# Thursday Afternoon, November 9, 2023

#### Manufacturing Science and Technology Group Room C120-122 - Session MS+AP+AS+TF-ThA

#### Machine Learning for Microelectronics Manufacturing Process Control

**Moderator: Tina Kaarsberg**, U.S. Department of Energy, Advanced Manufacturing Office

#### 2:20pm MS+AP+AS+TF-ThA-1 Human-Machine Collaboration for Improving Semiconductor Process Development, Keren Kanarik, LAM Research INVITED

Although chips have been designed by computers for decades, the processes used to manufacture those chips are mostly developed manually – a costly endeavor using highly trained process engineers searching for a combination of tool parameters that produces an acceptable result on the silicon wafer. To assess whether Al could be beneficial in accelerating process engineering innovation and reducing costs, humans and machine algorithms were benchmarked on a virtual high aspect ratio plasma etch process [Kanarik, et al. Nature 616, 707–711 (2023)]. This talk will review results and take a behind-the-scenes look at the study, which showed a "human first, computer last" approach could reach process engineering targets dramatically faster and at half the cost compared to today's approach. While human expertise and domain knowledge are essential for the foreseeable future, the results point us to a path to foundationally change the way processes are developed for manufacturing chips.

3:00pm MS+AP+AS+TF-ThA-3 Machine Learning-based Atomic Layer Deposition, Kanad Basu, University of Texas at Dallas INVITED Atomic Layer Deposition (ALD) is dependent on a host of process parameters. These independent parameters can be set to a particular value to create customized recipes for growing films. Although they are considered to significantly influence the ALD process, existing research does not provide a methodology to quantify the impact of these parameters on growth rate and final thickness of a film. Moreover, process parameterbased thickness estimation is a resource- and time-intensive approach, requiring numerous experiments. To address these challenges, we propose a machine learning (ML)-aware strategy that generates "feature importance maps" to determine the most critical process parameters. In our study, we utilize a Veeco® Fiji Gen2 ALD system to grow a CeO2 film. Specifically, our study is associated with 78 process parameters, which include chuck temperatures, chamber temperatures, line temperatures, precursor temperatures, gas flow rates, among others. Our approach utilizes a random forest classifier, which is identifies the top-10 features (parameters) that affect ALD processes. The proposed approach furnishes promising results of up to 99% thickness prediction accuracy using the deduced top-10 features. These results are subsequently validated using in-situ spectroscopic ellipsometry, thereby advocating its effectiveness in generating the feature importance maps. We posit that only these ten features can be utilized to monitor and control ALD processes. Furthermore, in this analysis, we demonstrate the robustness of our solution, which is independent of the type of ALD process considered standard ALD process or temperature-dependent Temperature-Time-Thickness (TTT) ALD processes. Moreover, by monitoring just ten of the 78 process parameters, the proposed approach has implications of reduced data dimensionality (up to 87.2% reduction in feature space).

# 3:40pm MS+AP+AS+TF-ThA-5 Rapid Optimization of Gap-Fill Recipes Using Machine Learning, Sebastian Naranjo, L. Medina de Oliveira, M. Chopra, Sandbox Semiconductor

Creating and optimizing deposition recipes for nanostructured devices is costly and time-consuming. A major source of defects and device performance degradation is the formation of interior voids. These voids can have a number of causes, including non-uniform deposition rates along the substrate surface due to imperfect seeding and/or mass transport and reaction kinetics factors, as well as critical dimension variations in the initial profile due to imperfections in preceding processing steps. For example, during electroplating, the substrate surface is seeded before material deposition is set to fill the gap. Non-conformal seedings can cause the deposited material to accumulate at different rates and lead to localized voids. Void defects can also occur in highly conformal processes such as atomic layer deposition or chemical vapor deposition due to critical dimension variations such as bowing or tapering in the pre-deposition profile. Current methods for optimizing process performance rely largely on trial and error. Here we present a cost-effective and systematic computational approach to optimize recipe conditions using Sandbox Studio AI, which employs a combination of feature scale modeling and machine learning to rapidly predict process outcomes for a given electroplating system using a minimal number of experiments. In this approach, we first use critical dimension information about the fill height and void defects from a set of experiments to calibrate a feature scale model. We then use the calibrated model to predict critical dimension outcomes for thousands of possible process parameter combinations. These predictions are used to maximize process window stability and provide recipe recommendations that minimize the formation of voids even in the presence of seeding or initial profile imperfections. The showcased approach demonstrates how computational modeling can be used to accelerate learning cycles, improve process quality, and reduce development costs.

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