Metrology target design simulations for accurate and robust scatterometry overlay measurements

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ABSTRACT

Overlay metrology target design is an essential step prior to performing overlay measurements. This step is done through the optimization of target parameters for a given process stack. A simulation tool is therefore used to improve measurement performances. This work shows how our Metrology Target Design (MTD) simulator helps significantly in the target design process. We show the role of film and Optical CD measurements in improving significantly the fidelity of the simulations. We demonstrate that for various target design parameters we are capable of predicting measured performance metrics by simulations and correctly rank various designs performances.

Keywords: optical metrology, target design, overlay, scatterometry, overlay simulations, SCOL, DBO, OCD, MTD

1. INTRODUCTION

The ongoing reduction of printing resolution in the semiconductor industry has been demanding the ongoing attempts of tightening the overlay measurements specs. In recent years the lithographic resolution has not been reduced and the resolution reduction has been done by additional process and lithography steps, by applying multiple-patterning methods. This has led to the combination of two challenging consequences in the requirements for overlay measurements: the measured targets resolution has not been reduced due to the unchanged illumination light wavelength scale (of visible light) that enables the penetration of light through the process film layers, while the additional process steps have added a larger number of layers to be penetrated in order to perform the tight required alignment (overlay) between two patterned layers.

The difficulties described above have led both to the challenge of designing overlay targets that would enable sufficiently accurate measurements and to the sensitivity of measurements to process variations across and between wafers. This has raised the need to account for far deeper considerations in target design, and ultimately to the essential need of using simulations for target design optimization. In fact using simulations for estimating the accuracy and robustness of various metrology target designs in a given process stack has become a common requirement by cutting-edge leading microchip manufacturers [1],[2],[3].

Overlay targets are required to be printable, to have a relatively large process window, a sufficiently good TMU (Total Measurement Uncertainty) for repeatability specs, small overlay residual errors and sufficiently good accuracy. Finding targets that meet all these requirements demands an advanced simulation tool. The work described here demonstrates how our Metrology Target Design (MTD) simulator helps in successfully dealing with several of these challenges, and through an ongoing work will be dealing with all of them ultimately.

In this paper we restrict ourselves to overlay measurements by scatterometry (SCOL). In the following subsections we describe the basics of SCOL measurements followed by the fundamentals of our SCOL simulations.

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Section 2 will be devoted to the comparison of simulations to measurements for a specific stack. This section contains a work that has been aimed to test the capabilities of the simulations in enabling a successful target design.

Finally, in section 3 we will draw conclusions and give a short description of some of the remaining and ongoing objectives for our Metrology Target Design (MTD) simulator.

1.1 Scatterometry Overlay (SCOL) Measurements

The tool that is applied for our overlay measurements is based on an angle-resolved scatterometry [4]. It consists of a monochromatic light source, and the illumination spot is limited by a field-stop to a single target cell at a time. Several single-wavelength sources (λ_1, λ_2,…) are available in the range of visible light (400-800nm). A given target cell consists of a grating-over-grating structure, where the two gratings have a pitch of the order of magnitude of the light wavelength. This allows capturing in the collection pupil plane the intensities of the first order diffractions of the illuminating spot, such that all or most of the ±1st order diffracted spots are not overlapping with the zero order spot (see figure 1).

The tool light source and optical elements enable three main knobs for determining a certain tool setup for measurement: illumination wavelength (λ), illumination mask or apodizer (mainly choosing between on-axis illumination, as depicted in figure 1, or off-axis illumination, as shown below in subsection 1.2), and light polarization angle, which determines the polarization angle of both the illumination and collected light with respect to the cells grating vector (in the grating vector direction we refer to the light as "H-polarized" and perpendicular to the grating vector direction we refer to the light as "V-polarized").

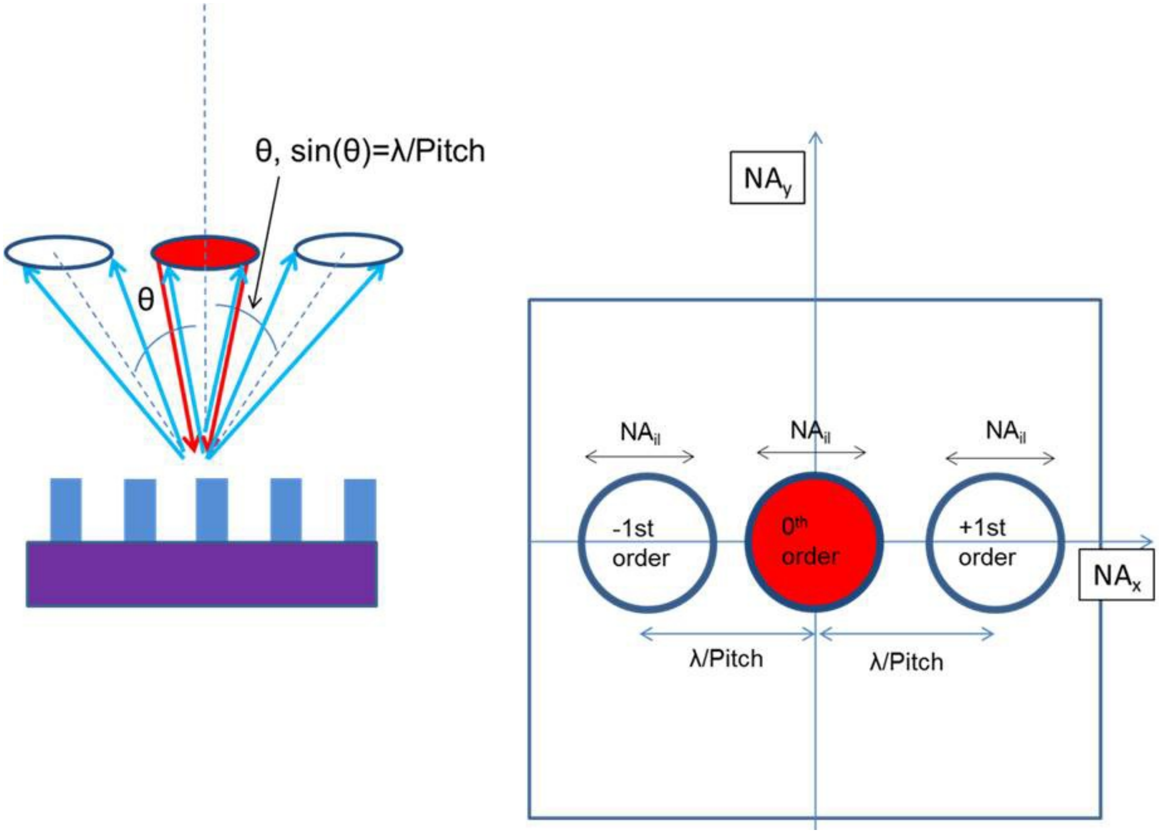

Figure 1. Collection pupil-plane for on-axis illumination in angle-resolved SCOL. The "NA" subscripts relate to Numerical Aperture coordinates, where the subscript "il" indicates "illumination". Wavelength is indicated by λ. (Figure in courtesy of Barak Bringoltz, KLA-Tencor Corp - Israel).

The basic concept for measuring the overlay from the ±1st diffraction orders, by using target cells consisting of grating-over-grating structures, relies on the breaking of symmetry between the +1st and -1st diffractions. By assuming that the only asymmetry in the grating-over-grating structure is due to the overlay between the bottom and the top gratings, the difference between the +1st signal and the -1st signal (while accounting for a 180 degrees rotation of the -1st signal with respect to the +1st one) is a measure to the overlay. Therefore we define the term of a "differential signal", which relates to the subtraction of the -1st order signal from the +1st one:

$$D_i\,(p) = S_i(p,+1) - S_i(p,-1) \tag{1}$$

where p indicates the index of a pixel in the collection pupil plane, corresponding to an illumination angle. The subscript i (= 1 or 2) refers to a target cell; in order to be able to quantify the overlay measure, two cells are required for each measurement direction. For each cell we induce a certain shift, f_0, in opposite directions, such that the total misalignment between the top and bottom gratings for the two cells is:

$$\begin{aligned} &\textbf{cell1:} \quad +f_0 + overlay \\ &\textbf{cell2:} \quad -f_0 + overlay \end{aligned} \tag{2}$$

Typical values of f_0 are ~20nm. From the two differential signals corresponding to the two cells we extract the overlay value [4]. This is done for each pixel, and a weighted average, which amplifies the contribution of the more sensitive pixels, is then applied for getting the single result of the overlay value.

A typical SCOL target consists of four cells, two for each measurement direction. A scheme of a typical target is shown if figure 2.

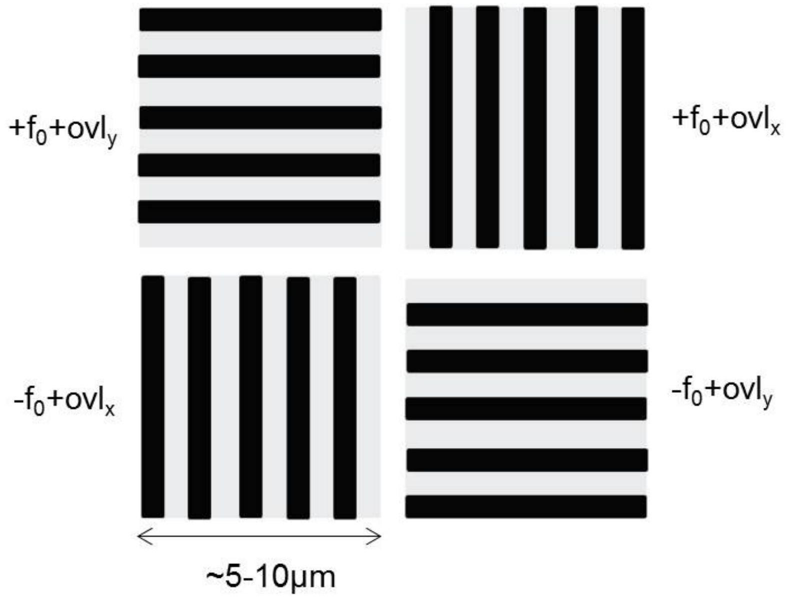

Figure 2. Typical SCOL target, where each pair of diagonal cells is used for the overlay measurement in its grating vector direction.

1.2 Electro-Magnetic (EM) Simulations

Simulations of the reflected light from a given wafer stack are done by solving Maxwell's equations for an input which consists of a spot of light having a certain wavelength and intensity distribution. Our measurements were done for two different illumination apodizers, an on-axis illumination (as depicted in figure 1) and an off-axis one. Figure 3 presents schematically the two illuminations; the on-axis is unapodized and is termed "Top Hat", whereas the off-axis is apodized (as shown in figure 3) and is termed "Quadrupole".

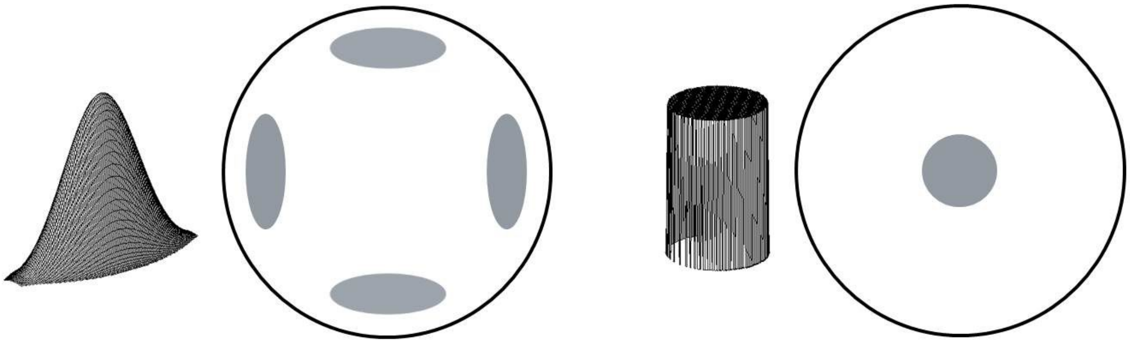

Figure 3. The two illuminations that are used in the measurements and simulations: (a) Quadrupole (QP) off-axis illumination and Top Hat (TH) on-axis illumination. The right-hand side figures for each illumination type depict the illuminating area in the illumination pupil plane and the left-hand side figures show the apodization applied to the illumination intensity.

Additional inputs to the EM simulations are the parameters that define the stack structure; these are given as two distinct types of parameters: layer thicknesses and materials dispersions, which depend on the certain stack processes, and target design parameters, which are variables that are chosen for optimizing the overlay measurements for that specific stack. The latter include pitch of the bottom and top patterned layers, CD (Critical Dimension) for the bottom patterned layer and for the top patterned layer (typically a photo-resist layer), half-pitch shift (see figure 4) which distinguishes between a "bar-over-bar" (indicated by us as *F=0*) and a "trench-over-bar" (indicated by us as *F=1*) configurations, and different segmentations of the gratings bars. Figure 4 presents the stack which has been used for comparing results of simulations to measurements (see section 2).

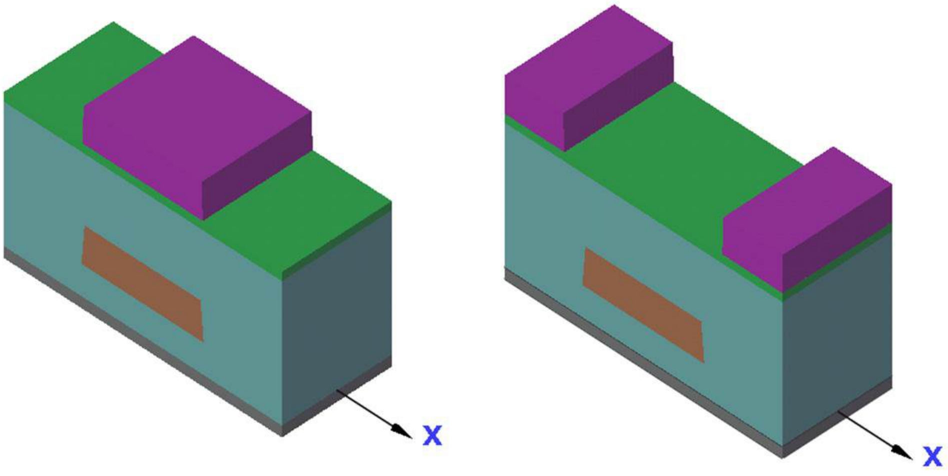

Figure 4. Schematic isometric drawings of a unit cell for a stack of a test wafer, showing two distinct target design configurations: (a) "bar-over-bar" and (b) "trench-over-bar".

Having setup all of the above mentioned inputs (stack geometry, materials dispersions, light wavelength and light illumination angles and apodizers), we then determine some numerical approximation parameters which are related to the applied numerical method (e.g. grid densities or other characteristics associated with the discretization due to the numerical computation.

The EM part of the simulation basically computes the Jones matrix associated with each illumination angle for each relevant (far field) diffraction order. In our case these are the $\pm1^{st}$ and 0^{th} orders. We then account for the contributions of the relevant optical system elements (such as lenses and polarizers) to convert the Jones matrices into intensities. In particular we account for a polarizer (in the illumination path) and an analyzer (in the collection path), which are set to 0 or 90 degrees depending on the designated tool setup of "H-polarized" light or "V-polarized" light.

Ultimately, the outcome of the EM simulations is the collection pupil plane of diffractions up to the $\pm1^{st}$ orders, or in other words the collection pupil images, similar to the ones that one expects to obtain on the CCD camera of the measurement tool.

1.3 Performance Metrics

Since the role of our simulations is to predict the better performing target designs, appropriate metrics indicating on performance need to be determined. Various metrics have been defined to indicate on the level of measurement precision (which indicates on measurement repeatability and is part of the common metric of TMU), accuracy and robustness. For the demonstrated comparisons of the current work two main metrics have been accounted for: Sensitivity-to-Overlay (which we term *SE*) and Diffraction Efficiency (which we term *DE*).

The definition of Sensitivity-to-Overlay, *SE*, is mathematically the partial derivative of the differential signal with respect to overlay. If we approximate the differential signals from the two cells by the first term of a Fourier series (of anti-symmetric terms only) [4]:

$$\begin{aligned} D_1(p) &= \sum_n A_n(p)\sin\left\{\frac{2\pi n}{Pitch}\left(f_0 + overlay\right)\right\} \approx A_1(p)\sin\left\{\frac{2\pi}{Pitch}\left(f_0 + overlay\right)\right\} \\ D_2(p) &= \sum_n A_n(p)\sin\left\{\frac{2\pi n}{Pitch}\left(-f_0 + overlay\right)\right\} \approx A_1(p)\sin\left\{\frac{2\pi}{Pitch}\left(-f_0 + overlay\right)\right\} \end{aligned} \tag{3}$$

and furthermore by assuming a small misalignment between the patterned layers with respect to the pitch:

$$\begin{aligned} D_1(p) &\approx A_1(p)\frac{2\pi}{Pitch}\left(f_0 + overlay\right) \\ D_2(p) &\approx A_1(p)\frac{2\pi}{Pitch}\left(-f_0 + overlay\right) \end{aligned} \Rightarrow D_1(p) - D_2(p) \approx A_1(p)\frac{4\pi f_0}{Pitch} \tag{4}$$

we obtain for the Sensitivity-to-Overlay (per pupil pixel):

$$\frac{\partial D_i(p)}{\partial(overlay)} \approx \frac{D_1(p) - D_2(p)}{2f_0} \tag{5}$$

for each one of the cells (i=1,2). From this result we derive an averaged metric, *SE*, which is a form of a signal-normalized summation over the pixels, such that *SE* has the dimensions of [1/length]. This metric indicates how sensitive a stack structure is with respect to the overlay between the top and bottom gratings. The value of that metric will be indicating the capability of measuring overlay with good precision.

The definition of Diffraction Efficiency (*DE*) is the ratio between the $\pm1^{st}$ orders signals and the 0^{th} order signal:

$$DE = \frac{1}{2}\frac{\sum_{p=1}^{N_p}\left\{S_1(p,+1) + S_1(p,-1)\right\}}{\sum_{p=1}^{N_p} S_1(p,0)} \tag{6}$$

This is defined for a specific cell (cell 1 in that case), but would give similar results for both cells (since the small shift between the gratings which distinguishes the two cells does not affect much that ratio). This metric indicates on the amount of spatial noise that might be affecting measurements due to various imperfections of the target which cause to the contamination of light originated from the 0^{th} order diffraction to the $\pm 1^{st}$ orders that are used for extracting the overlay; small values of *DE* would be indicating that only a fraction of the 0^{th} order diffraction could damage (through target edge diffractions, target noise etc.) the $\pm 1^{st}$ order signals significantly.

2. PREDICTION OF MEASUREMENTS BY SIMULATIONS

For testing our simulator and in order to be able to assess the level of success of the simulations in their assistance in target design, we have tried some attempts of comparing the simulation results to measurements. Previous work of comparisons was done first for a single grating stack [3]. That initial work, however, was done mostly for the purpose of verifying the capability of the simulator to predict correctly and accurately the measurements done by the overlay tool. At this stage we have tried comparisons for proper SCOL targets. That has been done on a test wafer, which included many designs of targets. The stack for this wafer is shown in figure 4 and figure 5 for isometric view and front view, respectively. The process of performing the comparisons included several steps, as described in the subsections below.

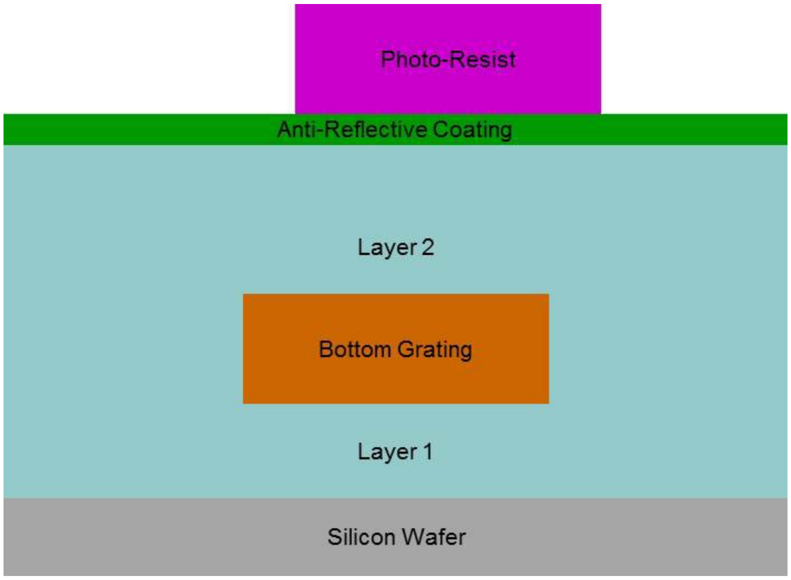

Figure 5. Schematic front view drawing of a unit cell for the stack of the investigated test wafer.

2.1 OCD and CD-SEM Measurements

An accurate and reliable simulator is essential for achieving well behaved predictions of actual measurements, but is not sufficient. This becomes important in particular when the level of accuracy in predicting measurement needs to be sufficiently high for distinguishing between various target designs. Another crucial condition is having the correct and sufficiently accurate inputs to the simulation, or alternatively excluding exceptional cases for which small variations in inputs might result large differences in the computed signals or metrics.

We have noticed that frequently intended stack information is significantly different from the actual printed stack. We therefore have chosen to take a preliminary step of OCD (Optical measurement of Critical Dimension) verification. This step helps in verifying the stack layer thicknesses and the stack material dispersions.

The OCD verification could adjust the layer thicknesses and dispersions, but could not verify the CD (grating bar width) differences, since these are typically different between designated OCD and SCOL targets. Therefore, by simulating various CD values (for the test wafer targets all top and bottom grating CD values were identical) and rechecking with

CD-SEM measurements we could confirm a significant bias in the CD values, as shown in figure 6 for two target designs. Figure 6 demonstrates how the matching between simulated and measured signals significantly were improved by accounting for that bias; in that figure the cross-sections of the measured signals are plotted (in blue) for two different targets (where each one was measured with different tool setups), and the simulated corresponding signal cross-sections are plotted on the same figures (in black) for the designated CD value (on the left), and for the biased CD value (on the right) found through the simulation of many CD values for multiple tool setups. Having a match in signals between simulation and measurement as shown on the right of figure 6 implies on a definite sufficient accuracy of the simulation in predicting measurement performances.

In figure 7 the found biased CD values (normalized by pitch) are plotted versus the CD designated values, and it is shown that a systematic bias exists for all investigated targets. This bias is known to be a type of bias that occurs as a result of certain lithographic exposure rules.

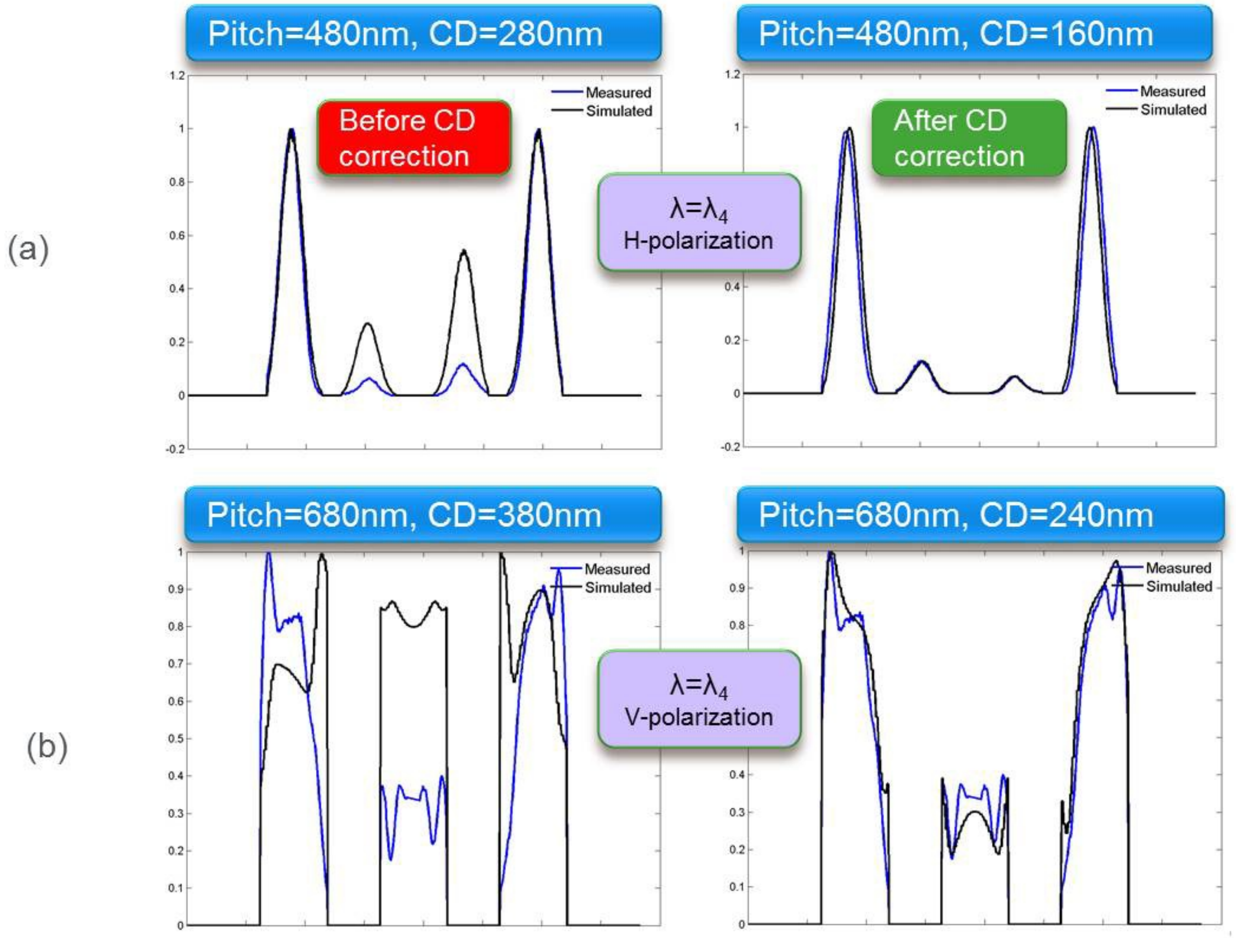

Figure 6. Comparisons of simulated-to-measured signals before correcting the CD bias and after the correction, for two targets: (a) a 480nm pitch target measured with Quadrupole illumination, and (b) a 680nm pitch target measured with Top Hat illumination.

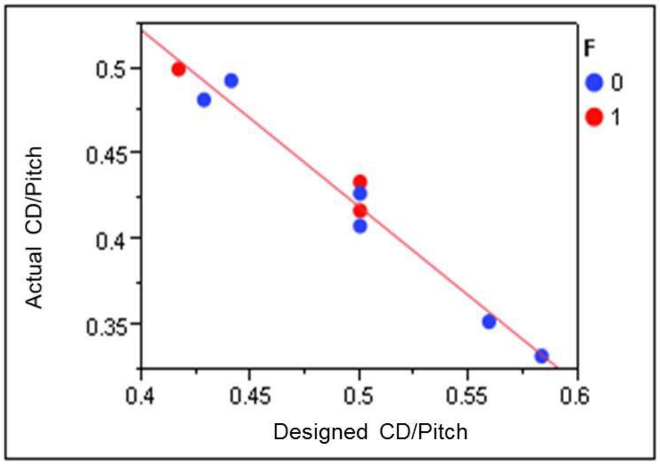

Figure 7. Biased CD vs designated CD (normalized by pitch) for multiple target designs. *F* refers to “bar-over-bar” design configuration (*F=0*) or “trench-over-bar” design configuration (*F=1*). Top and bottom CD for these targets are identical.

2.2 Signal Simulation-to-Measurement

Simulation validation has been done for our test wafer for many different target designs. After the verification step described in the previous subsection, an excellent agreement has been achieved. Figure 8 present a comparison of a full pupil image for the measured signal (top figure) and the simulated signal (bottom figure) for given target and tool setup. By comparing the measured and simulated images the agreement of fine details can be identified. The spatial noise that can be clearly observed in the measured signal is presumed to be a consequence of both finite cell-size and target noise diffractions effects.

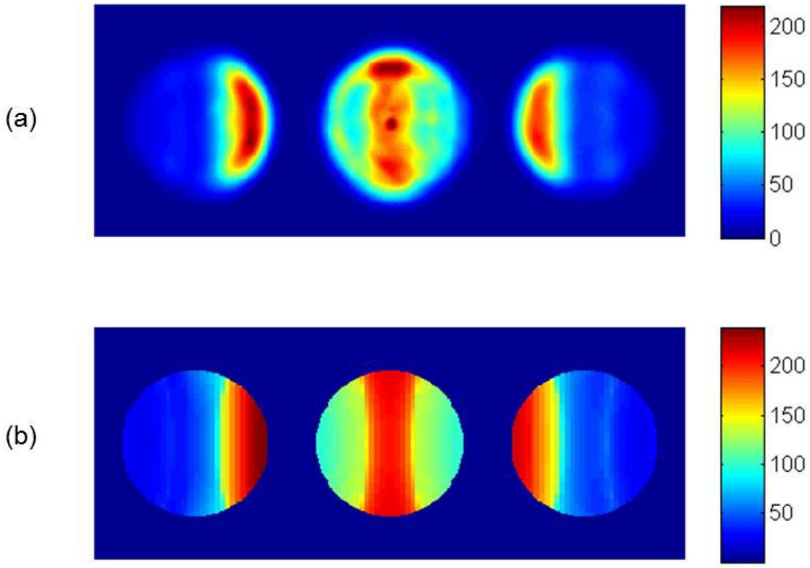

Figure 8. Pupil image for (a) measured signal and (b) simulated signal, showing the -1st,0th,+1st diffraction orders from left to right. The false color bar indicates intensity in Gray-Levels. The target in this case is for pitch=760nm, top/bottom CD=330nm and *F=1*. The tool setup is Top Hat illumination, $\lambda=\lambda_1$ and H-polarization.

Figure 9 presents the comparison of simulated-to-measured signal cross-sections for three different targets and for multiple tool wavelengths. All three cases are for target configurations of "bar-over-bar" (*F=0*), and for tool light set to H-polarization. Note that the choice of illumination (on-axis Top Hat or off-axis Quadrupole) depends on the ratio wavelength/pitch; for larger target pitches most of the wavelengths require the on-axis illumination, whereas for small target pitches most of them require the off-axis illumination (for the same reason for the smallest pitch of 480nm the longer wavelengths of ~600-700nm cannot be used for measurement at all). The matching of signals between simulations and measurements shows very good agreement for most targets and tool setups. In cases where we see some noticeable differences (such as in figure 9c for $\lambda=\lambda_1$) the reason typically could be high sensitivity of the signal to the specific wavelength, or to small changes in the stack structure (since the light optical path is determined by either one of them).

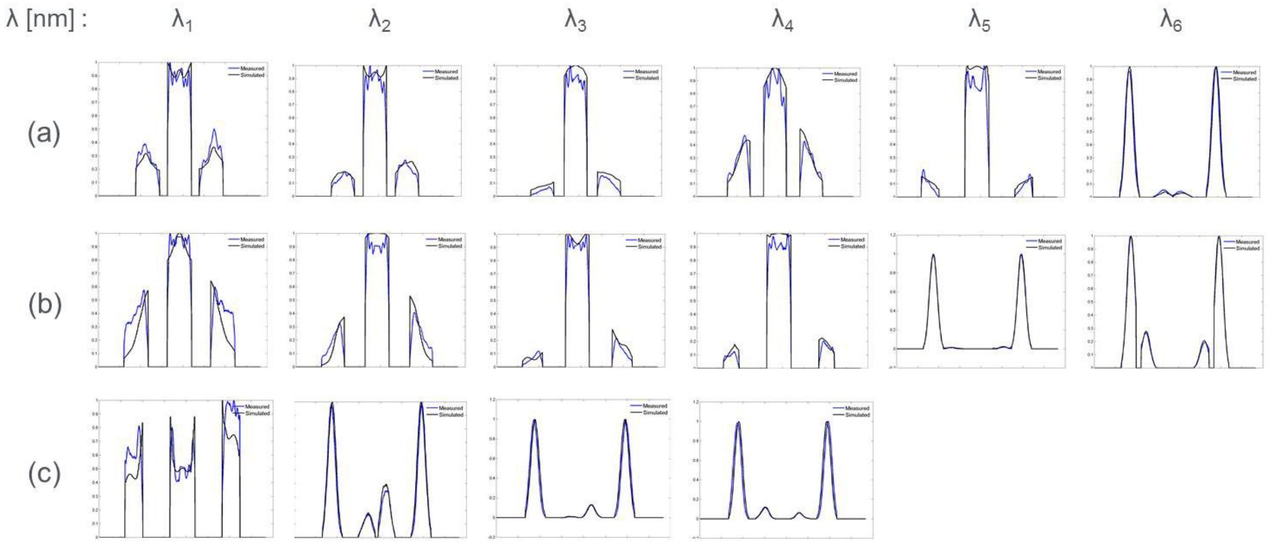

Figure 9. Simulation-to-measurement signal cross-sections for multiple tool setups (wavelength in this case) for three different targets: (a) pitch=760nm and top/bottom CD=325nm, (b) pitch=560nm and top/bottom CD=270nm, and (c) pitch=480nm and top/bottom CD=160nm. For all three cases *F=0*, and tool light is H-polarized. Measured signals are in blue lines and simulated signals are in black lines.

2.3 Metrics and Ranking Performances

After reviewing the comparisons of the simulated signals with the measured ones, it is of great interest to us to test the matching of main performance metrics. Furthermore, since we have the objective of using simulations for optimizing target designs, it is important for us to be convinced that the matching of metrics could be shown to be sufficiently accurate such that the ranking of target designs based on simulations would be consistent with the one that is based on measurements. We therefore compare for the various targets and various tool setups the two performance metrics that were defined and discussed in subsection 1.3. Figure 10 presents the comparison of *SE* (Sensitivity-to-Overlay) and *DE* (Diffraction Efficiency) between these two metrics computed from the simulated and from the measured signals. We can see that the consistency of the simulations with the measurements is very high.

In figure 11 scattered plots are shown on a log-log scale for both Sensitivity-to-Overlay *SE* and Diffraction Efficiency *DE*. Each circle marks simulated versus measured value for a certain target design and tool setup. We can observe that the deviation from the 45 degrees slope is relatively small, and this can be seen quantitatively by the linear fit and the R-squared that are given on the upper left side of the figures. All together the correlation between simulated and measured metrics is very high.

Overall, it can be observed that even for some cases where the matching between simulation and measurement is not very high, the consistency in ranking the targets based on these metric performances is not being damaged crucially.

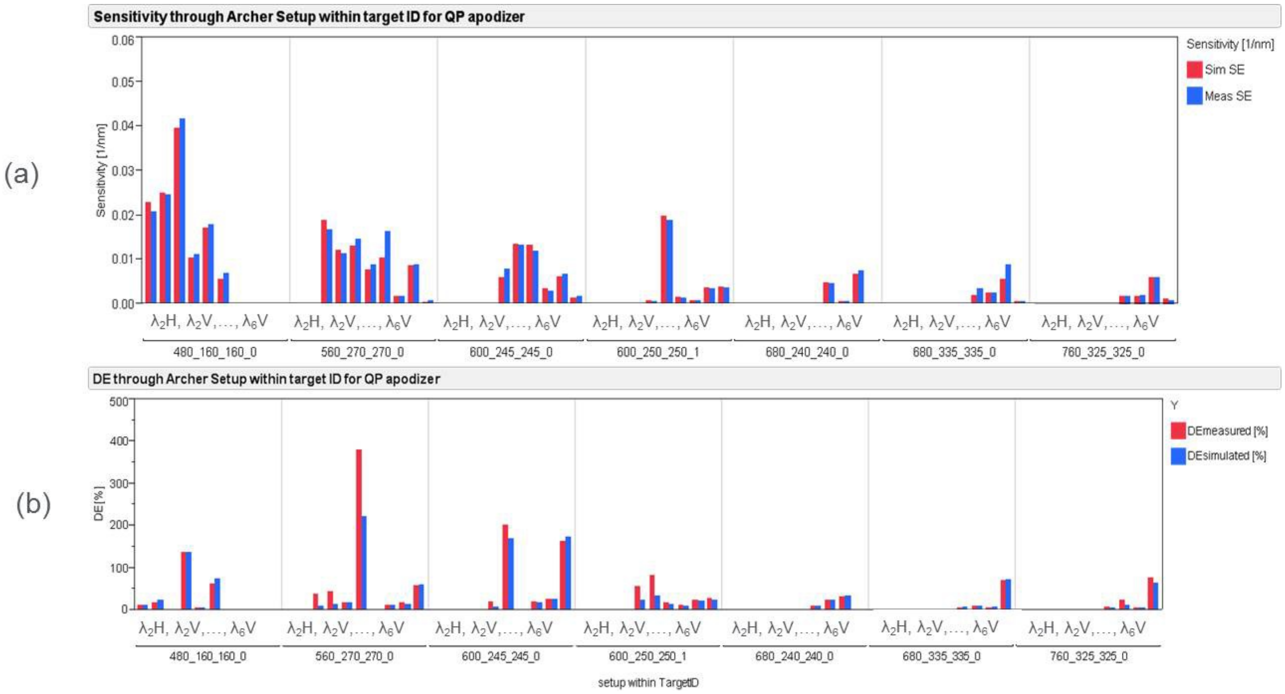

Figure 10. Measured vs simulated metrics: (a) Sensitivity-to-Overlay *SE* and (b) Diffraction Efficiency *DE*. The inner horizontal labels are for various tool setups, and the outer labels indicate the target design: [pitch]_[top CD]_[bottom CD]_[F]. These results include only the tool setups for Quadrupole illumination.

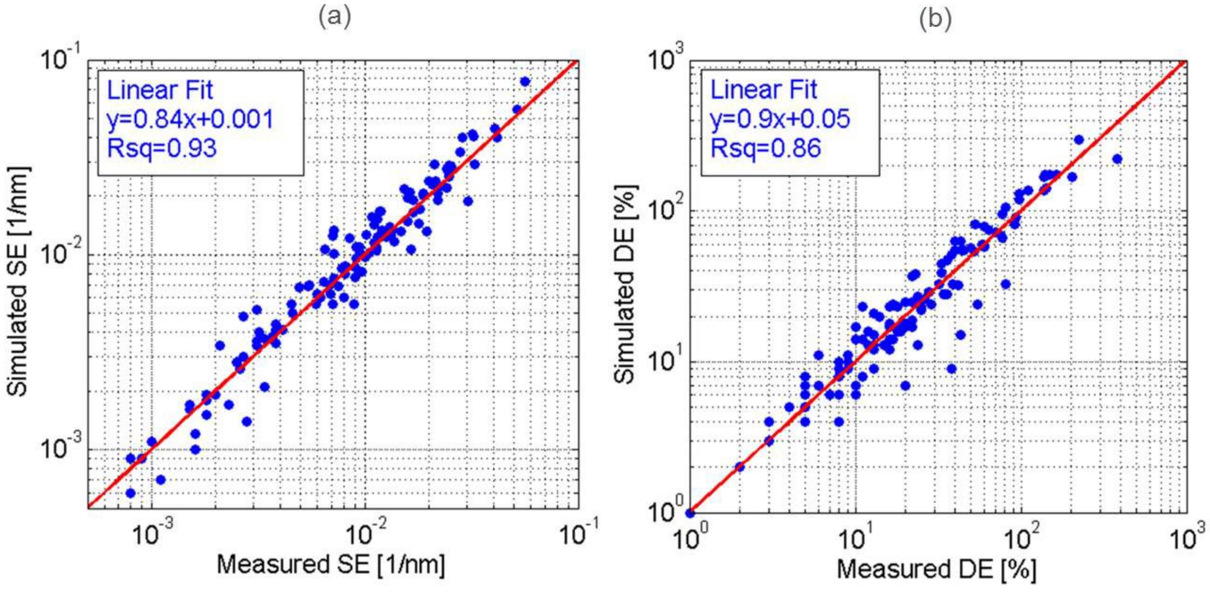

Figure 11. Scattered plots for simulated vs measured metrics: (a) Sensitivity-to-Overlay *SE* and (b) Diffraction Efficiency *DE*. The solid line marks the perfect correlation and is a reference for the dotted results. The legend boxes on the upper-left provide a linear fit for the dots and the R-squared result.

3. CONCLUSIONS AND ONGOING WORK

We have demonstrated the capability of correctly simulate reflected signals from a wafer stack and to match them accurately with measured signals from a scatterometry overlay tool. Moreover, we have shown that main target performance metric match well and we are able to rank target designs correctly if we base our ranking on simulations instead of on measurements. This important outcome suggests that the use of simulations for target design is feasible for scatterometry overlay measurements. This use of simulations, instead of relying on experimental measurements only, is an important part in achieving successful overlay measurements in general and in particular in being able to measure overlay for challenging stacks.

The current work, however, has been done for a rather simple stack test wafer. It is expected to be more difficult for stacks that include more layers, or for stacks that might be more challenging in the sense that their performance metrics ranges for various target designs and tool setups will be significantly narrowed and restricted to a low values. The simulations of more challenging and multilayer stacks is therefore currently under investigation. We have learned through this work how crucial the verification of stack geometry and dispersion is. Therefore, the preliminary part of OCD measurements (or other type of film measurements for that matter) is an important step in achieving successful prediction of measurements by simulations. That step could be used on regular bases prior to the step of using simulations for target optimization.

The performance metrics that have been calculated for this work are basic measures for overlay measurements capabilities, but more metrics are required to assist in predicting the capabilities to measure an accurate overlay and to overcome problems that are associated with process variations. Some more such metrics are already in use, and in an ongoing work we calculate additional performance metrics for both our simulations and measurement.

Finally, it is important to be aware that the successful matching between simulations and measurements for whatever performance metrics that we have, there still might be some effects on measurements that are not accounted for through those metrics. Some effects that are known to us are the diffractions from target cell edges, target surrounding contaminations and target noise. For the first two we have an ongoing work for modeling the effects of finite cell-size targets. The latter one is a more vague effect, and could be addressed with some more limitations.

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