Modeling and Analysis of Scatterometry Signatures for Optical Critical Dimension Reference Material Applications

Heather J. Patrick[1,2], Thomas A. Germer[1], Michael W. Cresswell[1], Richard A. Allen[1], Ronald G. Dixson[1], and Michael Bishop[3]

[1]National Institute of Standards and Technology, Gaithersburg, Maryland 20899 USA
[2]KT Consulting, Inc., 2545 10th Street, Suite A., Antioch, CA 94509 USA
[3]International SEMATECH Manufacturing Initiative, 2706 Montopolis Drive, Austin, Texas 78741 USA

Abstract. We use an optical critical dimension (OCD) technique, matching modeled to measured scatterometry signatures, to obtain critical dimension linewidth of lines in grating targets fabricated on SIMOX (separation by implantation of oxygen) substrates using the single-crystal critical dimension reference materials (SCCDRM) process. We first compare experimentally obtained reflectance signatures for areas of the unpatterned substrate with signatures modeled using Fresnel theory, and show that the buried oxide (BOX) layer of the SIMOX is not well described optically by a single homogeneous layer of SiO_2, but can be so described if a mixed Si-SiO_2 boundary layer is included between the Si wafer and the BOX layer. We then obtain linewidths from OCD measurements on a series of grating targets with a range of design linewidths and pitches, and show that the linewidth obtained from the OCD technique is linearly related to the linewidth obtained from scanning electron microscopy (SEM), with a slope near unity and zero offset. While these results are very promising, further work in improving the fit of the simulated signatures to the measured signatures for some of the targets, reducing the target line roughness, and analyzing the uncertainties for potential optical critical dimension reference materials, is anticipated.

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PACS: 07.85.Jy Diffractometers, 06.30.Bp Spatial dimensions, 07.60.Hv Refractometers and Reflectometers

INTRODUCTION

We report on optical critical dimension (OCD) measurements of grating targets fabricated according to the single-crystal critical dimension reference materials (SCCDRM) process.[1] In OCD, the geometrical parameters (such as CD linewidth, line height, etc.) that best describe the lines of the target grating are determined by comparing measured optical signatures with modeled signatures. Here, the optical signatures consist of the reflectance of the grating at a fixed wavelength versus angle of incidence, measured for both s-polarization (the incident light is linearly polarized with E-field perpendicular to the plane of incidence) and for p-polarization (incident light linearly polarized with its E-field in the plane of incidence), a method that is often referred to as angular scatterometry.[2] The SCCDRM implementation provides features with known geometries—typically vertical sidewalls—defined by the silicon lattice. While earlier work focused on CD measurements of isolated SCCDRM lines at a single point for use in atomic force microscopy (AFM) calibration,[1] OCD measures the linewidth over a large area of a grating target. Here, we consider the use of SCCDRM grating targets as potential OCD reference materials. For this investigation, we compare target linewidths obtained by OCD to those measured using scanning electron microscopy (SEM).

In addition to comparing measured and modeled signatures for grating reflectance, we have also compared signatures taken on unpatterned areas of the substrate with simulated Fresnel reflectance signatures. This allows us to parameterize the thicknesses and refractive indices of the SIMOX (separation by oxygen implantation) substrate used for the SCCDRM chips, where we refer to the silicon wafer, a mixed boundary layer (if present), and the buried oxide (BOX) layer as the substrate. While we recently reported on OCD measurements of a subset of the targets considered here,[3] the improved substrate description in the current work is a better match to substrate reflectance data, and improves the fits of the simulated optical signatures to measured signatures for the grating targets.

TARGET DESCRIPTION AND SEM MEASUREMENTS

The SCCDRM OCD targets were fabricated on SIMOX wafers. SIMOX material consists of a thin silicon device layer over a BOX layer on a silicon wafer. Fig. 1 shows the line profile (the cross-section schematic of an individual grating line) within the grating target. The grating lines are fabricated in the silicon device layer, and have vertical sidewalls defined by <111> silicon lattice planes. The perimeter of each target is a parallelogram such that all edges are aligned to the <112> lattice directions.[3] The targets used here measure 100 µm from top edge of the target to the bottom edge of the target. The design widths of the lines in the targets range from 350 nm to 1000 nm, and targets with a ratio of design linewidth to line space of 1:1 and 1:2 were used. The actual linewidths in the targets are significantly smaller than design, as the anisotropic etch technique used in the fabrication process exhibited a typical process bias of more than 400 nm. Targets from two SCCDRM chips labeled B1 and J1, which had identical feature heights but slightly different processing conditions, were used.

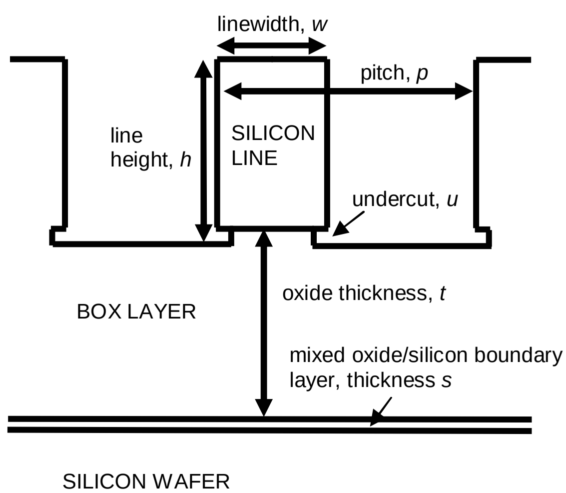

FIGURE 1. Line profile for the SCCDRM grating targets.

CD measurements were made by SEM on the targets from chip B1 in order to 1) provide an independent measure of the CD linewidth and 2) approximate the degree of line roughness for the grating. SEM measurements on chip J1 are in progress but were not available at time of publication. For these measurements, three SEM images were captured at three locations in the target. Each of these images was captured at 20,000X at a resolution of 2560 pixels by 1920 pixels, and included 6.4 µm long sections of two or three line segments (depending on the linewidths and spaces). The dimensions of the lines in these images were determined at 80 to 100 locations along the line. The edge roughness was estimated to range from 1.6 nm to 12.6 nm with an average value of 5.5 nm. The average CD linewidth, w_{SEM}, varied from 125 nm for a 1:2 target with 550 nm design linewidth, to 600 nm for a 1:1 target with 1000 nm design linewidth, as shown in Table 1. The typical uncertainty in w_{SEM} (the average linewidth of the target) was ± 2.5 nm (1-σ).

SCATTEROMETRY OCD

The optical signatures for the grating targets and the SIMOX substrate are obtained from angle-resolved reflectance measurements at a fixed laser wavelength using the NIST goniometric optical scatter instrument (GOSI).[4] Light from a λ = 532 nm laser is incident on the target at a variable angle of incidence θ. The light is focused on the target to a roughly Gaussian spot with a 20 µm full width at half maximum (FWHM). The laser polarization is set to either p- or s-polarization, and the detector angle is maintained at twice the angle of incidence (2θ) so that the specular component of grating reflectance is collected. Here, θ is varied from 5° to 55°. A small portion of the incident light is picked off before the final focusing lens to provide a reference intensity measurement.

The simulated signatures were obtained using the rigorous coupled wave (RCW) analysis for surface relief gratings.[5] This method solves the electromagnetic problem for a plane wave incident upon a medium having a dielectric function $\varepsilon(x,y,z) = \varepsilon_k(x)$, which is periodic in x, independent of y, and independent of z within each of a finite number of layers, indicated by index k. The solution requires Fourier series expansions of $\varepsilon_k(x)$ and $1/\varepsilon_k(x)$ for each layer. In practice, the Fourier series is truncated at some maximum order M, chosen here to be ±35. The modeled line profile is shown in Fig. 1 and was chosen because it is the simplest structure believed to adequately describe the grating, based on prior knowledge of the targets.[1] It is parameterized by the grating pitch p, line height h, the CD of the linewidth w, the undercut u, the SiO_2 film thickness t, and a mixed SiO_2-Si boundary film thickness s. Since the sidewall angles are vertical, it was not necessary to include sidewall angle as an adjustable parameter. The undercut arises during etching of the chip and is modeled as a square region with height and width u. When simulating signatures from the unpatterned SIMOX substrate, we set w and u equal to zero such that the Fresnel reflectance of the substrate is simulated.

TABLE 1. Summary of SCCDRM OCD targets used in the investigation.

Target ID	Target pitch, (μm)	Design Linewidth, (nm)	Linewidth from SEM, w_{SEM}, (nm)	Linewidth from OCD, w_{OCD}, (nm)	χ_r^2 of best-fit simulation
B1 00s 1:1	2	1000	596	579.5	137.9
J1 80s 1:1	1.6	800	-	281.5	109.5
B1 75s 1:1	1.5	750	320	319.5	117.0
B1 70s 1:1	1.4	700	260	259.0	29.5
J1 70s 1:1	1.4	700	-	161.5	10.3
B1 00s 1:2	3	1000	595	584.5	14.7
J1 00s 1:2	3	1000	-	581.5	38.3
B1 70s 1:2	2.1	700	301	297.5	35.4
J1 70s 1:2	2.1	700	-	301.0	40.5
B1 55s 1:2	1.65	550	125	114.0	122.1
J1 55s 1:2	1.65	550	-	116.0	244

The optical constant for the silicon wafer and the silicon lines is set at n_{Si} = 4.143 + i0.0283.[6] The optical constants for the oxide layer, n_{oxide}, and the thickness and composition of the mixed layer are determined from fitting the substrate reflectance (see "Results and Discussion", below).

In order to determine the best fit parameters for a measured target or substrate reflectance signature, the reflectance signature is compared with a library of simulated signatures for all combinations of the parameter space, and the parameter set corresponding to the simulation that minimizes χ^2_r is taken to be the best estimation of the target parameters. χ^2_r is given by

$$\chi_r^2 = \frac{1}{2N}\sum_{i=s,p}\sum_{j=1}^{N}\left(\frac{R_{meas,i}(\theta_j) - R_{sim,i}(\theta_j)}{\sigma_i(\theta_j)}\right)^2 \quad (1)$$

where N = 51 is the number of discrete angles where the reflectance is measured, σ is the estimated uncertainty in the measured reflectance, and the subscript i is used to denote that both s- and p-polarization reflectances are included in χ^2_r. We estimated $\sigma_i(\theta_j) = 0.01*R_{meas,i}(\theta_j)$ from the typical repeatability of the target signatures, as discussed further below. χ^2_r provides a relative measure of the quality of fit between the reflectance data and the simulation, with lower values indicating better agreement.

RESULTS AND DISCUSSION

Figure 2 shows the reflectance of the substrate near the grating targets on SCCDRM chip B1. We initially attempted to simulate the substrate reflectance using only the BOX layer and no mixed boundary layer ($s = 0$). The dashed lines show the resulting best fit curves, where we took n_{oxide} = 1.462, consistent with accepted values for SiO_2,[6] and where the best fit curves had oxide thickness t = 358 nm. As shown in the figure, the resulting fit is very poor. This was consistent with previous spectroscopic ellipsometry (SE) measurements on an unpatterned sample of SIMOX similar to that used for the SCCDRM chips, which showed that the oxide layer was not well described by a single layer of SiO_2, but required the addition of a mixed oxide/silicon boundary layer.[3] The solid lines in Fig. 2 show the resulting best fit reflectance when n_{oxide} was fixed at 1.462, the mixed boundary layer was taken to be a single Bruggeman effective medium layer[7] with a 50/50 mix of the oxide and silicon, and s and t were allowed to vary. This gave a much-improved fit, with s = 17 nm and t = 362 nm. Similar results were obtained for chip J1. Although we were able to further improve the fit by varying n_{oxide} and including more layers in the Bruggeman medium, this gave only modest improvement, and did not ultimately result in better fits to the grating target measurements.

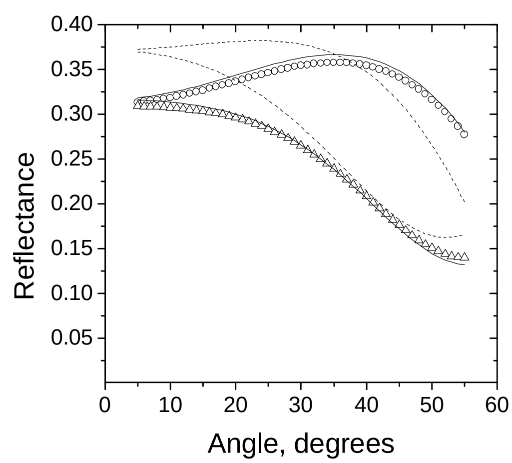

FIGURE 2. Measured substrate reflectance for s- (open circles) and p- (open triangles) polarization, and best fit simulated reflectance using BOX layer only (s = 0), dashed lines (upper, s-, lower, p-), and using an oxide layer plus a mixed oxide/silicon boundary layer, solid lines (upper, s-, lower, p-), as described in the text.

OCD line width measurements were made on eleven grating targets on chips B1 and J1. The pitch, design linewidth, and average linewidth as measured by SEM (where available) of each target are shown in Table 1. Fig. 3 shows the measured reflectance from one of the targets. Also shown in the figure is the simulated reflectance for the best fit linewidth, w_{OCD} = 259.0 nm, determined as follows. Only the pitch and linewidth were expected to vary from target to target. The pitch p of each target was well known and was fixed to the value shown in Table 1. Likewise, the height of the targets was fixed to h = 138 nm, consistent with AFM measurements of nearby isolated lines, and we fixed s = 17 nm from the substrate results. For the remaining adjustable parameters, initial exploratory libraries were produced where w was varied over at least 200 nm, u was varied from 0 to 15 nm, and t was varied from 350 nm to 380 nm. The best fit parameter sets from these libraries provided a rough value of w for each target and indicated that as expected, the values for t and u were consistent to within a few nanometers across the chip. For the final determination of w_{OCD}, we fixed u = 8 nm, t = 374 nm and h = 138 nm for all of the targets, then generated a set of fine step libraries for w where for each target, w was varied over a 40 nm range centered on its value from the exploratory libraries, in 0.5 nm steps. The best fit values for w are reported as w_{OCD} in Table 1.

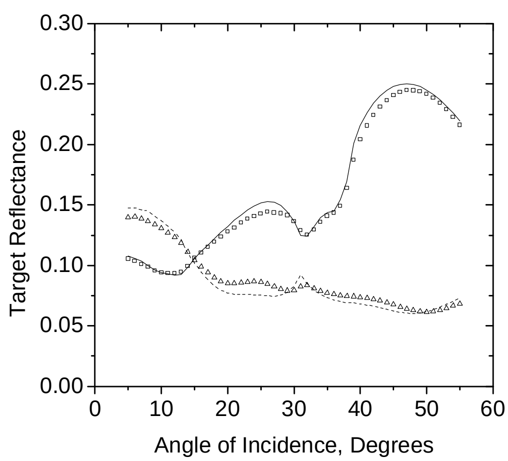

FIGURE 3. Comparison of measured and simulated OCD signatures for s-polarization (squares: measured, solid line: simulated) and p-polarization (triangles: measured, dotted line: simulated), for the B1 70S 1:1 target.

As seen in the Table, although we assumed the model line profile structure shown in Fig. 1 to be appropriate for all of the targets, there was a considerable range in χ^2_r values for the targets. For 1:2 line space ratio targets except the 550 nm design linewidth targets, and for 1:1 targets with design linewidths below 750 nm, the simulated signatures were in reasonable agreement with the data. Fig. 3 shows a typical data and simulation for this group. Unfortunately, the model was not as successful for the 800 to 1000 nm design linewidth 1:1 targets, or for the 550 nm design linewidth targets. One possible explanation for this is that the model does not take linewidth or line edge roughness into account. In the 550 nm design width B1 target, for example, the rms roughness seen in an individual SEM image was about 8 nm, a considerable fraction of the 125 nm linewidth. However, for the 1:1 targets with design linewidths over 750 nm, this fractional effect would be much lower. It is also possible that the chip processing resulted in a somewhat different line profile than that shown in Fig. 1 for the 1:1 targets.

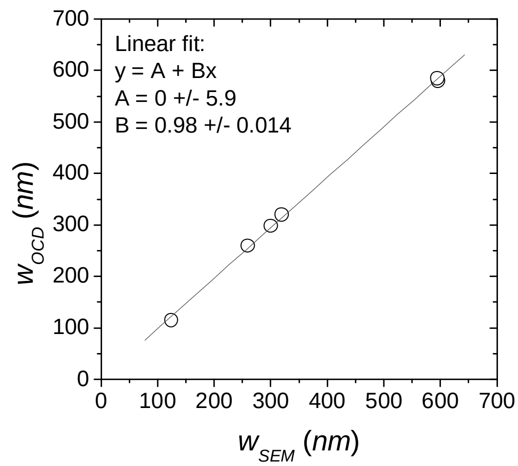

FIGURE 4. CD linewidth extracted from OCD, w_{OCD}, versus linewidth measured by SEM, w_{SEM}, for six targets on SCCDRM chip B1.

Figure 4 shows the value of w_{OCD} determined for each of the six targets on chip B1 versus the average SEM linewidth, w_{SEM}, measured for each target. The data were fit to a straight line using unweighted linear regression. Despite the above mentioned difficulties with the quality of the reflectance fits for some targets, we observed good correlation between SEM and OCD measurements, with the slope of w_{OCD} vs. w_{SEM} near unity with negligible offset. We believe this is due in part to the 90° sidewall angle of the silicon lines. In OCD targets with non-perpendicular sidewalls, cross-coupling between linewidth and sidewall angle in the optical signature is often a significant source of uncertainty in linewidth measurement.[8] In the current case, this source of uncertainty is not present. The slope between of w_{OCD} vs. w_{SEM} was also found to be very robust to changes in the substrate description. Although we have refined the substrate model in this work compared to our previous effort and have generally improved the χ^2_r values of the reflectance fits, our earlier substrate description also gave near-unity slope and very little offset between w_{OCD} and w_{SEM}.[3] However, the precise value of w_{OCD} for an individual target can vary for different substrate descriptions, particularly when χ^2_r for that target is large.

As previously mentioned, we have estimated the 1 sigma uncertainty in the measured reflectance as $\sigma_i(\theta_j) = 0.01*R_{meas,i}(\theta_j)$. This was obtained from the day-to-day repeatability of the reflectance measured from a target on 5 separate days, with the chip removed and replaced into the sample holder each day. In previous work, we have shown that the variation in w_{OCD} for this target from repeated measurements was very small, with a standard deviation of w_{OCD} over the data sets of only 0.4 nm.[3] We do not believe that the repeatability of the reflectance measurement is the only source of error in w_{OCD}, however. There may be additional systematic components to $\sigma_i(\theta_j)$. For example, on OCD targets the data were seen to be sensitive to the quality of the focus spot at the target, as excess light that is incident on the chip outside of the intended target could be collected by the detector and introduce a systematic error into the signature that would not necessarily be proportional to $R_{meas,i}(\theta_j)$. Another difficultly is the quality of fit between the experimental and simulated curves. Eq. 1 is approximately equivalent to calculating the reduced χ^2 of the fit to the data.[9] Ideally, we would like to use the value of χ^2_r in a χ^2 fit test to quantify a range of w_{OCD} and other model parameters that give acceptable fits to the data for each target. However, for the current level of agreement between simulation and measurement (see for example, Fig. 3) we do not believe the χ^2 fit test to be valid. Even the best fits have many points in the simulated curves which fall outside the estimated uncertainties in the measurements, and the differences between simulation and measurement do not appear normally distributed. For example, we could decrease the values of χ^2_r in Table 1 by increasing the number of angles measured, which should not be the case for normally distributed data. One avenue towards improving the reflectance fits may be to account for the line edge variations in the targets. One of us has recently shown[10] that the presence of random edge variation can reduce the amount of structure seen in a target's reflectance signature compared to the signature produced by a target with no edge variation. Efforts to address this issue, and the more general problem of error analysis in OCD, are ongoing.

CONCLUSIONS

In this work, we have obtained optical critical dimension linewidth on grating targets fabricated using the SCCDRM implementation, and have shown that the linewidth obtained from optical critical dimension scatterometry is very well correlated to that obtained from scanning electron microscopy. While these results make a significant first step towards development of reference materials for OCD standards, considerable work in improving the fit of the simulated signatures to the measured signatures for some of the targets, reducing the target line roughness, and in developing suitable uncertainty analysis for OCD applications, is required.

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