Scatterometry-informed machine learning study to determine bi-directional intercorrelation of adjacent patterning steps

Pádraig Timoney*[a], Stefan Schoeche[a], Daniel Schmidt[a], Will Parkin[a],
Aron Cepler[b], Ilya Osherov[c], Amit Godel[c], Igor Turovets[c]
[a]IBM Research, 257 Fuller Rd, Albany NY 12203
[b]Nova Measuring Instruments, 3342 Gateway Blvd, Fremont, CA 94538, USA
[c]Nova Ltd, 5 David Fikes St., Rehovot, 7632805, Israel

ABSTRACT

The use of machine learning has been well documented in recent years in a wide variety of optical scatterometry applications. Machine learning can either be used in a 'modeless' manner to directly correlate measured spectra to reference metrology without an optical model or serve as a complementary technique together with conventional scatterometry modeling to improve the sensitivity of specific parameters.

This work presents both modeless and AI augmented scatterometry modeling applications in the gate-all-around nanosheet process flow. AI augmented scatterometry models were generated for measurements at adjacent patterning steps and were validated by conventional TEM correlation. A concept is introduced to utilize modeless machine learning solutions as a complementary technique with AI segmented scatterometry models at consecutive process steps. The forward and backward prediction of selected measurement steps is studied to identify possible inconsistencies between the outputs of the associated scatterometry models.

An intercorrelation matrix is assembled to tabulate average correlation of 6 modeless machine learning models to the corresponding previous / future step scatterometry model output. This bidirectional machine learning assessment proves to be a simple methodology to reveal the intercorrelation between past and future process steps and helps to identify both model and process stabilities.

Keywords: Machine Learning, scatterometry, modeless, AI augmented scatterometry, reference metrology, bidirectional intercorrelation, replacement metal gate

*Corresponding author: padraig.timoney@ibm.com

1. INTRODUCTION

The technology requirement for advanced logic CMOS transistors continues to drive reduced transistor size and advances in device architecture. The transition from planar to FinFET, and now to nanosheet transistor architecture, results in increased complexity of optical scatterometry measurements [1]. The complexity arises from an increasing number of geometric degrees of freedom, along with reduced optical sensitivity to a variety of critical structural dimensions. Frequently, the key measurement parameters in nanosheet scatterometry models are located beneath the surface and therefore significant portions of the incident light may be absorbed by the structure above the degree of freedom of interest. For example, monitoring of the inner spacer formation processes requires analysis of the dimensions and dielectric material volume beneath the dummy gate structure as shown in Figure 1 (a) [2]. The lateral indents in the silicon germanium sheet stack and subsequent filling of these indented shapes with inner spacer dielectric material present a challenge to optical scatterometry due to the small volume changes and the depth below the surface at which these small changes occur.

The Replacement Metal Gate (RMG) module features a number of optical scatterometry applications, including process steps such as dummy gate removal, channel release, high k / interfacial layer (HK/IL) depositions, and work function metal (WFM) deposition. Referring again to Figure 1 (b) and (c), after the dummy gate material is extracted and the sacrificial silicon germanium in between the inner spacers is removed at the channel release step (b), monitoring of the empty gate profile together with the remaining silicon nanosheet thickness and remaining spacer thickness parameters is challenging to accurately characterize in an optical scatterometry model.

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Monitoring of the dummy gate structure throughout the consecutive replacement metal gate processes is explored further in this paper by leveraging both AI augmented scatterometry modeling and modeless machine learning solutions.

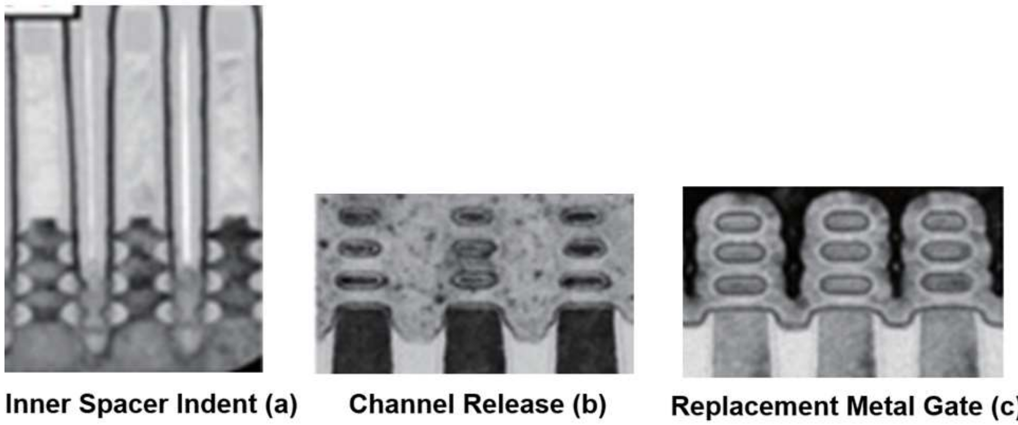

Figure 1: Sample cross section transmission electron microscopy (TEM) images illustrating the metrology challenges in nanosheet process flow for inner spacer indent (a), channel release (b) and replacement metal gate (c) [2].

2. MODELESS MACHINE LEARNING AND AI AUGMENTED SCATTEROMETRY

Increased adoption of machine learning methods, both as a replacement to conventional rigorous coupled wave analysis (RCWA), and as an aid to RCWA, can help improve application performance.

In AI augmented scatterometry, a conventional geometric model is enhanced by machine learning algorithms leveraging a variety of user inputs. This be beneficial in a scenario where the available reference metrology is limited. Such solutions also constrain inter-relationships between geometric parameters as with conventional scatterometry modeling, providing a comprehensive representation of the full structure whilst leveraging the user inputs to boost sensitivity to the parameters of interest.

Modeless machine learning may also be utilized in a scenario where variation in the scatterometry spectra can be related to a suitable quantity of accurate reference metrology. Such modeless solutions can be developed quickly once sufficient reference metrology has been collected. However, it is not typically utilized in a scenario where a variety of measurements are required with interrelated physical quantities or where suitable reference metrology is not available for the key measurement parameters.

In prior work, sheet-specific measurement of the lateral silicon-germanium indentation depth was demonstrated by modeless machine learning as well as AI augmented scatterometry [3,4]. The primary goal of this measurement is to obtain the lateral indentation of the three SiGe nanosheets with respect to the silicon nanosheets. The amount of silicon germanium removed is critical for optimal device performance, however it is challenging to quantify with conventional RCWA analysis due to the very small volume change in Ge and the significant absorption of the incident light that occurs above the indented SiGe from the dummy gate structure. This measurement sensitivity challenge can be mitigated by augmenting the scatterometry model with artificial intelligence, using reference data from transmission electron microscopy (TEM). Figure 2 illustrates the parameterization used for the AI augmented scatterometry model and the resulting correlation to TEM that was obtained.

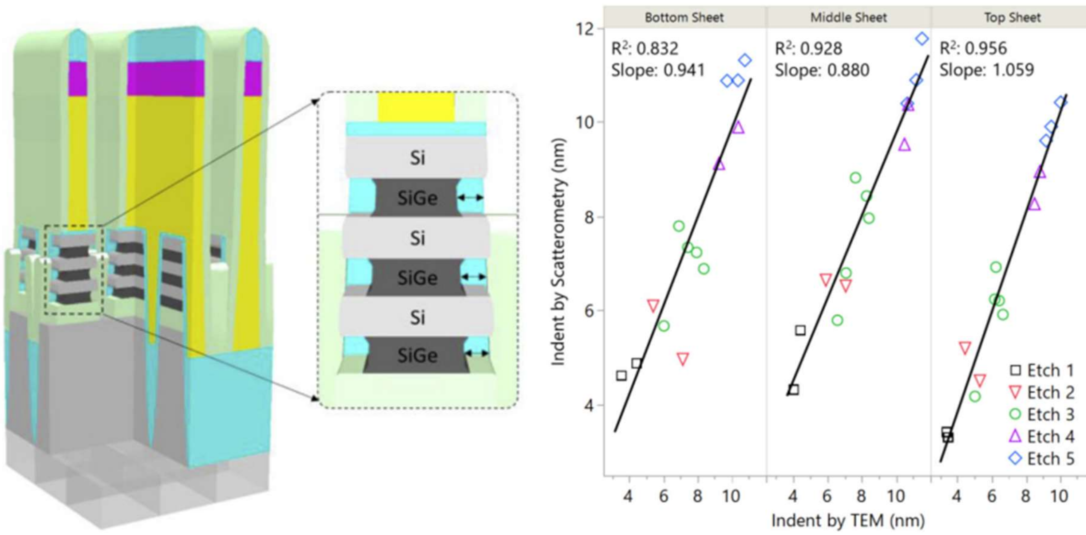

Figure 2: Demonstration of AI augmented scatterometry model to measure SiGe sheet specific indent depth. Adapted from [3].

Monitoring of the average silicon germanium indent depth has also been reported using a modeless machine learning approach [5]. The modeless solution was trained using the difference in measured XRF Ge Lα counts between pre and post lateral indentation etch. In the data presented, the R^2 improved by utilizing the modeless machine learning solution as compared to a conventional RCWA solution.

3. AI AUGMENTED SCATTEROMETRY MODEL SETUP AND VALIDATION

In this work, AI augmented scatterometry models are developed in adjacent Replacement Metal Gate (RMG) patterning steps. In many RMG scatterometry measurements there are similar challenges to those previously reported for inner spacer indent depth – namely, limited spectral sensitivity of key parameters and correlations between height and CD parameters. Improved scatterometry model performance can be obtained with AI augmented scatterometry models, which help to minimize cross-parameter correlations and boost sensitivity to key parameters of interest. These models describe the physical variations of the full structure and are useful when limited reference metrology samples are available. However, it can be difficult to assess the long-term model reliability with such limited samples. Figure 3 shows the correlation to TEM that was obtained from one of the AI augmented scatterometry models developed in this work for Height (Ht) and critical dimension (CD) parameters, as part of a well-established practice to validate the solution in the typical scatterometry model development work.

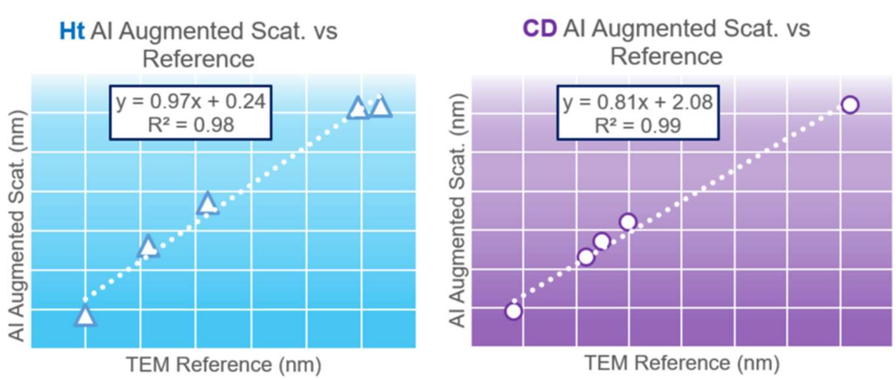

Figure 3: Correlation of AI augmented scatterometry model parameters height (Ht) and CD to TEM reference metrology.

In the next section, the concept of a scatterometry informed forward-backward intercorrelation matrix will be introduced leveraging modeless machine learning solutions to study the performance of inline conventional scatterometry and AI augmented scatterometry models at adjacent patterning steps.

4. SCATTEROMETRY INFORMED INTERCORRELATION MATRIX

Modeless machine learning methodology allows the prediction of output data from raw spectra, assuming that the spectra from that process step can be associated with the input reference data. For example, in the RMG sector applications studied in this work, the primary changes in consecutive patterning steps concern the extraction of sacrificial dummy gate and silicon germanium nanosheet material followed by deposition and patterning of HK, IL, and work function materials. Therefore, the assumption is made that output data from scatterometry measurements at such adjacent process steps can be leveraged as suitable reference metrology with which to train modeless machine learning solutions at the steps before or after the step at which the reference metrology was derived.

Figure 4 introduces this concept, where spectra acquired at the process step 1 measurement are trained to predict downstream metrology from the process step 2 measurement. Data from approximately 50 wafers were utilized to train the modeless prediction. The predicted CD achieves a correlation of R^2=0.78 to the actual downstream CD for 150 wafers not included in the training of the model.

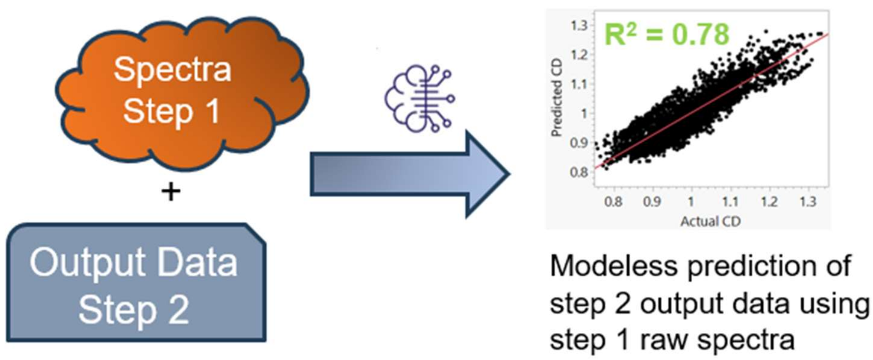

Figure 4: Prediction of downstream metrology data at process step 2 by a modeless machine learning measurement at process step 1. Blind test data from 150 wafers validates the feasibility of this approach.

In this study, measurement data is generated from 3 process steps, the first 2 of which utilize AI augmented scatterometry models while the 3rd step utilizes a conventional scatterometry model to output the data. Since each measurement step can have a predicted value generated at the 2 other process steps, there are 6 modeless machine learning prediction vs actual plots to consider. The same training wafers and blind test wafers were used to minimize the contribution of the real wafer process variation on the results.

In Figure 5, the prediction vs actual CD plots are arranged in a matrix format. The diagonal line may be also thought of as the movement of the wafer from top left to bottom right of the chart. This also helps to visualize the concept of downstream prediction vs upstream prediction. For example, in the case of the top right cell of the matrix, spectra acquired at the measurement after process step 1 are generating a modeless prediction of the measured CD after process step 3, whilst at the bottom left cell, spectra acquired after process step 3 are generating a modeless prediction of the measured CD after process step 1. It is noteworthy that most of the R^2 values are largely symmetrical on both sides of the diagonal line. However, one unexpected result is that the step 2 prediction of the CD at process step 3 has a better R^2 (0.9) than the step 3 prediction of the CD at process step 2 (0.73).

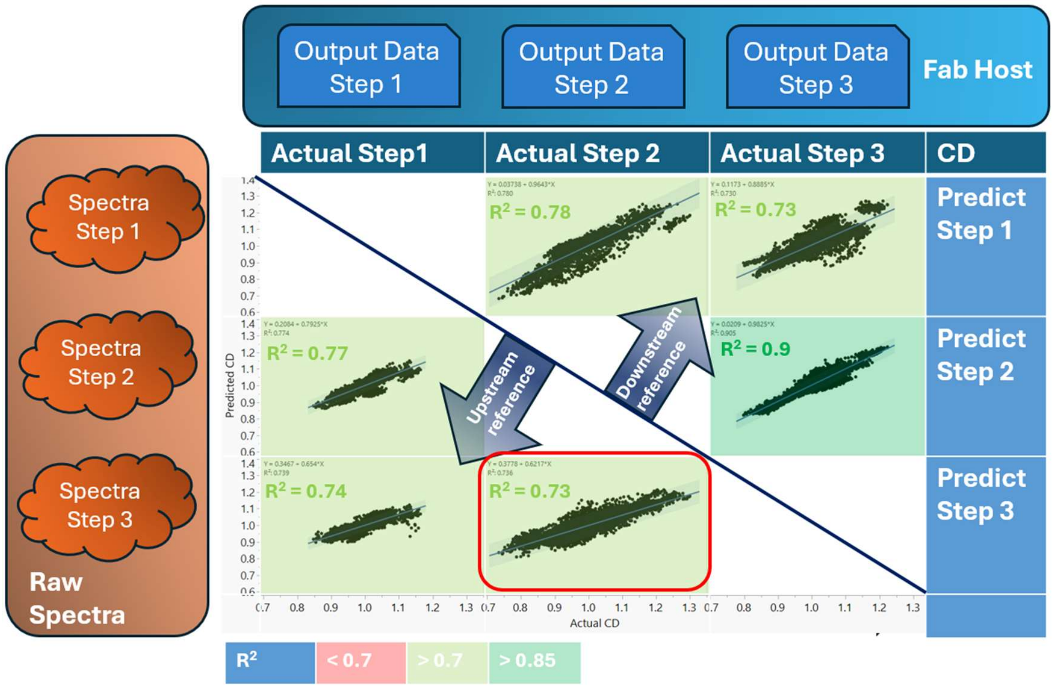

Figure 5: Scatterometry informed intercorrelation matrix representing the upstream and downstream prediction of the CD parameter to the output CD values form each of the scatterometry models.

Figure 6 depicts the improvement of the step 2 model; the actual step 2 reference data was regenerated to train the modeless prediction at step 1 and step 3. The results demonstrate that after step 2 model optimization, the step 3 prediction of step 2 CD R^2 value (0.93) is now similar with the step 2 prediction of step 3 CD R^2 value (0.9). Figure 7 shows the updated intercorrelation matrix for the predicted CD vs actual CD R^2 values after step 2 model optimization. Together with the improvement in step 3 predicted step 2 R^2 illustrated in Figure 6, it can also be seen that the step 1 predicted step 2 CD improves, albeit very slightly.

It has been assumed thus far that the parameter represented in the scatterometry informed intercorrelation matrix does not change very significantly through the consecutive process steps 1 to 3 and that the variation of the parameter of interest is mostly a property of the incoming process variation. In such an example, the intercorrelation matrix is useful in detecting a scenario where there may be an opportunity for additional model optimization as demonstrated in Figure 6.

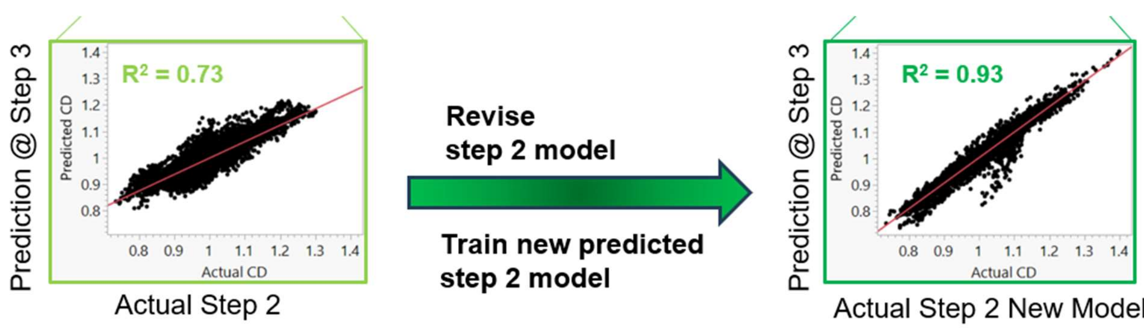

Figure 6: Improvement in step 3 predicted step 2 CD achieved by optimization of the AI augmented scatterometry model at process step 2.

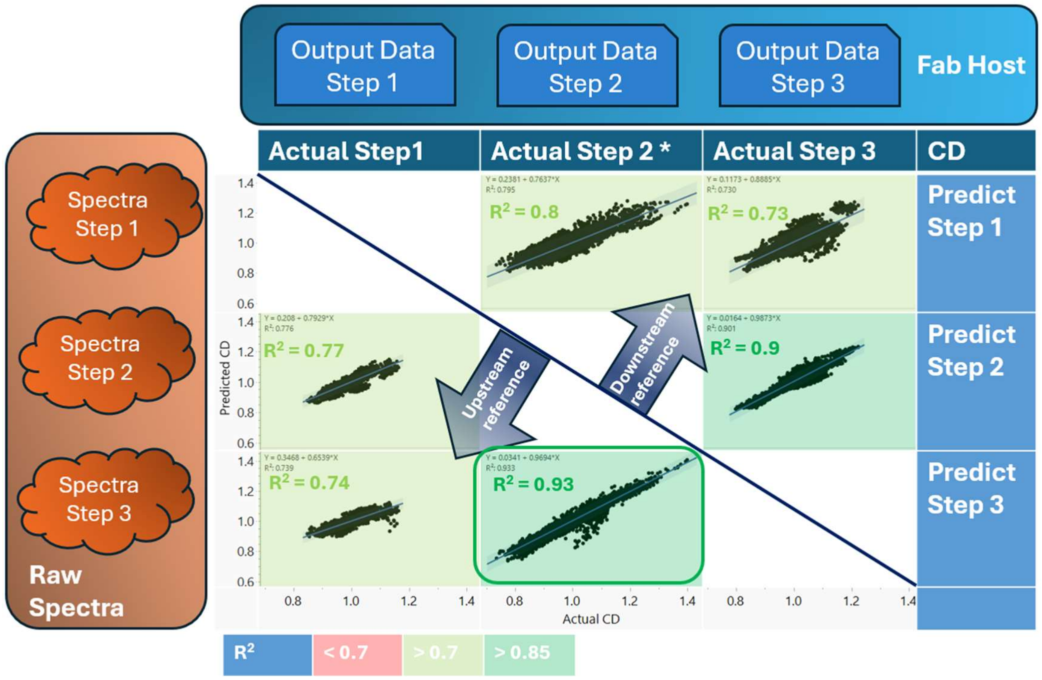

Figure 7: Updated scatterometry informed intercorrelation matrix after optimization of step 2 model representing the upstream and downstream prediction of the CD parameter to the output CD values form each of the scatterometry models.

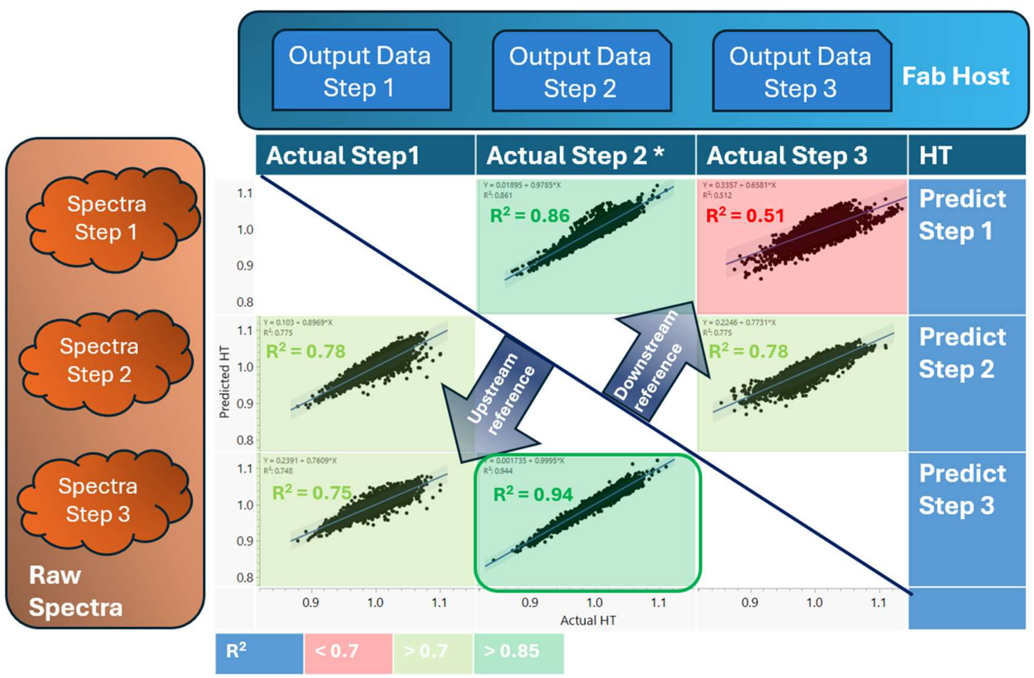

Figure 8: Scatterometry informed intercorrelation matrix after optimization of step 2 model representing the upstream and downstream prediction of the Ht parameter to the output Ht values from each of the scatterometry models.

In Figure 8, the intercorrelation matrix of the Ht parameter is shown. Although the results demonstrate high R^2 values for step 1 predicted step 2 Ht ($R^2 = 0.88$), downstream prediction of step 3 appears to be less successful. This result appears to suggest that the step 3 Ht data is not a reliable source of reference metrology which to train a modeless machine learning solution at process step 1. This indicates that the height is physically changing between step 1 and step 3 in a manner that is no longer possible to predict using the initial training set that was used for the machine learning solution. Such observations could prove valuable in identifying sources of variability in the process flow.

5. CONCLUSIONS

AI augmented scatterometry models are developed to help address concerns about models with limited sensitivity to key parameters in the nanosheet RMG sector. These models are validated by correlation to reference metrology, albeit with limited availability of reference metrology. A scatterometry-informed intercorrelation matrix concept is proposed as a methodology to monitor the performance of scatterometry models utilizing modeless machine learning. The results presented in this work demonstrate successful prediction of downstream scatterometry data with high confidence, as demonstrated with R^2 values > 0.85.

The scatterometry informed intercorrelation matrix was successfully used to identify potential candidates for model improvement and was also utilized to quantify the improvement achieved by regenerating the reference metrology for the modeless solutions with the improved scatterometry model. The results demonstrated an improvement in step 3 predicted step 2 from $R^2 = 0.73$ to $R^2 = 0.93$.

The study presented in this work demonstrates the feasibility of modeless machine learning to identify process and metrology model variation across adjacent process steps. It is worth noting that this study considered only the output from other scatterometry models as reference metrology with which to train the modeless solutions, there is a wide variety of alternative reference metrology sources to be considered in future studies provided that the reference metrology can be associated with the corresponding measurement spectra that is used to train the model. Studies of forward and backward intercorrelation may also be considered for future process improvement work.

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