Virtual Metrology White Paper - INTERNATIONAL ROADMAP FOR DEVICES AND SYSTEMS (IRDS)

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EXECUTIVE SUMMARY

This white paper provides an overview of virtual metrology (VM) and the benefits it can provide, with cost reduction (both capital expenditure and cycle time) being the primary benefit. The white paper also examines some of the issues preventing wider adoption of VM, and offers some possible solutions. The key adoption issues identified in this white paper primarily came from a survey of advanced process control (APC) users, implementers, and managers, conducted by the International Roadmap for Devices and Systems (IRDS) Factory Integration focus team, to help understand the current state of VM adoption.

The main factors described as preventing wider adoption of VM are based on consensus opinions of the survey respondents. These include: confidence in models, customer data quality, lack of process knowledge and correlation with metrology, model maintenance, cost, and intellectual property (IP) security.

Possible solutions include development of a standardized prediction quality metric, improved data communications and data quality for model building and model maintenance, better training data, correlation with real metrology when possible, and improved interaction between yield and VM, which will allow VM to leverage some of the metrology data that yield depends on. The whitepaper also describes some current and potential applications of VM.

The following recommendations are summarized in the conclusions

- *Standards are needed to evaluate customer data quality*. A set of criteria on the minimum level (type and completeness) of data required for VM models would be helpful. Although the wide range of current and possible applications preclude exact specifications, guidelines on how to select an initial data set would be helpful.

- *Standards or guidelines are needed on how to evaluate model quality and how to communicate model quality via a model quality metric*. Issues involving model quality are some of key factors limiting VM model development and adoption. A model quality metric (or a number of possible metrics) will not only increase confidence in models, but also provide governance for use and enhance model portability and reuse. A platform to host, maintain and manage models would also be useful.

- *Where applicable, industry roadmaps should identify processes that could benefit from specific VM applications.* A wide range of processes could benefit from VM if there is wider understanding of how VM should be applied and what benefits could be achieved. The development community and industry roadmap developers should highlight applications beyond the current ones that could benefit from VM. Use cases that clearly illustrate different applications should also be highlighted.

- *Solutions for VM model robustness and maintenance should be identified* Challenges with maintaining models in the face of process dynamics and context shifts should be identified along with potential solutions and a roadmap for implementation. The relationship between model robustness and maintenance requirements, and how it applies to specific VM application types should be identified.

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1. INTRODUCTION

This whitepaper explores some of the relationship between real and virtual metrology (VM). The goal is to better understand the needs, challenges and opportunities for virtual metrology. Virtual Metrology is defined by SEMI E133[1] standard as

> "*…the technology of prediction of post process metrology variables (either measurable or nonmeasurable) using process and wafer state information that could include upstream metrology and/or sensor data."*

Virtual metrology is not a direct measurement. It requires a set of data that characterizes an environment to make a prediction. VM can be applied to answer questions such as - *what post process metrology variables are critical, how are these variables related to the input data, and how are the input variables transformed by the current process. Hence, what data must be collected to help predict those variables?* VM plays a limited role[2-6] in improving process knowledge and yield, but this could be larger if it is applied to other areas. Currently, process parameters such as etch rate and deposition rate are seen as easily adaptable to VM, while uniformity, particle detection and characterization, chemical mechanical polishing (CMP) scratches, and stress are seen as more difficult. Figure 1 shows a run-to-run (R2R) control approach using VM for a semiconductor manufacturing process[4].

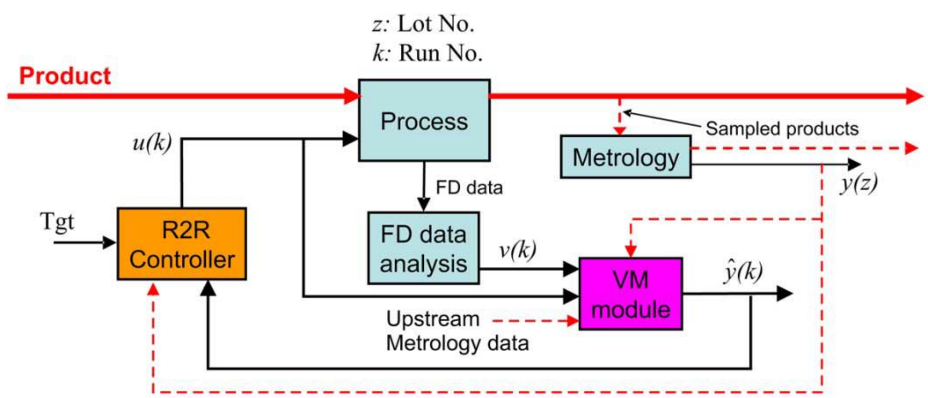

Figure 1: A generic R2R control diagram for VM for a semiconductor manufacturing process. u is an input, v is a process variable, y is measurement output from metrology, ŷ is prediction from the VM module. Illustration taken from Ref. # [4]. Both real metrology (RM) measurements and VM predictions are used as feedback data to the R2R controller. The RM measurements are also used to update the VM model.

Real metrology (RM) on the other hand provides an actual measurement of wafer or other parameters; this information about the current state of the wafer is typically used to help keep the process under control. The issue of whether the right type and amount of data is being collected is a reoccurring one in metrology[7]. Possible solutions for most of the metrology challenges listed in the International Roadmap for Devices and Systems (IRDS) Metrology Difficult Challenges table [8] would involve an increased use of modeling, simulation, and data analytics. The vast amount of data already collected could be used to increase the benefits of both real and virtual metrologies, and could be applied more widely to other areas of debug and diagnostics[9].

Although closer interaction between VM and RM could greatly increase the return on investment (ROI)[10, 11] for both areas, there are barriers. In this whitepaper, we examine some of the issues preventing wider adoption of VM, some possible solutions, and potential areas of application. This information represents a collaboration between the Metrology and Factory Integration focus teams within IRDS. The information presented is partly from a survey of advanced process control (APC) users, implementers, and managers[12], conducted by IRDS Factory Integration focus team, to help understand the current state of VM, and possible solutions.

2. KEY BENEFITS OF VIRTUAL METROLOGY

The primary benefits of VM are cost and cycle time reductions. This includes savings from reduction of both capital expenditure and cycle time. The latter can result from leveraging VM as part of smarter metrology and dynamic sampling techniques. In this case, VM is able to predict what and how much to sample to get the desired results. Other key benefits include augmenting run-to-run (R2R) control, and the ability to predict something that cannot be measured directly or non-destructively. These same benefits currently constitute the main ROI. Table 1 lists the primary benefits, ROI order, and the order in which VM is usually adopted. For importance of VM, a value of 1 indicate the most important.

TABLE 1: BENEFITS OF VIRTUAL METROLOGY

	Importance of VM- (Ultimate ROI)	Order of VM adoption
Metrology excursion detection	4	1
Use of smarter metrology sampling / dynamic sampling.	3	2
Augmenting run to run (R2R) control	2	3
Ability to predict something that cannot be measured directly or non-destructively	1	4

3. SOME ISSUES PREVENTING WIDER ADOPTION OF VM AND POSSIBLE SOLUTIONS

3.1. CONFIDENCE IN MODELS

Virtual metrology relies on models, and as such most of the issues identified as preventing wider adoption revolve around confidence in models. Models could be hard to validate prior to initial deployment and especially as part of a model maintenance effort. Given that VM may sometimes be used to predict parameters that real metrology cannot measure or verify, confidence in models is most important. Currently, there is no standard or generally accepted method to validate or adopt VM models, or to communicate model confidence.

3.2. CUSTOMER DATA QUALITY

This includes not measuring the relevant parameters, not using the right sampling strategy (i.e., amount and frequency of sampling needed to accurately predict post process information), including the necessary context data (such as product ID and maintenance indication) along with parameter data, and the quality of the training data. In some cases, data integrity in older tools and changes of state of models after major tool maintenance often leads to excessive error or poor repeatability. So robustness of models over time and across context due to data drifts and shifts is a problem. Other causes of poor data quality include measurement noise and process noise.

3.3. LACK OF PROCESS KNOWLEDGE AND CORRELATION WITH METROLOGY

In addition to data issues raised above, there may not be a full understanding of the processes being modeled, or a lack of incorporation of process knowledge in modeling solutions (i.e., models are purely statistical or data-driven). Although the main effects of a process may be well known, a full mechanistic understanding of all the process variables, especially to the level needed to add value, may not be available. As a result, when model parameters cannot be directly measured, correlation with real metrology is not always possible. This leads to a lack of acceptance by the metrology and yield groups.

3.4. MODEL INDEPENDENCE AND MAINTENANCE

Virtual metrology model portability across different chambers (chamber matching), recipes, products and other context is often low and inconsistent due to chamber differences, dynamics, context differences, and sensor calibration drift, etc. Methods of porting models need to be developed to reduce the startup cost of model development. VM models must also continue to provide predictions in the face of process dynamics and context changes such as process drift, product changes, and maintenance events. This usually requires VM models to have an ability to adapt to these changes in the environment. Challenges and potential solutions for VM model adaptation to maintain model quality and robustness must be identified.

3.5. Cost and Intellectual Property (IP)

Cost and Intellectual property are two of the overarching problems that cut across all aspects of VM. Although VM could have a lower capital cost, it is an additional investment. Intellectual property protection and confidentially also mean that VM models and associated data and interfaces cannot be shared easily.

4. Some Possible Solutions

Possible solutions would include addressing the global problems outlined above, but also finding ways to make implementing VM more practical in the field. This requires a clear indication that the ROI is worth the effort. To do this, use cases that clearly illustrate different applications, and robustness over time and context are needed. Ideally, this would be for cases where VM could make a unique impact.

The development and use of a prediction quality metric would be very helpful in increasing the confidence of models and defining their use. A lot of the issues that prevent wider adoption has to do with model reliability, confidence, and repeatability. A prediction quality metric would at least give users an indication of model quality. Understanding better ways to communicate data for model building, better training data, and correlation with real metrology (when possible) would be helpful.

An area or approach that could help VM is predictive maintenance (PdM)[13]. Both VM and PdM largely use the same modeling approaches, and have a lot of the same requirements for model development, implementation and maintenance (historical data, communication infrastructure, data merging, etc.). However, while VM has been around longer, PdM seems to be receiving more attention. Simple PdM models can be more portable and robust, and it is easier to show ROI. PdM also has more relaxed requirements with respect to functionality. For example, even if PdM predicts an earlier schedule, the end result is still okay. In spite of differences in expectations, the success of PdM suggest that there could be things VM could learn from PdM. Methods to integrate VM and PdM has also been proposed[14].

The relationship between yield and VM could be better. Currently, yield analysis relies heavily on real metrology rather than VM. Although the benefits described above have a direct impact on yield, VM's interaction with fault detection (FD) and APC could be further improved to increase yield. Specifically, similar models used to predict metrology metrics could be used to predict and improve yield. The impact of good sampling techniques on measurement uncertainty are well known[15], and should be applied more widely. Better sampling techniques developed for VM would be particularly useful in predicting yield excursions, especially if the models come with a prediction quality metric. This will result in a smaller data set being used for yield correlation. FD also needs to be more yield aware, i.e. FD process excursions linked to yield excursions.

5. Applications Of Virtual Metrology

Virtual Metrology can be applied to a variety of applications where the relationship between process parameters and results are well understood and can be predictable. VM has been applied to the following areas with varying degrees of success: etch rate, deposition rate and film thickness, chamber matching, chemical mechanical polishing, carrier profiles prediction and uniformity among others. We highlight two uses that cut across different applications: R2R control and smart sampling.

5.1. Run To Run (R2R) Control

R2R Control is defined as "*the technique of modifying recipe parameters or the selection of control parameters between runs to improve processing performance. A run can be a batch, lot, or an individual wafer*"[16]. R2R control uses process, equipment, and metrology data with historical knowledge of the same parameters to suggest changes to the recipe after each run. The goal is to capture and correct process shifts and drifts and to reduce process variability between runs, which in the end reduces cost. R2R control is used due to lack of in-situ or real-time information about a process, especially one that could drift out of control. R2R control has been successfully implemented in lithography, CMP, and chemical vapor deposition amongst other areas, and could be extended to other uses. Some benefits include improved process capability (increased accuracy to target and reduced variability), early detection of process drifts, reduced process downtime, better process control, and scrap reduction among others. R2R control utilizes both feedforward and feedback information for process control. This information usually comes from pre and post-process metrology respectively. Unfortunately, in a large number of semiconductor processes, not all wafers are measured, so the controller must operate without 100% wafer sampling, reducing controller effectiveness. As shown in Figure 1, VM can be used to augment real metrology, enabling essentially 100% sampling for pre and post metrology. Issues of VM prediction quality complicate the control modeling and execution process.

5.2. Smart Sampling

Smart sampling (also known as dynamic sampling) is the ability to change the sampling details (frequency, size, etc.) based on prior observations. This enables the ability to know what to sample, how much to sample, and when. Generally, the sampling frequency increases when the process looks as if it is drifting from the intended value, and decreases when the process is under control. With adaptive sampling, a key part of the implementation is to make sure that the algorithm is robust enough to respond to small process shifts during low sampling periods. Smart sampling has been applied to different areas such as etch and deposition and is usually one of the first VM techniques to be adopted. When used as part of a VM scheme, data from smart sampling is used along with other process data to feedforward information[17, 18].

6. Potential Applications Of Virtual Metrology

Increasingly, machine learning and predictive analysis are used for metrology applications [10, 11, 19-21]. Although this is not always referred to as VM, it is part of a trend towards autonomous and semi-autonomous evaluation of metrology data for pattern analysis, prediction, and decision making. The following examples are areas where the predictive nature of VM could be used to enhance the usefulness of real metrology. In some cases, this would help streamline current measurement processes, in other cases it would predict outcomes for parameters that cannot be measured non-destructively based on training data. This is not meant to be an exhaustive list, just a few examples to highlight the broad applicability.

6.1. Directed Self Assembly

Directed self-assembly (DSA) is based on the use of self-assembling materials (mostly block copolymer films) for nano-patterning[22]. Although there are a variety of potential applications in nanotechnology, a considerable body of work has been devoted to semiconductor lithography[23-25]. Although DSA is a promising technique for nano-patterning, it is mostly at the research stage, so a large body of process monitoring data is not widely available. In addition, there is no clear information on material and system dependent measurands. However, key metrology challenges have been identified, and their solutions for a factory environment could benefit from VM. Prediction techniques could be used to determine where DSA defects are most likely be, and also correlate certain types of defect with process issues in other steps. Some examples include:

DSA Defects: Metrology techniques to detect low densities of surface and buried defects over a large area are needed for DSA. Low densities and small defect sizes mean that optical inspection tools do not have the required sensitivity for detection. A better understanding of the material and system dependent defects would help predict the most critical post metrology variables, defect position and location, defect density, and possible impact on the process.

DSA: CD and Overlay: Another issue is overlay metrology for DSA. Overlay shifts in DSA are not systematic, so more sampling at higher rates is needed to fully capture overlay shifts. Metrology issues such as position and critical dimensions (especially over a large area) are yet to be addressed.

6.2. Virtual Standards and Test Structures

Virtual Metrology could play a role in the development of virtual test structures. The data to model the relationship between instrument parameters, measurement data, performance and yield is available but rarely used for such purposes. This is mostly due to lack of knowledge about process variables that could affect the results. This could change if predictive models are used to verify the "calibration" or suitability of an instrument for specific measurements. The goal is not to replace physical calibration. This approach will model the relationships between frequency of calibration, process shifts, and post metrology parameters. This will provide information on when best to physically calibrate the instrument, and when to use virtual standards. Virtual standards could be combinations of instrument and system models, parameters, and calibrated images[26] used to define the best operating status for a set of measurements. Although developed for different applications, the use of model based libraries for Scanning Electron Microscopy (SEM) linewidth analysis[27] and data fusion models[28] could be refined for this application.

6.3. HYBRID METROLOGY

Hybrid metrology is the complementary use of several techniques to measure parameters, where no single instrument has the capability, resolution or low levels of uncertainty needed to characterize all the parameters. At least two or more instruments are used, and the results combined to get the final values. *Note that the hybrid metrology discussed here is the use of multiple instruments, rather than the combination of VM and RM.* The need to use multiple techniques[29-32] comes from the increased use of 3D devices such as fin-based field effect transistors (finFETS), where the number and complexity of parameters make it impossible for any single instrument to measure. For example, in measuring critical dimensions with scatterometry [29, 33, 34]regression models that include parameters such as width, sidewall angle, height and pitch are developed. The uncertainty of the models could be reduced if values for some of the parameters are included and allowed to float with their specified uncertainties. Values from specific parameters would come from instruments that are better at such measurements than scatterometry. So sidewall angle values from atomic force microscopy could be included in the optical regression model, with the uncertainty providing a smaller floating range. Similarly, for failure analysis, two or more techniques can be combined on the same device to obtain sub-nm structural and electrical information as in the case of AFM and TEM[35, 36]. Figure 2 shows a conceptual diagram of hybrid metrology. Critical dimension –small angle X-ray scattering (CD-SAXS)[37, 38], atomic force microscopy (AFM)[39, 40], SEM, and optical critical dimension (OCD) contribute information based on specific measurands or parameters based on their capabilities. This is used to develop a generalized measurement model. This model can also be applied to dedicated site-specific analysis and failure studies[35]. Applications of hybrid metrology could also involve just two instruments such as AFM and SEM or TEM[35, 41-44] and SEM and CD-SAXS. In some applications, one of the instruments could also provide calibration and traceability for specific measurands.

The data intensive nature of Hybrid metrology lends itself to some degree of virtualization. Also, some of the analysis tools could be used for prediction. Hybrid metrology involves instrument calibration, instrument selection, measurement systems modeling, data analysis and synthesis. Virtual metrology could be used to predict which instrument should be included in the group based on past performance, or knowledge from training data, and robustness of the generalized model. For example, VM training data would be able to predict if an increase in overall outcomes (model performance, better process control, etc.) associated with the use of certain instruments justifies the cost. Rigorous uncertainty analysis could also enhance the effectiveness of smart sampling[15]. Research on ways to incorporate virtual metrology, hybrid metrology, and machine learning are currently underway[20, 21, 45-47].

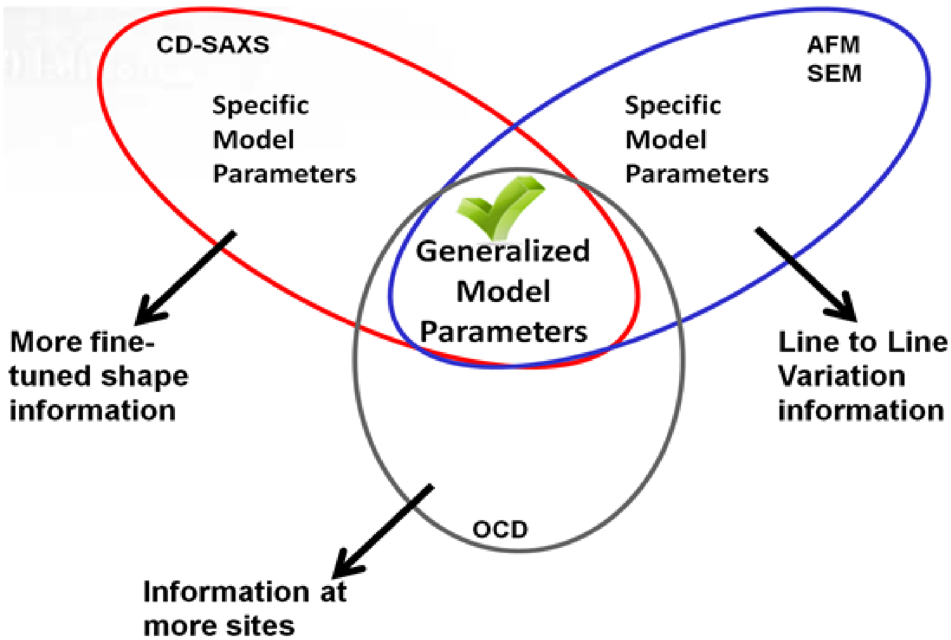

Figure 2: Conceptual diagram of hybrid metrology. Information from different instruments is used to develop a generalized model of the measurement. Image courtesy of Richard Silver (NIST).

6.4. ESH/S

Some of the analytical methods developed for metrology could be applied to environmental, health, safety and sustainability monitoring. This could be used for nanomaterials, effluent and contamination monitoring, and more broadly to a wide range of analyte evaluation issues. Given that the analyte being monitored is either a process material or a by-product, some of the methods developed for materials metrology and contamination characterization when suitable could be applied to ESH/S. Materials metrology data could be used to predict expected levels of specific materials and their compounds. In some cases, this would involve modeling data from metrology, ESH/S, assembly and packaging on issues such as chemical sensing.

7. Conclusions and Recommendations

This white paper examined the relationship between virtual metrology and real metrology, some issues preventing wider adoption of VM, and possible solutions. Overall, confidence in models, customer data quality, methods for model maintenance, and lack of incorporation of process knowledge and correlation with metrology were identified as some of the key issues preventing wider adoption of VM. A possible solution would be to develop a model quality metric. This would give users an indication of model quality, and help increase confidence in models. Another possible solution is to improve the collaboration between yield and VM. Yield relies heavily on real metrology rather than VM. VM's interaction with FD and APC could be further improved to increase yield. Similar models used to predict metrology metrics could be used to predict and improve yield.

In order for VM to gain wider acceptance, certain steps could be taken by the VM development communities, standards developers, and industry roadmap developers to increase the wider adoption of VM. These steps include:

- *Standards are needed to evaluate customer data quality*. A set of criteria on the minimum level (type and completeness) of data required for VM models would be helpful. Although the wide range of current and possible applications preclude exact specifications, guidelines on how to select an initial data set would be helpful.

- *Standards or guidelines are needed on how to evaluate model quality and how to communicate model quality via a model quality metric*. Issues involving model quality are some of the key factors limiting VM model development and adoption. A model quality metric (or a number of possible metrics) will not only increase confidence in models, but also provide governance for use and enhance model portability and reuse. A platform to host maintain and manage models would also be useful.

- *Where applicable, industry roadmaps should identify processes that could benefit from specific VM applications.* A wide range of processes could benefit from VM if there is wider understanding of how VM should be applied and what benefits could be achieved. The development community and industry roadmap developers should highlight applications beyond the current ones that could benefit from VM. Use cases that clearly illustrate different applications should also be highlighted.

- *Solutions for VM model robustness and maintenance should be identified*. Challenges with maintaining models in the face of process dynamics and context shifts should be identified along with potential solutions and a roadmap for implementation. The relationship of model robustness and maintenance requirements to specific VM application types should be identified.

Overall the metric that matters most is cost reduction – both capital and cycle time. Increased awareness about the benefits of VM, and closer interaction between real and virtual metrology would ultimately lead to substantial cost savings.

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