Improved Scatterometry Time to Solution for Leading-Edge Logic Applications

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Abstract - **This paper describes an innovative approach to scatterometry modeling, significantly reducing time to solution compared to the industry's current best practices. One of the drawbacks to traditional scatterometry measurement techniques is the time required to optimize the model, which includes material optical constant extraction, model build time, initial model optimization, and model testing. A novel methodology that includes both stability and self-consistent scatterometry accuracy prediction can achieve an order of magnitude gain in productivity over prior methods. This technique creates opportunities among semiconductor chip manufacturers for wider scatterometry adoption at advanced technology nodes, where scatterometry is often the only reliable non-destructive metrology for device structure dimensions. The reductions in cycle time and improvements in accuracy prediction are keys to the success of scatterometry as an enabler for advanced process control and monitoring.**

This paper presents results on a conventional poly gate litho and final inspection and on leading-edge high-k metal gate after-etch applications. Spectroscopic ellipsometry is used to collect spectra from the gratings on the wafers. Then scatterometry results are obtained using the new approach and via traditional industry-accepted procedures to compare time to solution. To confirm the validity of the results, reference metrology data are collected on a CDSEM and TEM and the total measurement uncertainty is evaluated.

I. INTRODUCTION

In order to maintain Moore's Law, device dimensions are shrinking and new materials and device architectures are being introduced. Not only are entirely new types of metrology needed to meet the challenges associated with these new devices, but existing metrologies must improve to keep pace. Now considered an established metrology, scatterometry is one such metrology that has consistently improved since its introduction. An inherent challenge of scatterometry is that it is model based and requires a user to make a series of decisions on how to construct the model. The decisions include the choice of geometric model used to describe the device, the type of model to describe the dispersion of the materials, the parameters to fix and float in both the geometric and dispersion models, and the parameter ranges needed to cover the expected process range. Since the scatterometry signal is dependent on the entire structure, the user must include two types of parameters: critical parameters (also referred to as critical metrics) and required parameters. Critical parameters are defined as those parameters that need to be measured to control the device performance (e.g. the critical dimension (CD) of the poly-silicon gate, which directly impacts device speed) [1]. Required parameters are those parameters that when changed, due to process variation, significantly impact the spectra and thus the accuracy of the measurement. Ideally, the user would be able to float all of the parameters in the model. This was possible for some simpler devices used in previous nodes; however, as device complexity increases [2,3,4], the number of layers and number of gratings (as in double patterning lithography (DPL)) increases. This increased complexity forces the user to make compromises during model optimization. Such compromises are often subjective and require a high level of expertise which results in variation between users.

Current methodologies rely on the user to optimize the model using various metrics like parameter precision and model fit quality (e.g. ChiSq, GOF, etc). The user typically takes measurements on representative wafers to use during model development and to check across wafer trends, design-of-experiment (DOE) tracking and stability. To develop the model, the user starts off with generating an initial model that contains the critical parameters to be measured. The initial model is used to process the data and evaluate fit quality, DOE tracking and stability. After each model change, the user evaluates the model performance vs. the expected DOE trends and target stability. The user also evaluates the correlation between parameters in the model and typically fixes some of the highly correlated parameters to improve model stability. This iterative process is repeated until the model quality is deemed acceptable by the user based on the stability for critical metrics, the ability to track the DOE and the model fit quality. This process is time consuming due to the multiple iterations, subjective due to the user interpretation of the data and it does not provide any quantitative feedback to the user on the accuracy of the model. With increased complexity of structures and shrinking dimensions, industry is demanding more advanced configurations for scatterometry implementation like multi-azimuthal angle [5], DUV [2], etc. Even though these advancements in scatterometry technology are proving useful in meeting the measurement requirements,

they further worsen the subjective element of modeling optimization and increase the modeling optimization time (more modeling options means more iterations needed).

This paper describes a new method that is automated and uses both stability and accuracy to optimize the model performance. We will refer to it as Model Optimizer (MO) throughout the paper. The results of the automated method are compared to results obtained by expert users (EU) using the baseline open loop methodology.

II. STRUCTURES AND METHODS

A. Structures

Three applications were used to validate the robustness of the proposed automated Model Optimizer. The first one was a conventional gate stack measured at the after develop inspection (ADI) step. The schematic for this application is presented on Fig. 1(a). The parameter of interest for this application was the CD of the resist line, and CD-SEM measurements were available as reference metrology for calculating total measurement uncertainty (TMU) [6]. Spectroscopic ellipsometry (SE) was used for optical CD (OCD) measurement. A maximum of 11 geometric parameters or degrees of freedom (DOF) could be floated in the scatterometry model.

The second use case shown on Fig. 1(b) was the same gate stack measured at the final inspection (FI) step after etch. Poly gate CD was the critical parameter for this application. It was also measured with CD-SEM and spectroscopic ellipsometer to allow for a TMU study; dynamic repeatability OCD data were also available. Total number of potentially floatable geometric parameters in the scatterometry model was 9.

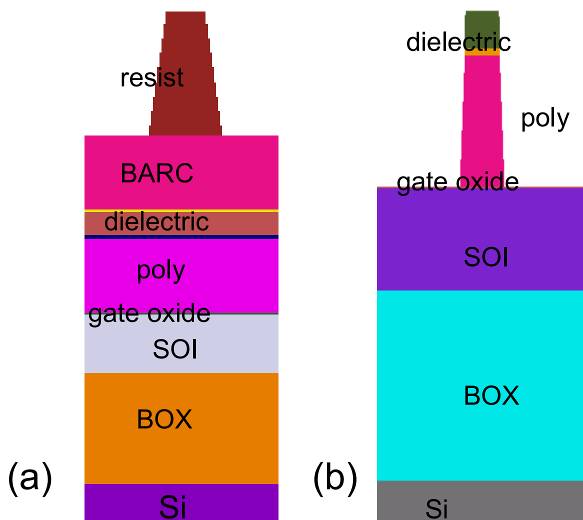


Fig. 1 Gate ADI and Gate FI applications used for characterization of the Model Optimizer - automated scatterometry model optimization method. The layers below the grating lines are not patterned.

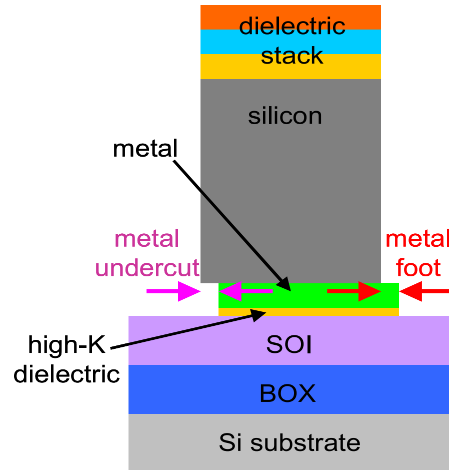


Fig. 2 The High-K Metal Gate (HKMG) post-etch structure. One of the critical parameters is the metal foot/undercut. Note that the unphysical scenario of a foot on one side of the gate and an undercut on the other is for demonstration purposes only. The SOI, BOX, and Si substrate layers are not patterned.

These two applications were run in production with integrated scatterometry metrology, allowing advanced process control and resulting in tighter CD uniformity cross-validated by electrical device performance [7,8]. They are well studied and provide excellent vehicles for careful characterization of the Model Optimizer methodology.

The third application was from a leading edge technology node high-k metal gate (HKMG) grating of nested lines, measured after the etching and cleaning processes. It was used to prove the extendibility of the automated scatterometry model optimization technique to more challenging applications [5]. The schematic is shown in Fig. 2, and one of the critical parameters was the metal gate undercut or foot. Transmission electron microscopy (TEM) provided reference metrology for the TMU characterization. Before wafer destruction for TEM, the same TEM measurement sites were studied with spectroscopic ellipsometry. Dynamic repeatability SE data were collected as well. The total number of geometric degrees of freedom that could be floated in the OCD model was 16, while two material dispersion parameters were also initially floated.

B. Methods

Scatterometry spectra were collected using spectroscopic ellipsometry and processed using rigorous coupled wave analysis (RCWA) for forward spectra simulation based on the modeled geometry of the structure and optical characteristics of the materials involved.

The focus of this paper is the automated method of optimization of the scatterometry model performed using a Model Optimizer feature in the OCD software. This method includes the following key components: i) model stability ii) quantification of model accuracy iii) algorithms for auto model optimization.

Model Optimization is a two step process where each step can be run separately or both can be combined into a one click model optimization routine. The initial optimization is performed based on the scatterometry model stability. Initial optimization is very quick even for very complex scatterometry models and results in a significantly reduced dimensionality of the problem and a good starting point for further optimization.

We refer to the next step of the model optimization as Enhanced Optimization with the goal of achieving the best possible measurement accuracy for the critical parameters. The Enhanced Optimization calculates Total Estimated Error (TEE) for each parameter, without the need for reference metrology as an input. We will show that TEE can be a good predictor of the total measurement uncertainty (TMU).

An automated feedback loop is used to minimize the Total Estimated Error of the critical application parameters, resulting in a self-consistent and accurate optimization method for the given scatterometry model. In order to evaluate the measurement performance and model optimization time, we generated models based on expert user and Model Optimizer, for each of the identified applications. In addition to these two models, several other iterations of the models were also generated to gauge the tracking of TEE predicted error and accuracy (TMU). Process variation ranges for all parameters was estimated and used as input to various scatterometry models.

III. RESULTS AND ANALYSIS

In this section of the paper we present results of the automated model optimization for the three structures described above and compare them to those obtained by the expert scatterometry user utilizing common industry practices for model optimization.

For the Gate ADI structure, the model created by an expert user after approximately one week of work had 7 floating parameters fixing thickness for all thin oxide layers and the silicon-on-insulator (SOI) layer thickness. The Model Optimizer scatterometry model optimized in less than one hour had 8 degrees of freedom including the 7 floating parameters from the expert user model and additionally letting the SOI thickness change. Model Optimizer also adjusted nominal values for two of the fixed oxide layers. Fig. 3 shows comparison of the TMU plots for the two scatterometry models described. Accuracy performance (TMU) is very similar for both models - Model Optimizer and expert user, even though there is a significant improvement (~ 97.5%) observed in the model optimization time when using the Model Optimizer approach. Several variations of the scatterometry model for Gate ADI were considered in order to validate the error prediction capability of Model Optimizer and compare this technique with the conventionally used spectral fit metric of model quality (ChiSq). They varied in the number and identity of the fixed parameters and represented a reasonable but not an exhaustive set of model variations that would be used by the expert user in the process of model optimization. As one can observe on Fig. 4, predicted TEE tracks fairly well with TMU obtained from the same model, with Model Optimizer 8 DOF model getting the lowest TEE and the lowest TMU. It is logically unclear in this case how to choose a model based on ChiSq as one can see that models with good and poor TMU achieve similar spectral fit quality.

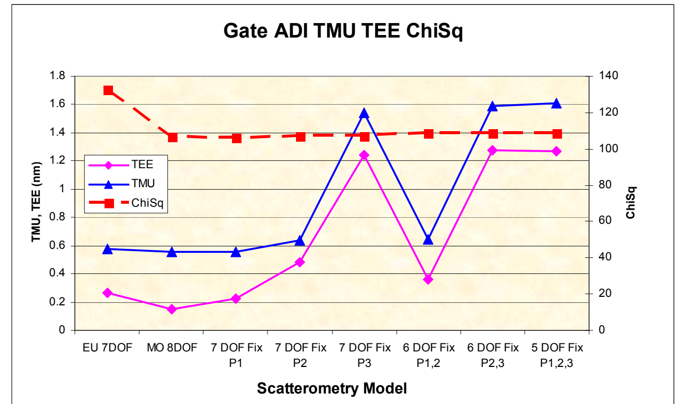
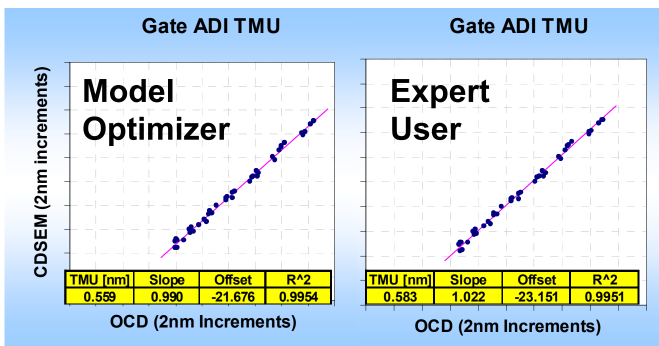


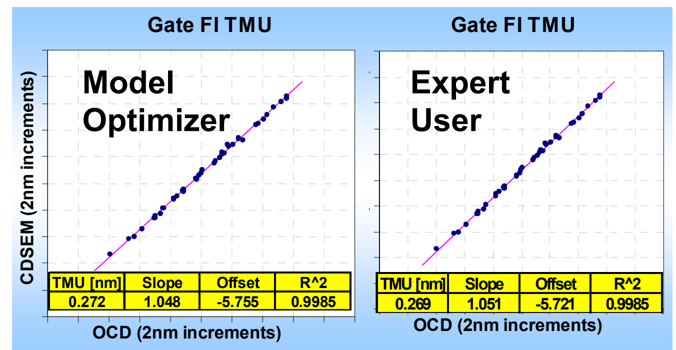
Fig. 4 Comparison of TMU, TEE, ChiSq for various scatterometry models for Gate ADI structure.



TMU [nm]	Slope	Offset	R^2
0.559	0.990	-21.676	0.9954

TMU [nm]	Slope	Offset	R^2
0.583	1.022	-23.151	0.9951

Fig. 3 Comparison of TMU for Gate ADI Model Optimizer and expert user scatterometry models.



TMU [nm]	Slope	Offset	R^2
0.272	1.048	-5.755	0.9985

TMU [nm]	Slope	Offset	R^2
0.269	1.051	-5.721	0.9985

Fig. 5 Comparison of TMU for Gate FI Model Optimizer and expert user scatterometry models.

For the Gate FI application both the expert user and Model Optimizer arrived at the scatterometry model with 6 DOF with a difference in the parameter of the remaining hard mask that was floated. The models are quite similar in terms of accuracy (Fig. 5). Similarly to the previous case, the expert user took about a week to optimize the Gate FI model while Model Optimizer needed less than one our to do the same.

We compared TEE, TMU and ChiSq for a number of variations of the Gate FI structure with different parameters fixed and floated (Fig. 6). In this case again good tracking of TEE and TMU was observed, while the worst ChiSq corresponded to the best TMU model. Optical correlations between parameters are to blame here for the poor predictive capability of the ChiSq metric, for which a small improvement is bought at the expense of making the model less stable and thus significantly increasing measurement uncertainty We also compared dynamic repeatability performance of the two models and results were quite similar (Fig. 7).

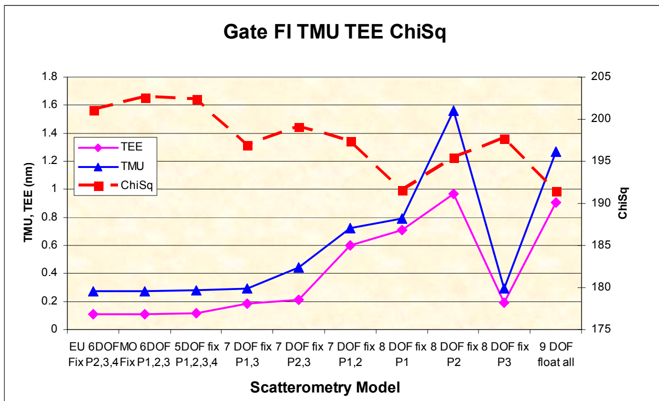


Fig. 6 Gate FI comparison of TMU, TEE, ChiSq. Expert User and Model Optimizer models are the first and the second respectively. Note anti-correlation of the ChiSq to the TMU

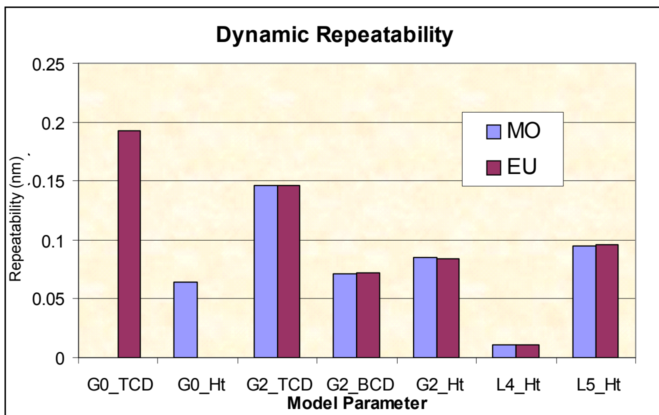


Fig. 7 Dynamic repeatability comparison for Gate FI shows similar performance for MO and EU models

The high-k metal gate structure proved the most challenging of the three for an expert user, and the optimization process took approximately two weeks. Model Optimizer still was able to finish the process within one hour. In addition to the overwhelming number of possible combinations with 18 degrees of freedom, the critical metric of the metal undercut/foot was a lower sensitivity parameter, raising the complexity of the problem. The expert user stopped at the model with 9 DOF while Model Optimizer reduced the number of floating parameters to 6. As seen on Fig. 8, accuracy (TMU) for the Model Optimizer 6DOF model is about 60% better than TMU obtained with the expert user 9 DOF model. Optical parameter correlations contributing to the higher measurement uncertainty are responsible for the accuracy difference. Again we studied several other variations of the HKMG scatterometry model and discovered that fixing 3 more parameters in the expert user model results in improved accuracy of the metal undercut/foot measurement.

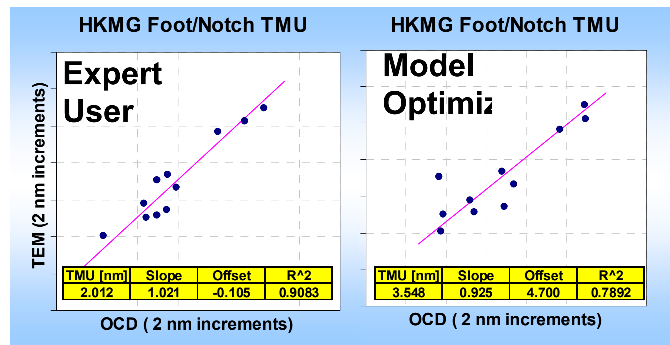


Fig. 8 Accuracy comparison for HKMG structure. Model Optimizer shows 60% improvement in TMU.

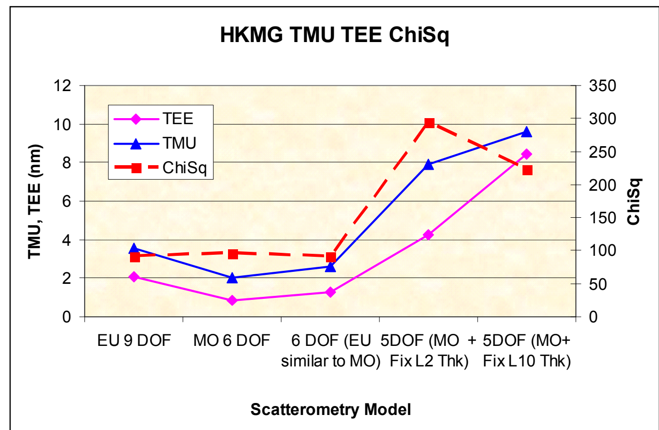


Fig. 9 High-k metal gate structure TMU, TEE, ChiSq. Graph shows good tracking of TMU using the TEE metric

In this case, the expert user model becomes the same as the Model Optimizer model except for two adjacent unpatterned layers that are correlated due to similar optical properties. The expert user model floats the upper layer whereas the Model Optimizer model floats the lower layer. The third data point in Fig. 9 corresponds to this 6 DOF version of the expert user model. The difference in TMU can be attributed to the larger

impact of fixing the lower layer since it has larger process variation. One can observe on Fig. 9 that fixing parameters in the 6 DOF model results in significant accuracy degradation, which in this case correlates to the worsening of the spectral fit quality (ChiSq). Yet in the set of the better TMU models ChiSq has no predictive value. Dynamic repeatability of the EU and MO models is compared on Fig. 10. With very respectable values for the dynamic repeatability one can infer that random tool noise is not a major contributor to the accuracy error for the measurement of the metal undercut/foot in the HKMG structure.

In this paper, we investigated accuracy (TMU) and TEE predictive error for only one critical parameter per application. Typically, there are 2-4 critical parameters per application with different priority. This study and the Model Optimizer approach could be potentially extended to more than one critical parameter, by possibly weighing the priority of parameters and using that as an input to the Model Optimizer algorithm.

IV. CONCLUSIONS

The new automated methodology for scatterometry model optimization was validated on three applications, including a leading-edge high-k metal gate structure. Accuracy of the critical parameter measurements achieved with the scatterometry model optimized with the new automated method was similar for two of the studied applications (Gate ADI and Gate FI), while for the HKMG application a TMU improvement of about 60% was obtained from the Model Optimizer model as compared to the model optimized by an expert user. Model optimization time was 40 to 80 times shorter (Table I) with the new methodology. Model Optimizer produces the final model based on only one measured spectra, which is usually the center point of spectral/process variation.

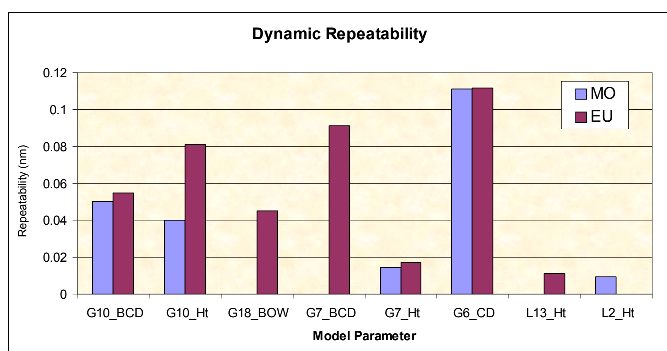


Fig. 10 Dynamic Repeatability comparison for HKMG shows that random tool noise is not a major contributor to the scatterometry measurement accuracy for this application

For certain applications, especially in a development environment where there is high process variation, it might be a good idea to investigate a few models derived from Model Optimizer based on multiple spectra (taking spectral variation into account). This might increase the model optimization time since it is directly proportional to the number of measured spectra utilized for calculations. Though the Model Optimizer methodology is still relatively new, the results obtained for all three studied applications are promising. Self-consistent scatterometry accuracy prediction capability of the Model Optimizer (TEE) that does not rely on external reference metrology was studied, and results suggest that it tracks well with the TMU, with scatterometry as the tool under test and CD-SEM or TEM as the reference metrology.

TABLE I
Measurement accuracy and scatterometry model optimization time comparison between the new Model Optimizer methodology and an expert user following standard industry practices. Note that the time to results shown here only apply to the model optimization phase. Other important phases of scatterometry application development which are not affected by Model Optimizer include wafer preparation, spectra collection, material characterization, model setup, library generation, and reference measurement collection and analysis.

Structure	TMU (nm)		Optimization Time (hrs)	
	MO	EU	MO	EU
Gate ADI	0.56	0.58	1	40
Gate FI	0.27	0.27	1	40
HKMG	2.01	3.55	1	80

In this paper we have evaluated the measurement performance of the Expert User and the proposed Model Optimizer using these key metrics: accuracy (TMU analysis), predictive error (TEE), and dynamic repeatability (wherever possible). Because of time constraints, some of the other metrics that are often utilized to gauge metrology performance, but were not included here, include tool matching, DOE tracking (though it is linked to accuracy), and sensitivity and correlation analysis for critical parameters. Even though the proposed methodology should be extendible to the scenario where multiple parameters are deemed critical, the Model Optimizer results presented here are based on optimization for one critical parameter per application. Furthermore, a limited set of DOE wafers were utilized for this study. A more thorough evaluation of Model Optimizer should include additional DOE wafers plus production wafers, and a variety of applications (e.g. spacers, metal trenches, vias, contacts, etc.).

It should be noted that the development of a scatterometry solution includes multiple steps – DOE wafer preparation, spectra collection, material characterization (n&k extraction), model setup, model optimization, library generation and reference measurement collection and analysis. The proposed Model Optimizer methodology should help to shorten one of these steps – model optimization – which is often the most critical and time-consuming step in the scatterometry workflow.

In the future we plan to increase the scope of the parameters that can be used in the model optimization process, including

hardware system characteristics, in addition to the geometry and material parameters of the scatterometry measurement targets.

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