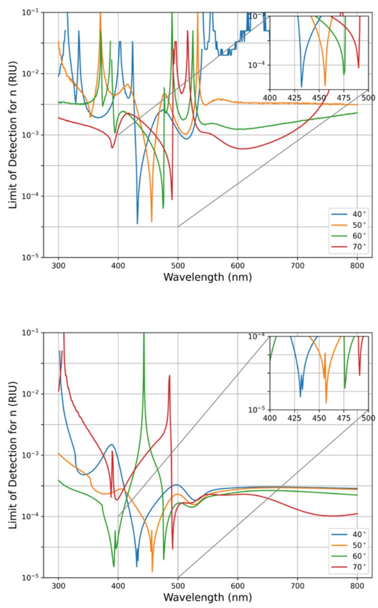

Figure 2. LOD graphs of n_a calculated from Ψ (top) and Δ (bottom) in refractive index units (RIU) for different angles of incidence and CD = 110 nm.

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