Optimization of Scatterometry Measurements by Enhancing with Machine Learning

AM: Advanced Metrology

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Abstract – In this study, we introduce a machine learning approach designed to augment the conventional Rigorous Coupled-Wave Analysis (RCWA) method used in scatterometry measurements. The utility of this approach is illustrated through two practical examples. Initially, we applied it to a recess structure in trench MOSFET. Following the application of our machine learning method to the RCWA model, the recess depth measurement exhibited improved stability and uniformity across the wafer. In the second example, we measured a 2D line trench in silicon (with a depth of 22 µm); here, both the top and bottom widths are parameters of interest. We show that our machine learning based model is more robust compared to the conventional RCWA method. Our results were then cross-verified using atomic force microscopy results and cross-section Scanning Electron Microscopy data, respectively.

Topics: Machine learning, spectral reflectometry, scatterometry, trench shape, CD, OCD, RCWA, recess depth

I. Introduction

The traditional use of electromagnetic simulations, such as Rigorous Coupled Wave Analysis (RCWA), has been primarily for scatterometric applications, to ascertain the geometry of various structures within a grid [1]. This proves beneficial when the spectroscopic reflectance spectra are sensitive enough to respond to small variations in the parameter of interest and when experimental data can be suitably characterized with an appropriate model. However, this method becomes considerably more challenging in certain situations, such as when dealing with a large pitch, an unfavorable aspect ratio between depth and critical dimension (CD), or a complex combination of different materials. In these instances, while the RCWA method may still provide the correct trend in variation, the uniformity or uncertainty of the measurements might be adversely impacted. In this context, machine learning (ML) based approaches have demonstrated promising results [2-3]. Furthermore, it has been observed that measurement accuracy improves significantly when utilizing a machine learning approach, as compared to traditional methods [4].

In this study, we illustrate this improvement through two distinct examples, demonstrating ML enhancement of the RCWA approach. The first case examines a recess in a MOSFET trench with a pitch greater than 2 µm. Here, it has been shown that the measurement of recess depth and sidewall oxide thickness is improved with the use of ML-enhanced scatterometry, as opposed to conventional RCWA. The second example involves a line trench in silicon with a pitch of 4 µm and a depth of 22 µm. The significant aspect ratio between the depth and critical dimensions presents a substantial challenge for RCWA simulations.

A. *Machine Learning Approach*

Initially, measured optical spectra are needed to determine the geometrical parameters of interest. Measurements in this work were carried out with a NOVA T600 MMSR tool, which has a vertical and an oblique incidence advanced scatterometry channels. The spectra consist of s-polarized (R_s) and p-polarized (R_p) reflection spectra collected from normal as well as oblique incidence channels with azimuth angles of 0 and 90 degrees.

In order to train the machine learning model, the collected reflectance spectra and reference measurement data, obtained from the RCWA method were used. We also incorporated external reference data such as inline Critical Dimension Scanning Electron Microscopy (CD-SEM) and cross-section (xSEM) measurements for cross-validation. NOVA software was used to build a ML model. Fig. 1 shows the ML model training scheme. The primary external references (used for model validation) are data from atomic force microscopy for the recess structure and xSEM data made at two locations per wafer for the line trench, respectively. For line trenches, in addition, the top widths of the trenches were measured at the same locations with inline CD-SEM.

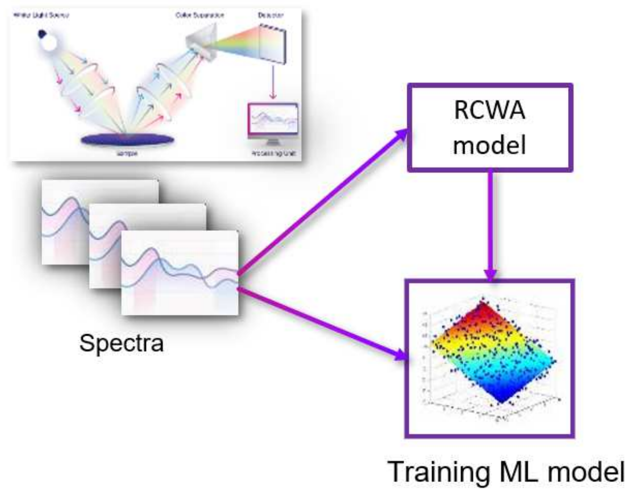

Fig. 1. ML model training scheme. Reflectance spectra are collected from several locations on each wafer in order to develop a RCWA model. The results are then further used to train the ML model.

The trained model is a mathematical estimator, which gives the parameters of interest (POI) from measured spectra (without reference data) as shown in Fig. 2.

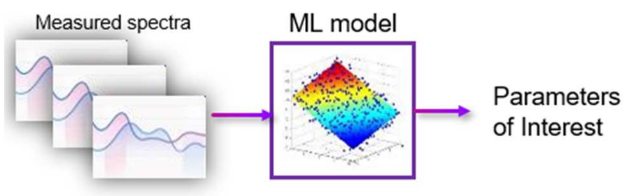

Fig. 2. Machine learning model is deployed to obtain multiple parameters of interst from measured spectra.

B. *Recess Depth of a Silicon MOSFET Trench from RCWA Method and Optimization done with Machine Learning Method*

As a first example, recesses in poly-silicon were etched for a silicon trench MOSFET in 300 mm silicon wafers. A schematic image of the structures is shown in Fig. 3. Three groups with different etch conditions were prepared. In this case, both recess depth as well as sidewall oxide (SWO) thickness were adapted, to generate the variation matrix. The first group represents process of record (POR) wafers. For the second group, recess depth was varied by +/- 8%, while maintaining a consistent SWO thickness. Lastly, in the third group, we kept the recess depth unchanged but modified the process to vary the SWO thickness. Each group comprised of two wafers.

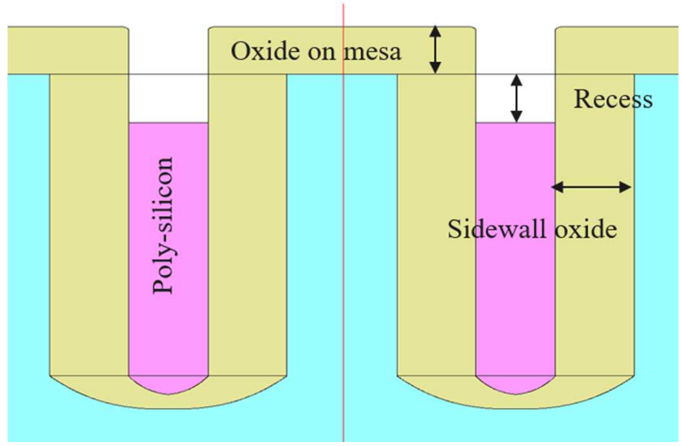

Fig. 3. Schematic image of the recess structure where the recess depth is the parameter of interest. The oxide on the sidewall is shown in yellow color and the poly-silicon in magenta.

At first, a RCWA method was developed and used to measure the recess depth. We have a substantial amount of experience with using the RCWA method for similar structures in the past [5]. However, the opening width to pitch ratio plays a significant role in determining the measurement sensitivity. If this ratio is below a certain threshold, then a robust measurement cannot be guaranteed. In this case, a suitable grating structure needs to be evaluated and used for a scatterometry solution. In this example, the relatively thick SWO in combination with a narrow recess opening width poses a challenge for this method. This challenge is evident in the recess depth measurement (13 sampling points per wafer) as shown in Fig.4.

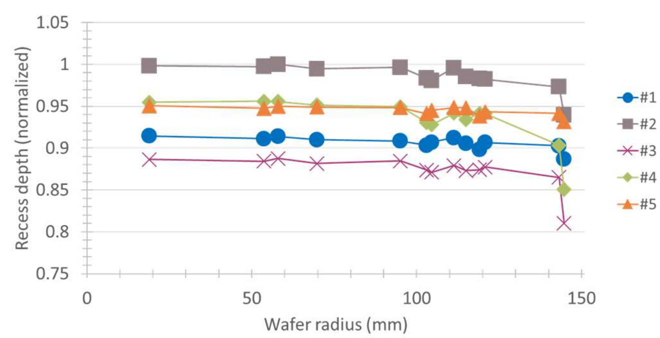

Fig. 4. Radial plot of the recess depth measured with RCWA based method. Wafer #1 is the POR, wafer #2 and wafer #3 represent one wafer each from the second group. Finally wafer #4 and wafer #5 represent one wafer each from the third group.

The radial plots for normalized recess depth in Fig. 4 display the data of one wafer from each group. Wafer #1 was processed under POR conditions. Wafer #2 and wafer #3 underwent a process variation to alter the recess depth by +/- 8%, respectively. However, one can notice the asymmetrical variation in recess depth for both wafers, wafer #3 being deeper than intended. Lastly, for wafer #4 and wafer #5, the process variation was implemented in such a way that only the SWO thickness was changed, while efforts were made to maintain the recess depth as close as possible to the POR target. As can be seen, the intended depth variation is noticeable which implies that the RCWA is capable of detecting the variation. We have ensured that the limits of the RCWA library are not violated. However, when the results are cross validated with SEM cross section data, particularly at wafer edges (e.g. last data points for wafers #2-#4 in Fig. 4), a mismatch between the RCWA measurement result and cross section data are observed. This correlation is shown in Fig. 5(a), where a large spread is observed with R^2 = 0.67. Subsequently, the ML approach was used to enhance the RCWA result. The measured spectra from all wafers were then re-evaluated using this ML model and an improved correlation has been demonstrated in Fig. 5(b) with R^2 = 0.98.

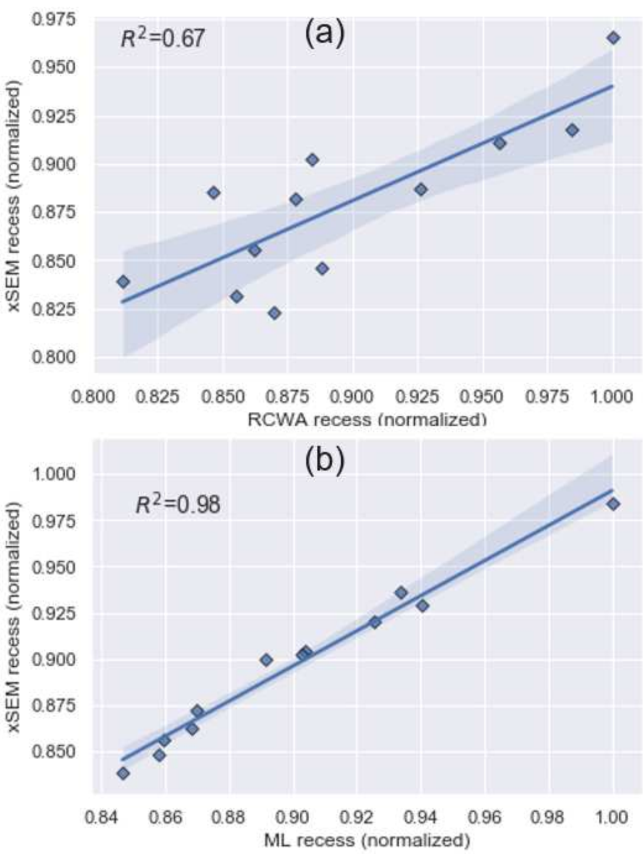

Fig. 5. Correlation plots between SEM cross section data and recess depths (normalized), (a) measured with RCWA and (b) after enhancing with ML approach.

To test this ML enhanced RCWA approach, a new set of wafers were prepared and measured. This new DOE set contained the same variations as in the previous DOE. That implies the new set of wafers again contains POR wafers, wafers with recess depth variation while maintaining fixed SWO thickness as well as wafers where the recess depths were not adjusted but the SWO thickness was varied. Fig. 6 shows wafer maps (105 sites) from a wafer belonging to the third group with shallower recess depth. In the RCWA case (Fig. 6 (a)), clear outliers are observed which are not observed when the RCWA is enhanced with ML (Fig. 6 (b)).

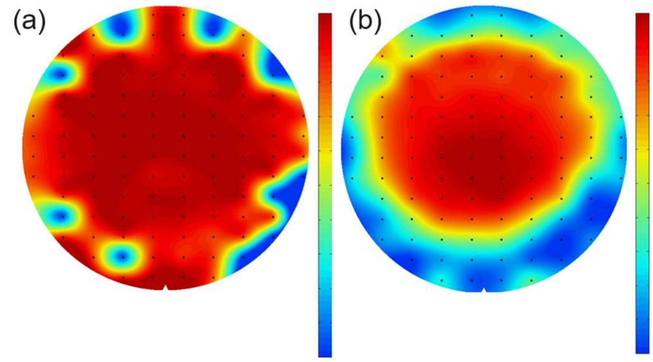

Fig. 6. Wafermaps of recess depth (a) using RCWA and (b) when enhanced with ML.

Finally, to carry out a cross validation, Atomic Force Microscopy (AFM) data were collected, but from fewer locations (13) on each wafer. We ensured that at those same positions, RCWA data were available. For this analysis, the recess depth and oxide thickness on the silicon mesa are added together, because only this combined depth can be obtained with AFM. Fig. 7 illustrates the correlation between the total depth measured using the RCWA method and the AFM results with R^2 = 0.72. Again, the recess depth values are normalized. The data points lying far away from the linear fit represent outliers in recess depth measurement from the RCWA method.

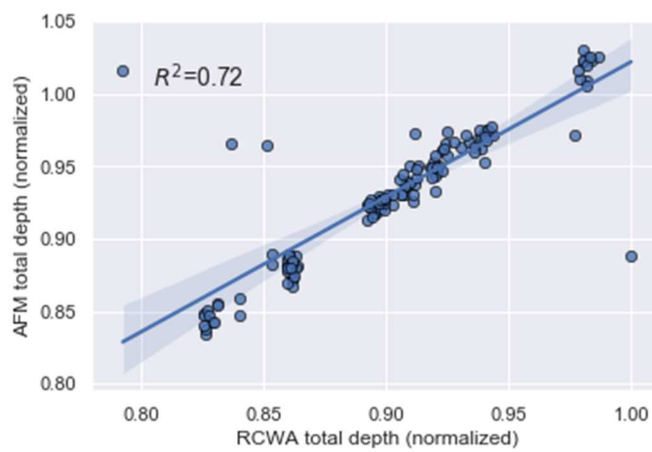

Fig. 7. Correlation plot between AFM data and total depth measured with RCWA only (normalized). Outliers result from insufficient sensitivity of the RCWA method in a few cases.

In contrast, the correlation between the ML enhanced RCWA data and AFM data have an improved coefficient of determination R^2 = 0.91 (Fig. 8), emphasizing the superior performance of the combined approach.

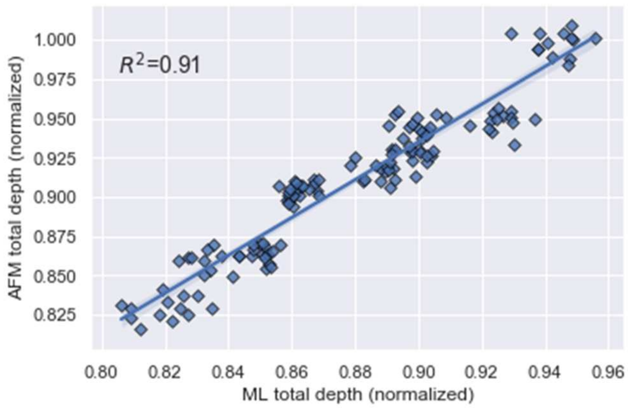

Fig. 8. Correlation plot between AFM data and total recess depth measured with ML enhanced RCWA approach (normalized).

C. *Top and Bottom CDs of 2D Line Trenches from RCWA Method and Optimization done with Machine Learning Method*

In the second example, five groups of silicon wafers were etched to have different sidewall angles for the line trenches, while keeping the depth on target. The first and second wafers had the largest deviation in trench side wall angle from POR of +/- 7%. The third and fifth wafers received an etch process variation of +/- 5% respectively. The fourth wafer in this DOE represents the standard process (POR). In this work, we focus on the top and bottom CDs, therefore, the trench depth data even though available, are not provided.

A RCWA model was developed using spectra collected from normal as well as oblique scatterometric channels. Full wafer scatterometry measurements (93 sampling points per wafer) were performed. In this model, the depth, top CD and bottom CD are varied sufficiently to cover the variation observed in cross sections. Radial plots of the top CD from all 5 wafers (wafer #1-5) are shown in Fig. 9 (a). However, outliers are observed which are positioned randomly for each wafer. Fig. 10 (a) shows the wafer map of top CD for wafer #5 with pronounced outliers at half radius and at the wafer edge. These are identified as artefacts from model interpretation rather than real outliers coming from the etch process.

In the next step, our ML approach has been implemented to develop an enhanced scatterometry model and the collected spectra are analyzed with this model. The ML model was trained using reference RCWA model data for trench depth, top CD, and bottom CD. In total 65 reference data points (13 sampling points per wafer) for each parameter were used to train a ML model. The trained ML model gives the top CD, bottom CD, and trench depth from measured spectra.

The top CD results are discussed first. Fig. 9 (b) shows a much smoother radial profile in comparison to the same data obtained with only RCWA model (Fig. 9 (a)). The improved radial profile is also observed in the wafer map (Fig. 10 (b)). Top CD values of line trenches decrease from wafer center, reach a plateau at 20-50 mm wafer radius, and increase towards wafer edge.

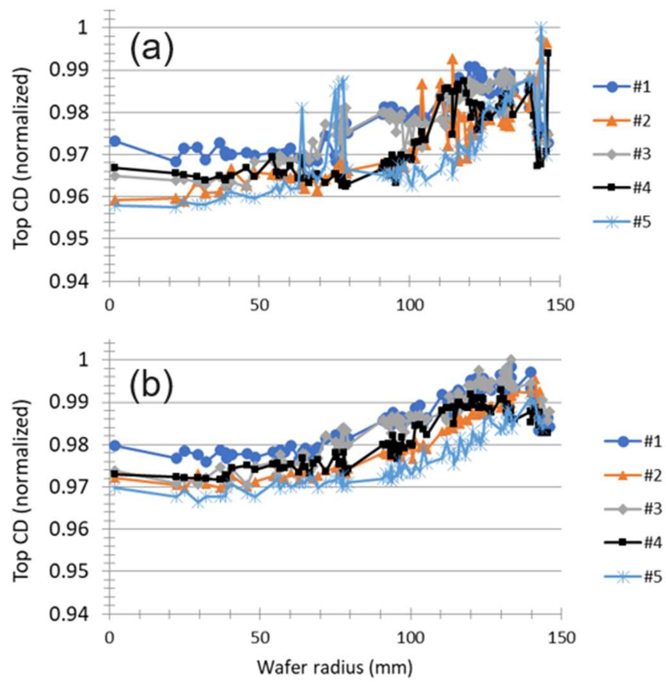

Fig. 9. Radial plot of normalized top CD for 2D line trenches obtained with RCWA (a) and ML (b) method for 5 wafers. There are outliers observed for top CD obtained with the RCWA method.

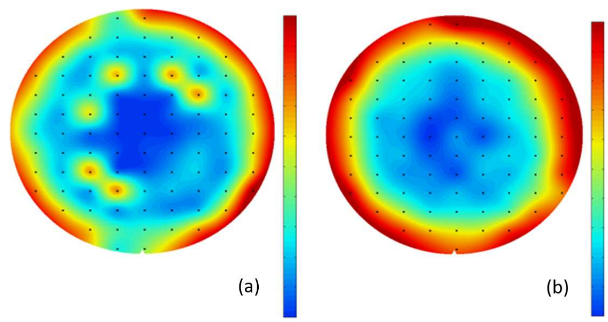

Fig. 10. Wafer maps of top CD for 2D line trenches obtained with RCWA (a) and ML (b) method for wafer #5. Outliers are observed for top CD which were obtained exclusively with the RCWA method (a). The ML enhanced RCWA method is able to remove these outliers (b).

A similar experiment has also been carried out for bottom CD. Measuring the bottom CD for such trenches is very challenging and building a suitable RCWA model requires large computational power. Despite that, a RCWA model was developed and the radial plot for normalized bottom CDs is shown in Fig. 11 (a). In the radial plot for the bottom CDs, the intended variation is somewhat observed. The bottom CD of wafer #4 which was etched with POR condition lies at the center, is shown with black squares. Bottom CDs of wafer #1 and 2 which received the largest process variation of +/- 8 %, are visible at the top and bottom of the graph, respectively. Finally, data from wafer #3 and wafer #5, which received a process variation of +/- 5% are observed just above and below wafer #4. However, outliers in the bottom CD are also observed, particularly around half-radius for wafer #5 and at the wafer edges for all wafers. These outliers are attributed to the artefacts from model interpretation.

Again, by using the ML enhanced scatterometry method, the results show improvement in uniformity and stability (Fig. 11 (b)). In the radial plot for the bottom CDs, the variation is nicely observed, the same color scheme as in Fig. 11 (a) is used. Radial plots of bottom CDs for wafer #3 and wafer #5 with +/- 5% process variation are closer to that for POR wafer #4. The radial plots for bottom CDs for wafer #1 and wafer #2 with +/-8 % process variation are at the top and bottom of the graph respectively. The bottom CD increase from wafer center up to 120 mm wafer radius and decreases slightly again towards the wafer edge. The drop in the bottom CD at the wafer edge has been confirmed with xSEM images. This is significantly smaller in comparison to the data obtained with RCWA method. Finally, 10 repetitions of the measurements were carried out and the standard deviation was calculated. The standard deviation calculated with our ML enhanced method was half of the standard deviation calculated with the RCWA method. This improved repeatability can enhance tool-to-tool matching as long as there is no significant offset between them. An offset is usually tool hardware dependent and does not originate from the used model for interpretation.

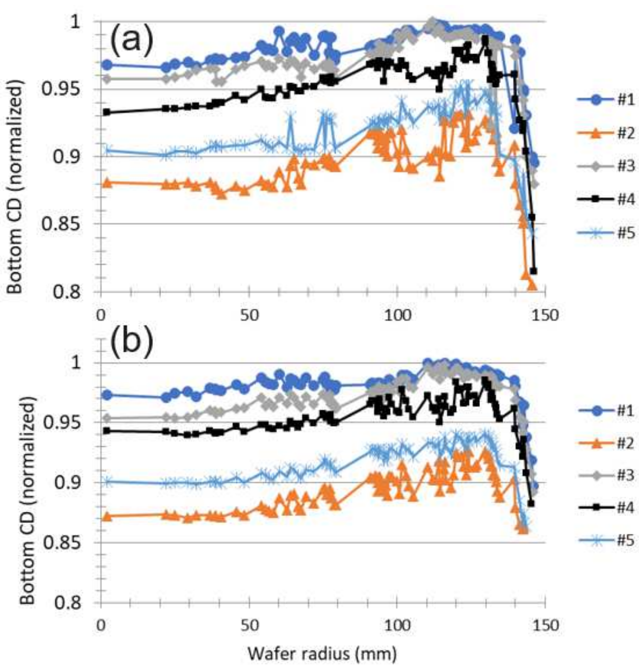

Fig. 11. Radial plot of normalized bottom CD for 2D line trenches obtained with RCWA (a) and ML method (b) for 5 wafers. Wafer #4 was etched with the POR process. Wafers #1 and wafer #2 were etched to have the largest and smallest bottom CDs (+/- 8%). Wafers #3 and #5 were etched to have slightly larger and smaller bottom CD than the POR wafer #4.

Next, cross section SEM measurements (2 points per wafer, center and edge) were performed at the same wafer locations as optical measurements in order to test the ML model. The bottom CD values obtained with the ML enhanced RCWA method agree well with the xSEM data (not used in the training set), with a correlation $R^2 = 0.89$ (Fig. 12). In our previous publication [2], we presented bottom CD measurement of deep trenches (depth > 40 µm), which was calculated using exclusively a ML model. In this case, it was not possible to develop a solution with RCWA. The ML model was developed using measured spectra and external reference data which were primarily xSEM data.

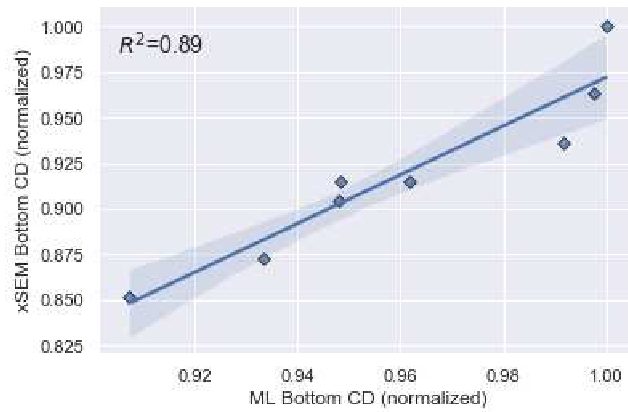

Fig. 12. Normalized bottom CD obtained from xSEM is plotted versus scatterometry results using the ML method. The xSEM data were not used in the training set.

In order to test the ML model for top CD, trench top CD were measured using a CD-SEM metrology tool (13 sampling points per wafer). CD-SEM measurements were performed at the same wafer locations as scatterometry measurements.

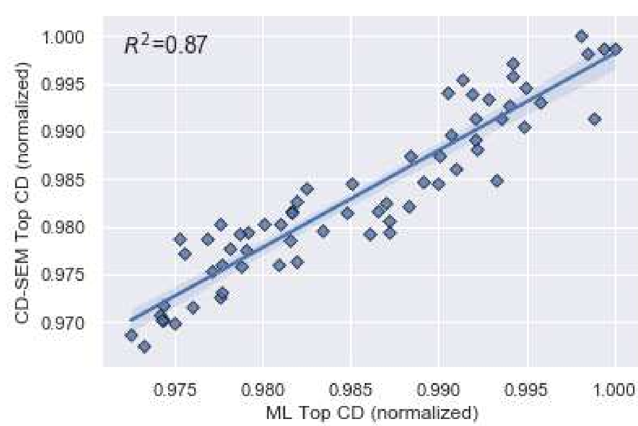

Fig. 13. Normalized top CD of trenches from the 5 wafers obtained from CD-SEM is plotted versus scatterometry results using the ML method. The CD-SEM data were not used in the training set.

Normalized top CD values obtained with the scatterometry enhanced ML model agree well with the CD-SEM data (not used in the training set), with a correlation $R^2 = 0.87$. The correlation plot for top CD obtained from the ML model and

CD-SEM reference data, which was not part of the training set, is shown in Fig. 13 for the 5 DOE wafers.

II. Summary and Conclusions

By using two vastly different examples, a recess in trench MOSFET and a 2D line trench, we have demonstrated the advantage of using an additional machine learning approach over only the conventional RCWA method. The ML enhanced RCWA method shows improved radial profiles for the recess depth of the trench MOSFET structure. The results have been independently cross validated with AFM measurements. A similar improvement was also observed for the top and bottom CD values of line trenches when traditional RCWA was augmented by the application of ML. These examples highlight how combining traditional methods with emerging technologies can lead to more reliable, and comprehensive results. The two structures could also be tackled using pure ML approach. However, this requires a significant number of external references such as xSEM images for developing a robust ML model. By using the ML enhanced RCWA method, the number of external references can be reduced.

In production environment, throughput is an important parameter. Therefore, it is imperative to address this when a combination method, as presented in this paper, is being used. For the two examples shown in this work, the measurement condition is not changed while using the ML enhanced RCWA approach and hence, the throughput is unaffected.

From our observations, the physical model remains a suitable tool for predicting the geometrical values. However, when complexity is increased, either the physical model becomes too complex or the sensitivity is compromised, leading to instability in simulation results. In a production environment, new complexities are frequently introduced and it is impossible to meet all the requirements for a suitable RCWA method (new structures, library calculation time etc.) at a fast pace. In these situations, ML can provide a valuable solution. It is equipped to enhance RCWA, improving the stability of measurement results in a shorter amount of time. Therefore, while traditional methods like the RCWA remain relevant, the integration of ML provides a promising and effective way to handle increasing complexity and maintain high productivity.

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