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Automated high throughput optimization of multistep and cyclic etch and deposition processes using SandBox Studio™ AI

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ABSTRACT

The development of new technologies and advanced nodes is capitally intensive due to process design strategies that involve dependent unit processes with different yields and performances. This has led to the exploration of model-based optimization to cut the cost and time of recipe creation; however, computational optimization of semiconductor processes is quite challenging due to multi-dimensional parameter spaces and limited experimental data. SandBox Studio™ AI is a computational tool that automatically builds a hybrid physics-based and machine learning model that can be used to predict optimal process recipes and explore novel process changes such as different incoming mask geometries and step durations. Herein, we show the utilization of SandBox Studio™ AI to build a computational representation of a cyclic etch and deposition process of a high aspect ratio channel etch with the following detrimental effects – bowing, resist over-etching, clogging via deposition, and twisting. The model was calibrated to a synthetic data set of thirteen experiments with five varying process parameters. Then, an optimal recipe was predicted that minimized the observed detrimental effects. The model was then used to explore different incoming mask geometries and step durations to improve the recipe even further. This capability is made possible by the software's foundational physics-based model and is not possible using conventional statistics and machine learning based tools.

Keywords: Etch, Deposition, Experimental Design, Process Optimization, High Aspect Ratio, Recipe Creation, Computation, Twisting, Clogging

1. INTRODUCTION

The continuous demand for device scaling and density improvements has led to significant development challenges across the semiconductor industry, which necessitate quantitative and qualitative advances in manufacturing techniques. Whether scaling is achieved by a shrinking of the process or three-dimensional design, the need for robust control of etching processes has emerged as a key prerequisite for progress on the state-of-the-art demands. In particular, the development of 3D NAND devices was proposed as a strategy for increasing areal density by stacking memory cells vertically [1], which entails the well-controlled etch of high-aspect ratio (HAR) structures. Etch at aspect ratios exceeding 50:1 faces unique difficulties and adequate device performance hinges on the ability to fabricate channels free of defects such as bowing, clogging, and twisting.

The compounding challenges of optimizing etch processes involving complex, multiscale, multi-physics phenomena have driven the development and use of computational tools to facilitate recipe development and alleviate some of the processing obstacles. Traditional machine learning/purely statistical techniques have shown themselves inadequate to the task. The complexity of the physics and chemistry of plasma etch processes together with the high dimensionality of process parameter spaces demands a large amount of training data that is time-consuming and expensive to acquire. At the same time, the deployment of purely physics-based models is hindered by industry secrecy, inadequate chamber characterization, and tool variability. A successful modeling approach must therefore be attuned to the realities of sparsely available experimental data and limited characterization of the relevant physics.

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Here we present an automated, high-throughput optimization strategy of multistep and cyclic etch and deposition processes using SandBox Studio™ AI. This software package uses a hybrid physics and machine learning approach to untangle the complex relationships between process parameters and critical dimensions of complex feature level profiles using a limited amount of experimental data. These relationships are then used to predict optimal process recipes.

2. METHODOLOGY AND MODEL INPUTS

SandBox Studio™ AI was used to develop a fully automated computational model of a 2D high aspect ratio channel etch consisting of a cyclic process that alternates etch and deposition steps each with a duration of 1 second. The incoming stack comprised a 300 nm tall hard mask with an aperture width of 50 nm on top of 3000 nm of substrate material (Figure 1a). The model was calibrated to a set of 13 synthetic experiments with five varying process parameters and used to optimize four critical dimensions: mask height, channel depth, bow width, and twist (Figure 1b). The process parameters and critical dimensions for each experiment were input to the software in tabular form and used to calibrate the model.

The optimization of twist deserves special mention. Twisting is a poorly understood process of a stochastic character [2], manifesting as a misalignment between the top and bottom of the channel. This is quantified as the (absolute) horizontal distance between the top and bottom of the channel. To treat the problem with a deterministic modeling strategy, we adopt a policy for selecting representative twist values for each combination of process parameters, which are then treated as deterministic calibration targets. For example, the standard deviation or 3σ value could be used as this representative. The key assumptions for the validity and usefulness of this procedure are that this chosen value faithfully represents variability in the distribution of twist measurements (which is straightforward if these values are normally distributed), and that the distribution of twists depends on the process parameters. This assures that twisting can be minimized without the need for a full characterization of its statistical behavior.

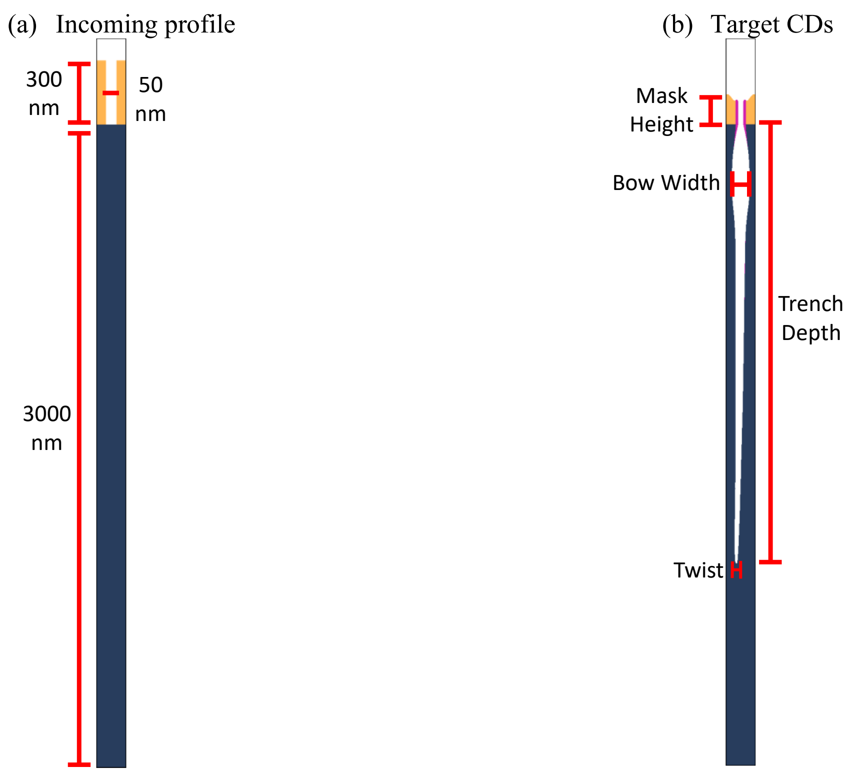

Figure 1. (a) Schematic of the incoming profile used to calibrate the model and (b) the target critical dimensions of interest.

3. MODEL CALIBRATION

Using the input data described in section 2, a SandBox Studio™ AI model was automatically built using the provided experimental process parameters and critical dimensions. The key governing mechanisms associated with the complex cyclic etch and deposition behavior were selected using a hybrid physics and machine learning approach. The calibrated model captured key defects that occurred in the experimental profiles, namely substrate under-etching, resist over-etching, bowing, clogging via deposition, and twisting. Visualization of the model prediction vs the experimental profiles for three of the experiments is shown in Figure 2. The model correctly replicated the deposition, bowing, and twisting effects. Parity plots of predicted CDs vs experiment for all thirteen data points is shown in Figure 3.

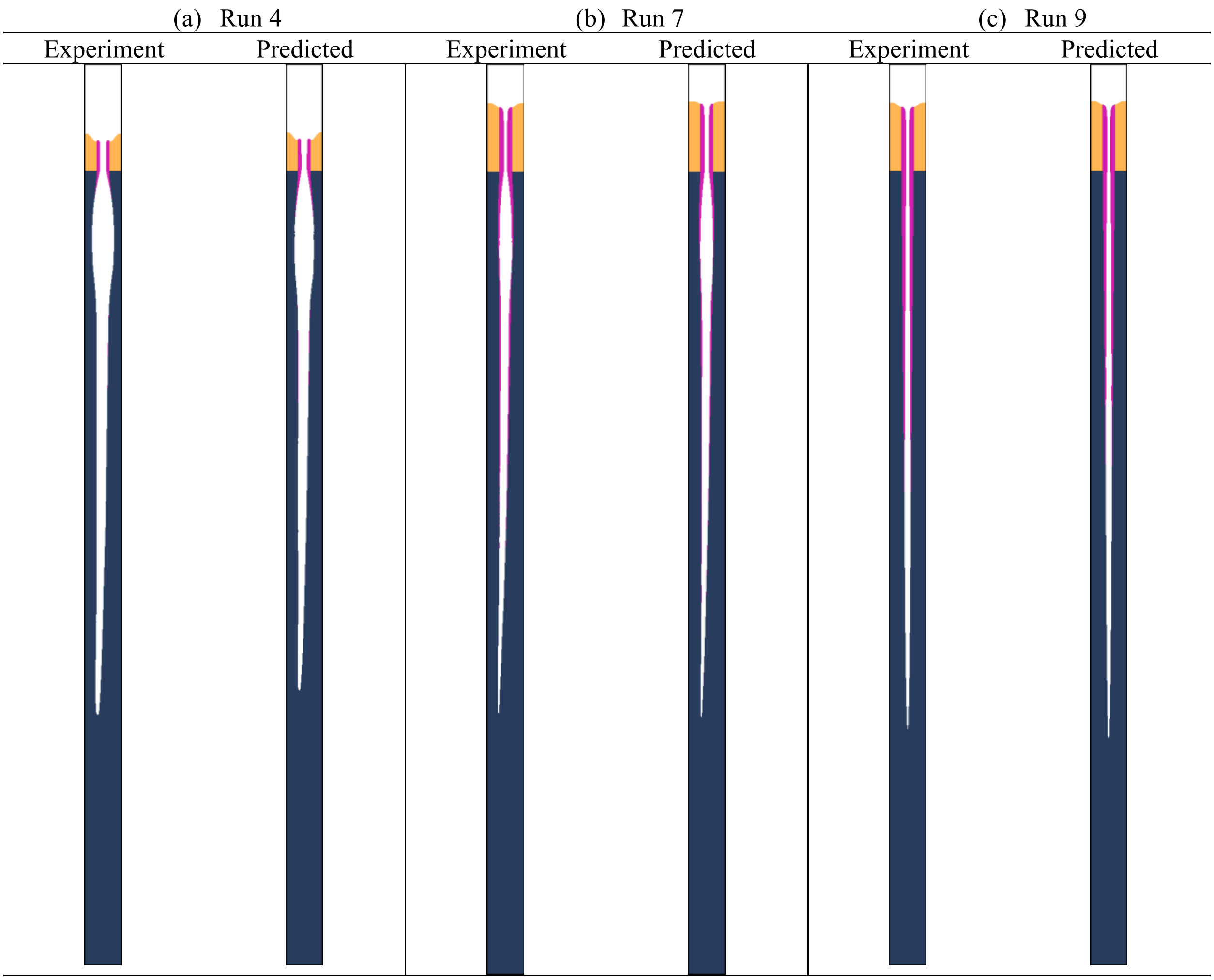

Figure 2. Comparison of experimental and predicted profiles. SBS AI predicts critical profile features including (a) bowing, (b) twisting, and (c) clogging

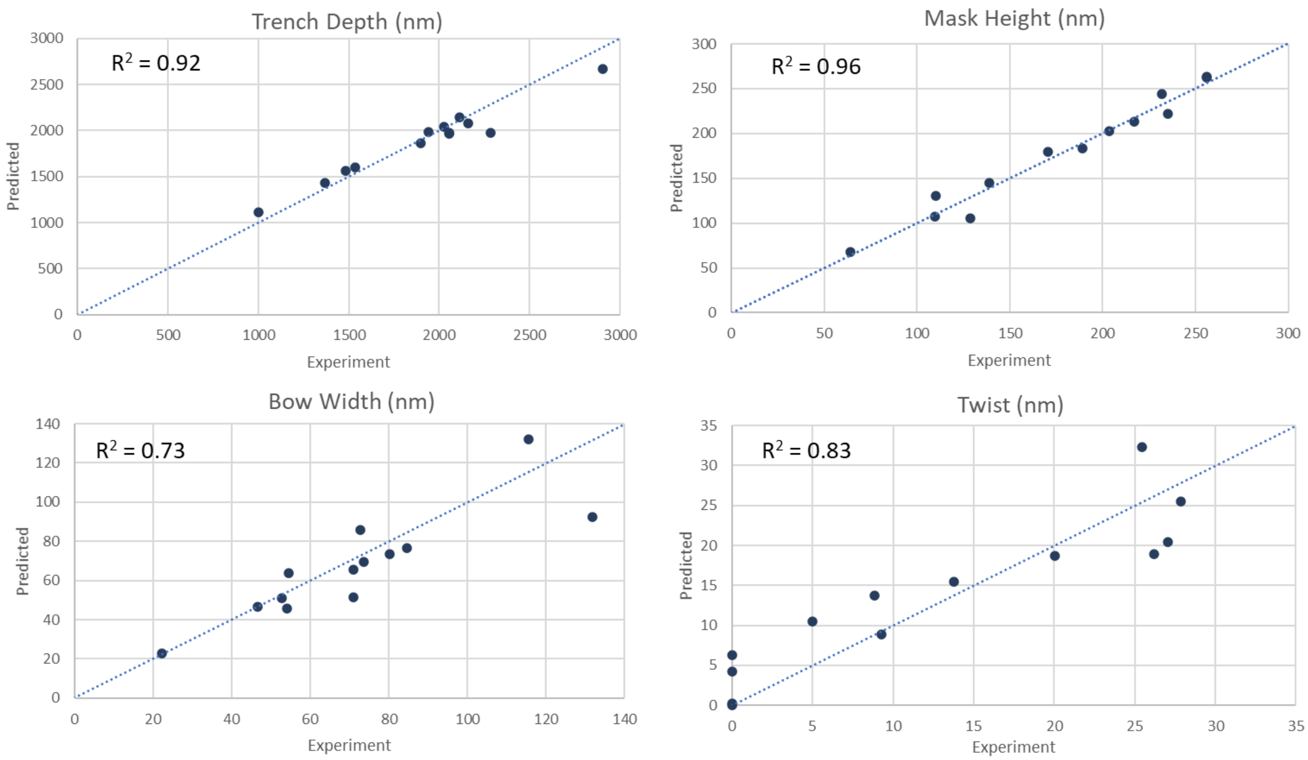

Figure 3. Parity plots of predicted critical dimensions vs experiment for all thirteen synthetic experimental runs.

4. RESULTS

4.1 Process Recipe Optimization

With a successfully calibrated model, SandBox Studio™ AI can be used to filter the process space and find process parameter combinations that achieve target critical dimensions within the required tolerances. SandBox Studio Quilt® is used to build process maps of each critical dimension across the process space as shown in Figure 4. These figures represent a flattening of the five-dimensional process parameter space into a two-dimensional density plot. This plot can be used to identify, for each critical dimension, the regions of process space that passes the design criteria within the required tolerances. These pass regions are combined, and an optimal recipe is selected from the largest region of process space that passes all criteria, as shown in Table 1 and Table 2.

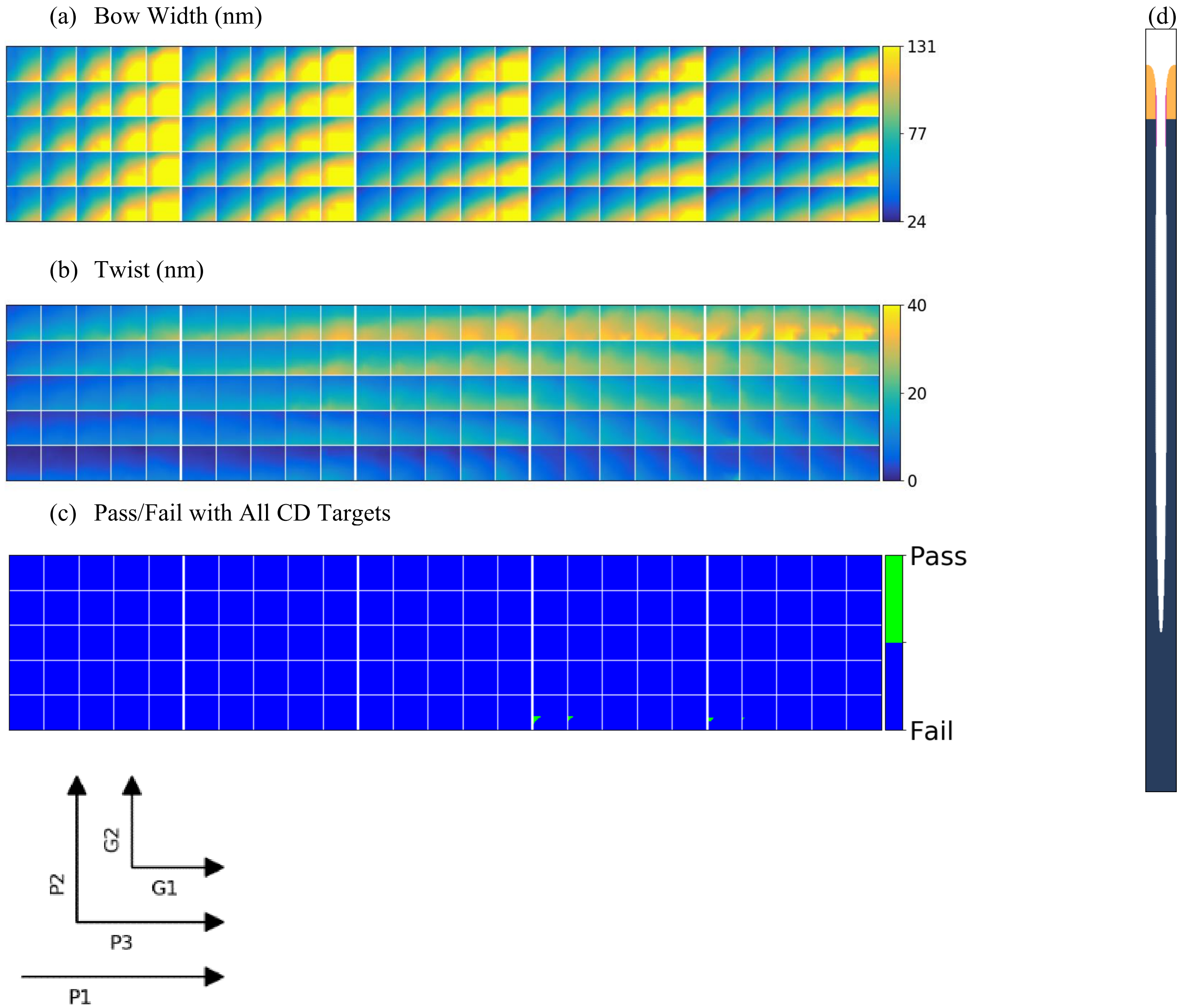

Figure 4. (a) Quilt process map for bow width. Low bow widths require low P3, low G2, and low G1, (b) Quilt process map for twist. Low P2 is required to minimize twist, (c) Pass/fail process map for all CDs of interest (Table 2), (d) predicted profile of the optimized process recipe (Table 1).

Table 1. Predicted Process Recipe

Process Parameter	Value (Normalized)
P1	0.75
P2	0
P3	0
G1	0
G2	0.30

Table 2. Target Critical Dimensions and Recipe Performance

Critical Dimension	Target Value (nm)	Experimental Value (nm)	PASS/FAIL
Channel Depth	> 2000 nm	2151	PASS
Mask Height	> 200 nm	241	PASS
Bow Width	40 +/- 10 nm	40	PASS
Twist	5 +/- 5 nm	8	PASS

4.2 Further Recipe Exploration

Trial 1: Modifying number of cycles

While the predicted optimized recipe meets all the target criteria, the channel has not reached the stop layer. A natural first attempt to push the recipe further would be to increase the etch duration by increasing the number of cycles. The calibrated model was used to explore this recipe alternation by running the physics-based model for a longer number of cycles than the predicted recipe. However, while the etch does reach the stop layer, excessive deposition results in the bow width not being met and the resist being over etched (Trial 1, Tables 3 and 4).

Trial 2: Modifying etch and deposition durations

One possible way to reduce the excessive deposition is to adjust the etch and deposition durations. In the original recipe, the etch and deposition phases were performed at 1 second each. In Trial 2, the calibrated model was used to explore this possible recipe adjustment by rerunning the model with the etch duration increased to 1.25 s and the deposition duration decreased to 0.75 s. This adjustment mitigated the clogging and resulted in recovering the bow width target criteria, but the mask resist was even further over etched (Trial 2, Tables 3 and 4).

Trial 3: Modifying initial mask height

Over etching of the mask might be mitigated by increasing its initial height. In the original recipe, a mask height of 300 nm was used. In Trial 3, the calibrated model was used to explore this possible recipe adjustment by increasing the starting mask height from 300 nm to 400 nm and rerunning the model. This adjustment resulted in minimizing the over-etching of the mask and all pass criteria being met (Trial 3, Tables 3 and 4).

Table 3. Recipes Performed

Process Parameter	Original Recipe	Trial 1	Trial 2	Trial 3
P1	0.75	0.75	0.75	0.75
P2	0.00	0.00	0.00	0.00
P3	0.00	0.00	0.00	0.00
G1	0.00	0.00	0.00	0.00
G2	0.30	0.30	0.30	0.30
Etch Duration (s)	1.00	1.00	1.25	1.25
Depo Duration (s)	1.00	1.00	0.75	0.75
Number of Cycles	100	200	200	200
Initial Mask Height (nm)	300	300	300	400

Table 4. Predicted Critical Dimensions. Red font indicates dimensions that are not meeting the desired criteria noted in column 1.

Critical Dimension	Original Recipe	Trial 1	Trial 2	Trial 3
Channel Depth (nm) (> 3000)	**2151**	**3000**	**3000**	**3000**
Mask Height (nm) (> 250)	**241**	**181**	**132**	**238**
Bow Width (nm) (40 +/- 10)	**40**	**24**	**54**	**50**
Twist (nm) (< 10)	**8**	**9**	**9**	**10**

5. CONCLUSIONS

SandBox Studio™ AI provides a hybrid machine-learning/physics-based toolset to accelerate etch recipe development. Here we demonstrated the automated development of a 2D model for a high aspect ratio channel etch. A model containing the key governing mechanisms was automatically selected and calibrated to a small batch of synthetic experiments with a high degree of accuracy. The calibrated model was used to find an optimized recipe minimizing defects such as bowing, clogging via deposition, and twisting. The model was then used to experiment with recipe modifications such as changes in the duration of etch and deposition steps and a different starting mask geometry, pushing the predicted recipe to an even better result. Such experimentation is not possible with purely statistical models, underscoring the power of combining physics with machine learning for etch recipe prediction.

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