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Generalized ellipsometry of artificially designed line width roughness

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ABSTRACT

We use azimuthally resolved spectroscopic Mueller matrix ellipsometry to study a periodic silicon line structure with and without artificially-generated line width roughness (LWR). We model the artificially perturbed grating using one- and two-dimensional rigorous coupled-wave methods in order to evaluate the sensitivity of the experimental spectrally resolved data, measured using a generalized ellipsometer, to the dimensional parameters of LWR. The sensitivity is investigated in the context of multiple conical mounting (azimuth angle) configurations, providing more information about the grating profile.

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1. Introduction

Line width roughness (LWR) represents one of the challenges of today's semiconductor technology process control [1]. With constantly decreasing pitch, the importance of LWR increases as the ratio between LWR and mean line width also increases. Optical characterization tools, proven invaluable for fast and non-destructive inline process control, require new methods and models in order to achieve the efficiency needed for the real-time quality measurement of the LWR [2]. There has been previous demonstration of an optical method for LWR assessment using reflectometer operating in the Fourier space [3]. More recent theoretical work on the sensitivity of angularly resolved data to LWR [4,5] demonstrated the significance of the problem and explored limits of effective medium approximations for the purpose of LWR modeling.

It is becoming even more challenging with new applications requiring measurements to be done in very small (usually less than 100 μm) targets. Such measurements using spectral ellipsometer techniques require significant focusing of the light beam (with few degrees wide incidence angles range) in order to access small targets and achieve sufficient light intensity. The numerical aperture of the incident light beam puts more demands on the optical modeling and requires reevaluation of the sensitivity of the optical methods to the LWR. The effects of the finite numerical aperture include non-coherent averaging over incidence and azimuthal angles that result in a "washing out" of the spectral features [6]. This may decrease the sensitivity of the data to imperfections in line shapes, namely to LWR.

In order to investigate the sensitivity of the Mueller matrix ellipsometry technique to the LWR, a sample with artificially designed periodic perturbation of the lines was manufactured using e-beam lithography. The periodicity does not exactly resemble the random nature of typical LWR, but it allows the origin of the change in the spectral optical response to be positively confirmed. The purpose of this work is to present an approach consisting of finding the proper parametric model for the unperturbed grating and determining the magnitude of the change in mean square error (MSE) due to the line perturbation. The periodic LWR can be modeled using a generalized biperiodic rigorous model [7]. This approach provides necessary certainty in order to confirm that the differences in the optical response are due to the line perturbation and are not due to some other imperfection or omitted feature(s) in the line grating model.

In Section 2 the basic experimental background is given, together with a description of the multi-azimuth Mueller matrix ellipsometric method. Special emphasis is put on the modeling of depolarization effects caused by the significant numerical aperture of the instrument. Section 3 summarizes results showing clear distinction between the quality of fits for the unperturbed and perturbed line gratings. Differences are explained using a rigorous model for biperiodic gratings which leads to a comparable quality of the fit for both gratings. Results are summarized in Section 3.

2. Experimental details and modeling methods

The sample studied in this work was manufactured at the University of North Carolina, Charlotte, using e-beam lithography to etch a 736 nm pitch line grating into the silicon wafer. Nominal heights of gratings are 400 nm with nominal middle widths are 300 nm. Samples with different levels of perturbation are situated into different 100 μm × 100 μm targets. A scanning electron

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microscope image taken from the top of the unperturbed sample is shown in Fig. 1(a). A second sample has its artificial LWR designed by periodic modulation (period of 512 nm) of the line-width with the nominal amplitude being 2% of the line-width [see Fig. 1(b)].

Both samples were measured using a generalized ellipsometer with an automatic rotating stage at different azimuthal configurations. Measured data consists of 11 elements of the spectrally-resolved normalized Mueller matrices, where elements in the last row of the Mueller matrix are not available. The instrument uses focusing optics in order to project the beam onto the sample with a spot size smaller than 60 μm at a fixed incident angle of 65°. Experimental azimuthal angles were chosen from the range between −90° and 90° with steps of 15° (where the planar configuration corresponds to the angle of 0°). Azimuths of opposite sign were used simultaneously during modeling in order to decrease the importance of systematic experimental errors which do not have the same symmetries as the natural physical symmetry present in the optical response of the grating. The information in off-diagonal elements is important for decorrelating some profile parameters from each other at different conical configurations (different azimuth angles) and for the sensitive determination of precise values of azimuthal angles offsets. Measurement errors provided by the instrument are in average usually smaller than 0.01.

Measurements of the unperturbed line grating and the sample with the nominal 2% perturbation were taken using exactly the same azimuthal angles in order to compare the data directly. Due to the perturbed grating having the same "average width" as the unperturbed grating, it is possible to directly compare measured data without using any model. Comparisons between data measured on both samples, shown in Fig. 2(a) and (b), illustrate small differences at two different azimuthal angles (0° and 90°) which are supposedly caused by the line perturbations. The magnitude of differences between data demonstrates sensitivity of the spectral ellipsometric method to the periodic line width perturbation. Differences are not very large, but are indeed observable and measurable. They also strongly depend on the azimuthal angle, making some configurations more sensitive than others.

The optical response of periodic gratings can be modeled using rigorous coupled-wave analysis (RCWA), which uses Fourier series expansions of the electric and magnetic fields inside layers within the structure in order to express and calculate propagating and evanescent modes. Afterwards, tangential field components are matched at boundaries between different layers and overall reflection and transmission coefficients are determined. Standard RCWA implementations are based on the original work of Moharam and Gaylord [8,9] using a staircase approximation of the grating profile. The convergence rate is significantly increased for lamellar gratings (especially in the case of absorbing materials) using factorization rules that appeared first in the work of Lalanne and Morris [10] and then mathematically proven by Li [11]. Another standard improvement to the original formulation [8] is to use the scattering matrix approach instead of the original transmittance matrix approach. This approach permits calculations for deeper gratings, which use more terms in the field expansions, and which otherwise suffer from finite numerical precision used in all modern computers. In the scattering matrix algorithm [12], the modes outside of the structure are organized into two subsets: modes approaching the structure and modes leaving the structure. This algorithm leads to a more consistent calculation of the modes propagating through the structure and to an increased stability of the numerical implementation. Both improvements, combined with the original work of Moharam and Gaylord (or work of Rokushima for anisotropic gratings [13]), are now considered as the standard rigorous method to calculate optical response of periodic gratings.

Although the optical response of the perfect grating to a plane wave can be completely described using the Jones matrix formalism [14], in some measurements, depolarization can appear as the direct consequence of some experimental imperfections and must be treated properly. The major source of depolarization considered in this work is the high numerical aperture (NA ≈ 0.065 [6]) of the incident beam. As the result, experimental data show depolarization

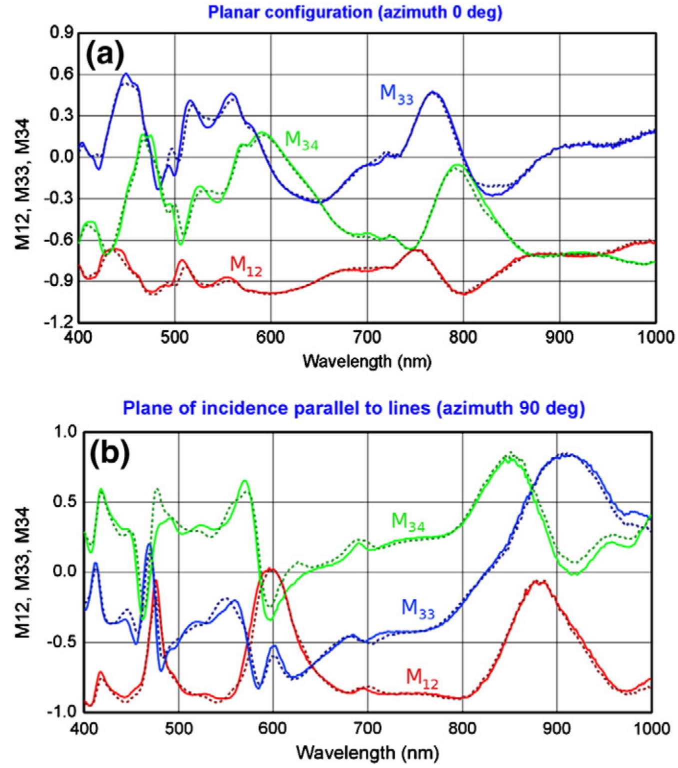

Fig. 2. Measured M_{12}, M_{33}, and M_{34} elements of the normalized Mueller matrices, plotted as functions of the wavelength of incident light, for the reference line grating (solid lines) and the grating with artificial LWR (dashed lines). Graphs show data acquired for (a) azimuth angle of 0° (planar configuration) and (b) azimuthal angle of 90°.

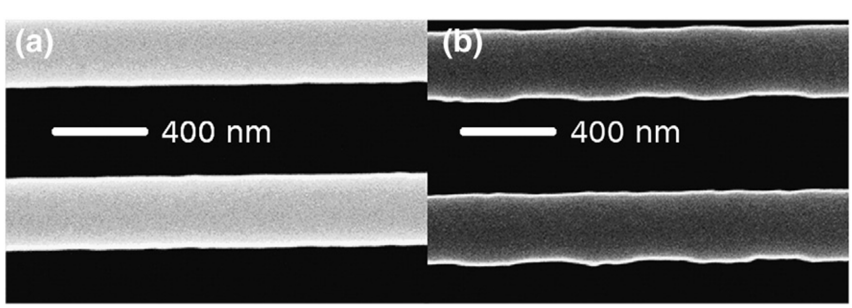

Fig. 1. Scanning electron microscope images from above (a) unperturbed and (b) perturbed line grating.

due to the incoherent superposition of the optical response over all incidence and azimuthal angles included within the numerical aperture. Depolarization effects are best treated using the Mueller matrix formalism, where the superposition is straightforward [6,15]. The most significant impact on the measured data can be seen in spectral regions with sharp spectral features. Neglecting depolarization effects caused by NA increases root mean square error values by a factor of about five. Modeling of depolarization in experimental data has substantial impact on the calculation time due to the necessity to perform calculations for multiple incidence configurations [6].

3. Results and discussions

In this work, we evaluate sensitivity of advanced ellipsometric methods to LWR represented by periodic perturbation of lines. The main goal is to confirm that observed differences between measured data obtained with and without LWR are solely due to the line width perturbation and not some other imperfection in the model or another physical difference between two samples. In order to do that, we have established a reasonably accurate and stable optical model of the unperturbed grating based on a multi-trapezoidal profile shape.

The grating profile is composed of four trapezoids on top of each other, with a thin silicon dioxide layer on the top of the first one (see Fig. 3). The profile is parameterized using eleven free parameters including: the total height, heights of top, and two bottom trapezoids; five trapezoid bases; offset to the nominal azimuthal angle; and the thickness of the silicon dioxide layer on the top. The absolute values of the correlations between parameters are very good, mostly much less than 0.7 with some exceptions leading up to 0.9. Except for 90° azimuth, there are no more than two correlations between parameters which reach values over 0.7, where the highest values (around 0.88) are typically connected to the heights of the bottom two trapezoids. At an azimuth of 90°, there are two correlations reaching 0.9 between the total height, the bottom trapezoid height and the bottom trapezoid base size. As a whole, correlations between profile parameters are very good with the best case being 75° azimuth, where all correlations were under 0.65.

The profile of the grating was determined for each incident azimuth separately by a least-squares optimization procedure that searches for optimal values of model parameters, which provide the best correspondence between experimental and modeled Mueller matrix data. Searching for the optimal values of parameters (values found at local minimum of the parametric merit function) is initiated using a numerical gradient based method, and the result is used as an initial guess for the Levenberg–Marquardt method [16,17]. The merit function is defined as a function of free parameter set p using all experimentally available elements of the normalized Mueller matrices as follows:

$$\mathrm{MSE}(p) = \frac{1}{11N_s - n - 1} \sum_{k=1}^{N_s} \sum_{i=1}^{3} \sum_{j=1}^{4} \left[M_{ij,k}^{m}(p) - M_{ij,k}^{e}(p) \right]^2 \Big|_{i \neq 1 \vee j \neq 1}, \quad (1)$$

where $M^x_{ij,k}$ denote the ij element of the k-th spectral normalized Mueller matrix and x stands for the modeled (m) or the experimental data (e), respectively. Numbers N_s and n denote the total number of spectral points and the number of free model parameters, respectively. Root mean square error (RMSE) used in the following text is defined as $\mathrm{RMSE} = (\mathrm{MSE})^{1/2}$.

The resulting profile of the grating defined by the lamellar layers as it is directly used by the RCWA is shown in Fig. 3 (blue lines) for the azimuthal angle of 45°. The profile is rather complex with significant overhang on the top which is crucial for the precise modeling of the measured data. In fact, it was not before the parameterization allowing this kind of overhang shape was used that the RMSE dropped to values smaller than 0.07 for all azimuthal angles. Due to some parameter correlations, there is some ambiguity about the exact shape of the overhang profile, but its existence and its significance are clear. An independent confirmation using atomic force microscopy (AFM) technique was performed using a critical dimension re-entrant tip. The results, shown in Fig. 4, clearly show this overhang.

The grating profile was determined for every measured azimuthal angle separately in order to confirm the stability of the profile and provide useful information about the accuracy of the model. The linewidth in the middle of the grating height has mean value of 291 nm with standard deviation of 0.9 nm calculated from 7 different azimuths. The resulting RMSE values achieved for all azimuths are shown in Fig. 5 (black boxes) with values increasing with increasing azimuthal angle (up to 90°). It is a typical trend which reflects the sensitivity of data to different profile features, where the higher sensitivity is usually closer to 90° as opposed to 0°. Fig. 5 suggests that there is still place for improvement for bigger azimuths where RMSE reach noticeably larger values.

Fig. 5 also shows RMSE values acquired by fitting the same profile model for the perturbed grating (red circles), showing significantly greater values than for the unperturbed one. Differences between RMSE values illustrate sensitivity of our method to the line perturbation, where larger contrast means higher sensitivity. The RMSE increases approximately 0.006 – 0.011 over the range of azimuths. From Fig. 5, we can say that the use of Mueller matrix ellipsometric methods is very promising for detecting the small line width perturbation, as there is very clear distinction between the results for unperturbed and perturbed line grating.

In order to further support the increase of RMSE values being due to artificial LWR, as opposed to other differences between the

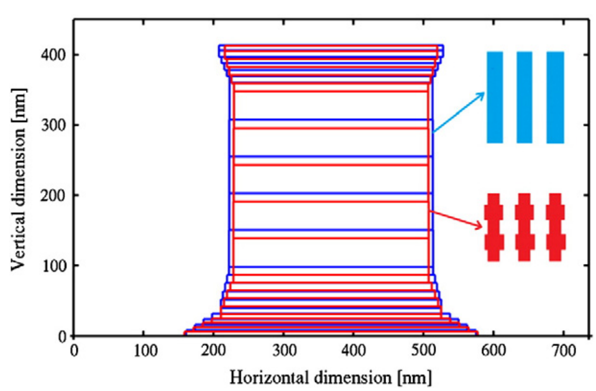

Fig. 3. Comparison between profiles acquired using the one-dimensional RCWA model on the reference grating (blue lines) and the biperiodic RCWA model of the grating with artificially designed LWR (red lines). Red profile represents perturbed grating in the narrow part.

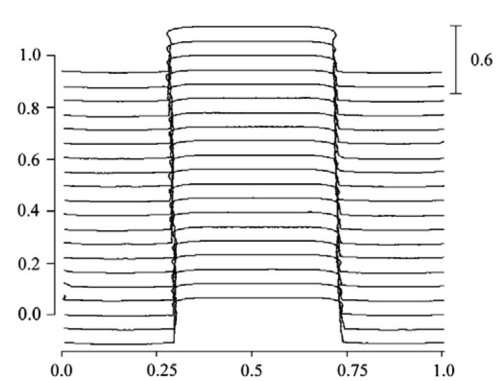

Fig. 4. Grating profile measured by AFM with all scales in micrometers. Line profiles show a clear presence of an overhang on the top of the grating.

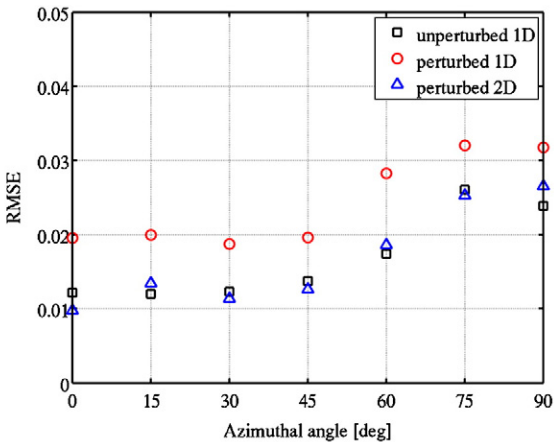

Fig. 5. Azimuthal dependence of RMSE from the best fits of the unperturbed grating using the one-dimensional RCWA model (black boxes) and the perturbed grating using the one-dimensional (red circles) and biperiodic RCWA model (blue triangles).

samples, the following study has been carried out. Taking advantage of the periodicity of our designed line perturbation, we have proceeded to apply a two-dimensional (biperiodic) model of the grating, adjusting two additional parameters (the perturbation feature length and depth) during the optimization process. The result of the fits is illustrated in Fig. 3 with two profiles compared at an azimuthal angle of 45°, where the narrower one corresponds to narrow places of the perturbed line. The mean value of the perturbation depth obtained by azimuthal fits was 20 nm (around 3.4% of the middle line-width) which is in a good agreement with 21 nm acquired from the original SEM image (see Fig. 1). The middle line width was reduced by 11 nm in the narrow part of the perturbed line.

Resulting RMSE values from the biperiodic RCWA modeling are shown in Fig. 5 (blue triangles) and compared with the unperturbed grating modeled using the one dimensional RCWA (black boxes). The comparison shows that the RMSE values are very close, which confirms that when the effect of the artificial roughness is correctly taken into account using the biperiodic model, the differences in the quality of fits disappear. This positive confirmation of the rising of RMSE values being solely due to artificial LWR allows us to conclude that the presented ellipsometric method is very sensitive to imperfections of grating lines. Moreover, it is apparent that even smaller artificial LWR can be detected and distinguished from other effects as there is sufficient difference between the RMSE values.

4. Conclusions

In this work we have presented an advanced ellipsometric method applied to the study of line-width roughness. Measurements and RCWA modeling were performed on the reference etched silicon line grating and the grating with artificially designed periodic line-width roughness. The multi-azimuth, Mueller matrix method used in this work allowed for a conclusive decision on the correctness of the proposed grating profile and helped to identify the overhang on the top of the grating line, which had a tremendous impact on the quality of the fit. The RMSE values for the reference and perturbed grating are acquired separately for multiple azimuths and show large differences. These differences disappear as soon as the proper 2D model of the artificial line width roughness is applied.

We can conclude that the ellipsometric method presented is very sensitive to artificial LWR and can be used to conclusively confirm origins of differences between optical responses of gratings with and without significant LWR. The multi-azimuth method improved the robustness of the method as there are different correlations between parameters at different azimuthal angles.

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