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Fast etch recipe creation with automated model-based process optimization

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ABSTRACT

A method for automated creation and optimization of multistep etch recipes is presented. Here we demonstrate how an automated model-based process optimization approach can cut the cost and time of recipe creation by 75% or more as compared with traditional experimental design approaches. Underlying the success of the method are reduced-order physics-based models for simulating the process and performing subsequent analysis of the multi-dimensional parameter space. SandBox Studio™ AI is used to automate the model selection, model calibration and subsequent process optimization. The process engineer is only required to provide the incoming stack and experimental measurements for model calibration and updates. The method is applied to the optimization of a channel etch for 3D NAND devices. A reduced-order model that captures the physics and chemistry of the multistep reaction is automatically selected and calibrated. A mirror AI model is simultaneously and automatically created to enable nearly instantaneous predictions across the large process space. The AI model is much faster to evaluate and is used to make a Quilt™, a 2D projection of etch performance in the multidimensional process parameter space. A Quilt™ process map is then used to automatically determine the optimal process window to achieve the target CDs.

Keywords: Etch, etch recipe creation, modeling, 3D NAND, experimental design

1. INTRODUCTION

Demand for 3D NAND flash memory continues to grow at a brisk pace [1-2]. Accompanying this growth are technologies with increasing memory density and number of layers [1-3]. Manufacturing of 3D NAND is very difficult especially for devices with as many as 128 or more layers. Etching is particularly challenging as high aspect ratio trenches must be created for the memory holes. The widths of these etches must be close to uniform throughout the entire structure for aspect ratios of 50 or more. Identification of the process conditions or recipe for the etch is an expensive and time-consuming task. Slow determination of recipes delays production and impedes product deployment. Here we demonstrate a model-based methodology to accelerate identification of the etch recipe which reduces development costs and shortens time to market.

Identification of optimal etch recipes for microelectronic manufacturing in general continues to be an arduous task. In fact, most etch recipes are discovered through trial-and-error experiments guided by the skill and experience of the etch engineer. It can take weeks to months to over a year to create an optimal etch recipe depending on the how challenging are the etch requirements and how new or novel are the material stacks. Despite decades of development of ever more sophisticated models and simulations of etch, they are rarely used to design or discover an etch recipe. This is because an enormous number of accurate model parameters are needed for the simulations to be predictive. They also take a significant amount of time to run on even fast computers.

Nonetheless, modeling and simulations provide an excellent framework to correlate, interpolate and extrapolate valuable experimental data in the search for an optimal etch recipe. Here we present an automated, efficient, and accurate methodology to do so for a channel 3D NAND flash memory. The process engineer only provides the data for the experiments and the model build, calibration, and subsequent optimization of the process is done automatically. We demonstrate this in SandBox Studio™ AI using synthetic experiments to demonstrate the effectiveness of the method to identify an optical process window for an etch recipe that achieves the target CDs.

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2. METHODOLOGY

2.1 Process flow for automated identification of etch recipe

The process flow to automate model development is illustrated in Fig. 1a and consists of three steps. The first is the model build where a reduced-order physics-based model is defined for predicting etch profiles based on process parameters. In this step, the process engineer provides the initial stack and subsequent profiles following several etch experiments. Using this data, the best model is selected based on its probability of being correct. The second step is the model calibration, where the parameters of the reduced-order physics-based model are calibrated using the experimental data. Given a calibrated model that accurately predicts the CDs from the experiments, one has a computational tool to probe the parameter space. In the third step, model optimization, an AI model of the etch process is developed based on the reduced-order physics-based model to efficiently search this large process parameter space. The optimal process parameters are then selected to give the largest process window to achieve the target CDs.

Once a model has been created, it can be updated with additional experimental data as indicated in Fig. 1b. Note that a process window predicted after a first round of experimentation may not in fact be correct when tested experimentally. However, these validation experiments and other experiments can be used to automatically update the calibrated model and update the prediction of the optimal process window.

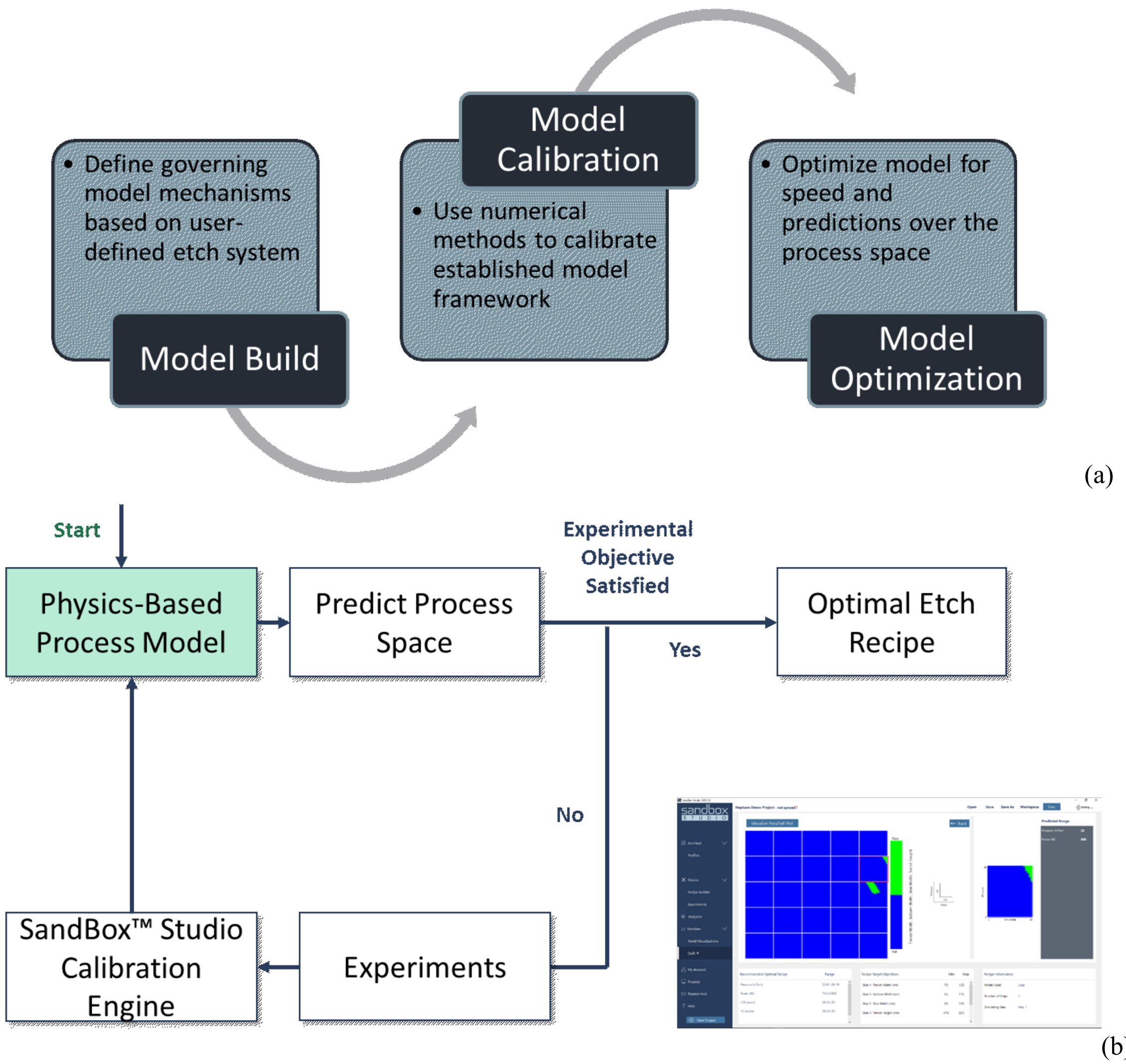

Figure 1. (a) Series of automated steps to build, calibrate and optimize a model for an etch process. Once the model has been identified and initially calibrated, it can iteratively be improved following the flow sheet in (b).

2.2 Channel etch

We will use the above automated methodology to identify the optimal recipe for a channel etch in 3D NAND. For the purposes of this demonstration, the stack will consist of 68 alternating layers of silicon oxide (O) and silicon nitride (N) or 34 layers of ON. The stack is assumed to rest upon a stop layer where it is assumed that no etch occurs. The method can be extended to 64 or 128 ON layers, but 34 layers is chosen for clarity in visualizing results and managing computational time. The initial structure is illustrated in Fig. 2. Due to the symmetry of the channel etch, it is modeled in 2D.

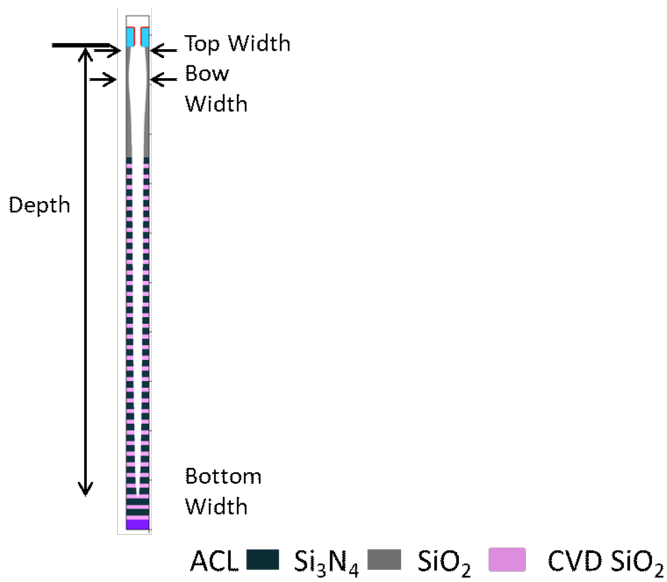

Figure 2. Cross-sectional view of a channel etch in 3D-NAND. Note for this view, the horizontal scale is expanded for clarity. The materials in the stack are resist (black), post-staircase oxide (pink), silicon oxide (light blue), silicon nitride (dark blue), and stop layer (gray).

2.3 Reduced-order models

There are several reduced-order physics-based models to simulate the channel etch. Details on the models have been discussed in detail elsewhere [4-6]. Briefly, the model accounts for fluxes of ions and neutrals from a 1D model of a plasma sheath. The chemical reactions of the plasma with the solids (here silicon oxide and silicon nitride) are also accounted for. Given the etch rate on the surface, the etch profile is evolved using the level-set method. Previous work has shown that the reduced order model and the profile evolution match experimental measurements well [4-6].

For the model selected by the model build step, we consider six process parameters, which consist of two gas flow rates G_1 and G_2 (a CxFy and Ar), and pressure, power, bias, and temperature (Table 1). All but time are normalized from 0 to 1, representing their minimum and maximum values.

Table 1. Process parameters and their ranges. Note that the gas flow rates G_1 and G_2 and pressure, power, bias, and temperature are normalized so that their minimum and maximum values range from 0 to 1. Later in the Quilt™ plots these parameters are assigned the variables P_1, P_2, …, P_6.

	G_1 (P_1)	G_2 (P_2)	Pressure (P) (P_3)	Power (PW) (P_4)	Bias (B) (P_5)	Temperature (T) (P_6)
Min	0	0	0	0	0	0
Max	1	1	1	1	1	1

Here experimental data (i.e., the etched profiles and measured CDs) are generated synthetically. We assume a set of parameters for the model embodying the etch rates and chemistry of the plasma. We then run the simulation using different process conditions taken from the ranges listed in Table 1. Gaussian noise with a standard deviation of ± 3 nm is added to the measured CDs from the synthetic etch profiles to simulate measurement and other errors. These noisy measurements constitute the experimental measurements for calibrating the model.

2.4 Critical dimensions for etch optimization

There are several critical dimensions for the trench etch. These are measures of the bow width, the widths of the etches at the top and bottom, and the depth of the trench. These critical dimensions are illustrated in Fig. 2. The target values of the critical dimensions are listed in Table 2.

To efficiently explore the process space using the calibrated, reduced-order physical model, a machine learning model is built. The machine learning model is trained using the physical model. The physical model is necessary for calibration, but even in its reduced form, simulations for a single process condition can takes a considerable amount of time. The machine learning model allows the user to quickly explore a range of process conditions and resulting outputs in the matter of a few minutes as opposed to tens of days with the physical model.

Table 2. Target values of the critical dimensions for the channel etch as illustrated in Fig. 2.

Critical Dimension	**Target Value (nm)**
Bow width (Bow)	60±15
Bottom width (BW)	60±15
Top width (TW)	60±15
Depth (D)	>2800

3. SYNTHETIC EXPERIMENTAL RESULTS

Typical etch profiles from the synthetic experiments are illustrated in Fig. 3. Common issues with the channel etch include bow formation (left panel), clogging of the mask when there is too much deposition (middle panel), and over-etching of the channel (right panel) which can occur when attempting to mitigate strong tapers and/or narrow bottom widths.

A summary of the target CDs of depth, bow width, top width and bottom width from the synthetic experiments is shown in Fig. 4. Of course, the values differ from experiment to experiment because of the varying process parameters. The green blocks delineate the ranges of the target CDs. Note there is no experiment where all four CD targets are met. The goal is to identify a set of process conditions that achieve all the target CDs using the automated steps described below.

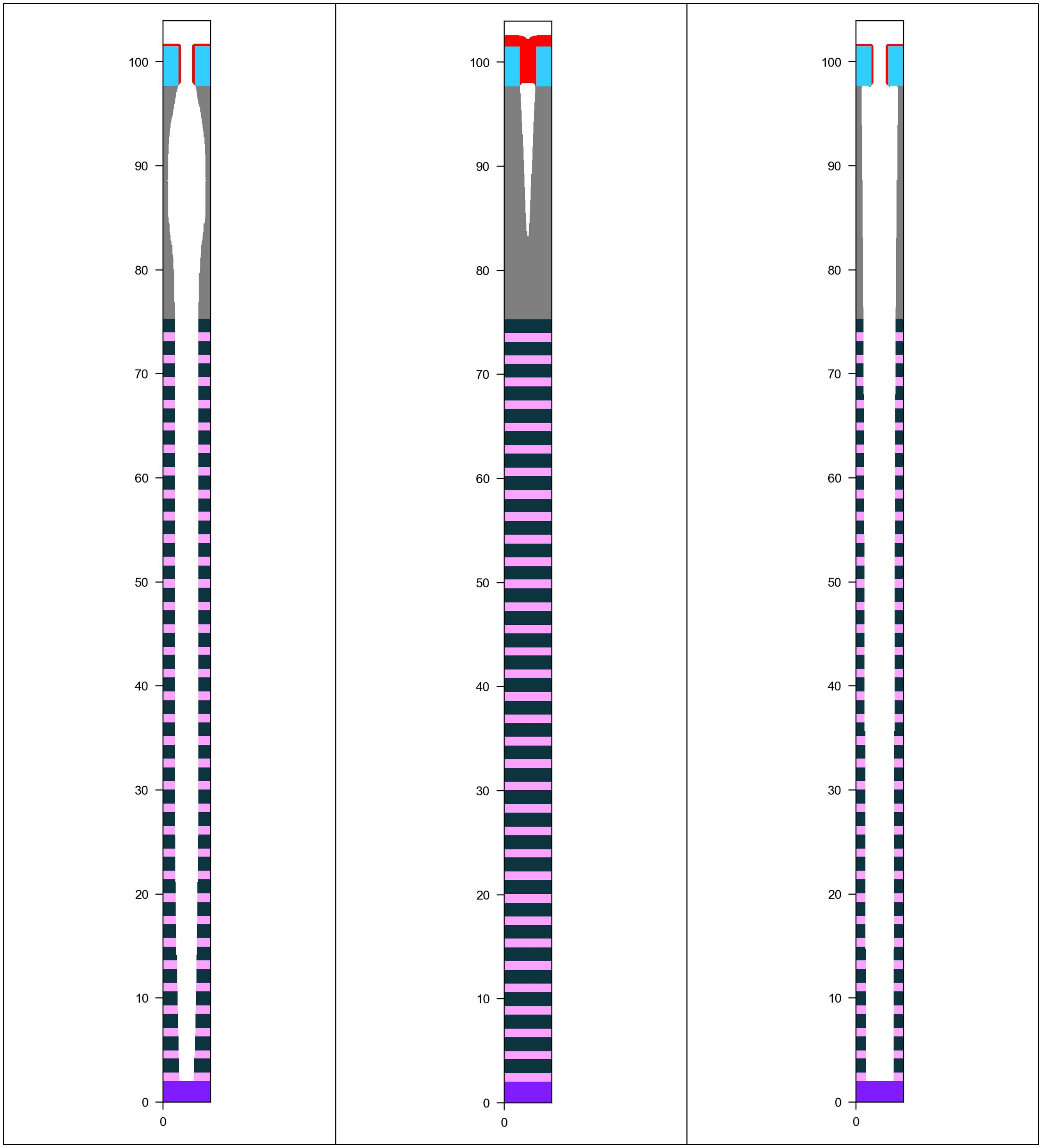

Figure 3. Examples of synthetic experimental data of trench etch: (l*eft panel*) Excessive bow width. (*middle panel*) Clogging of the mask, Over-etch of top, mid, and bow width (right panel).

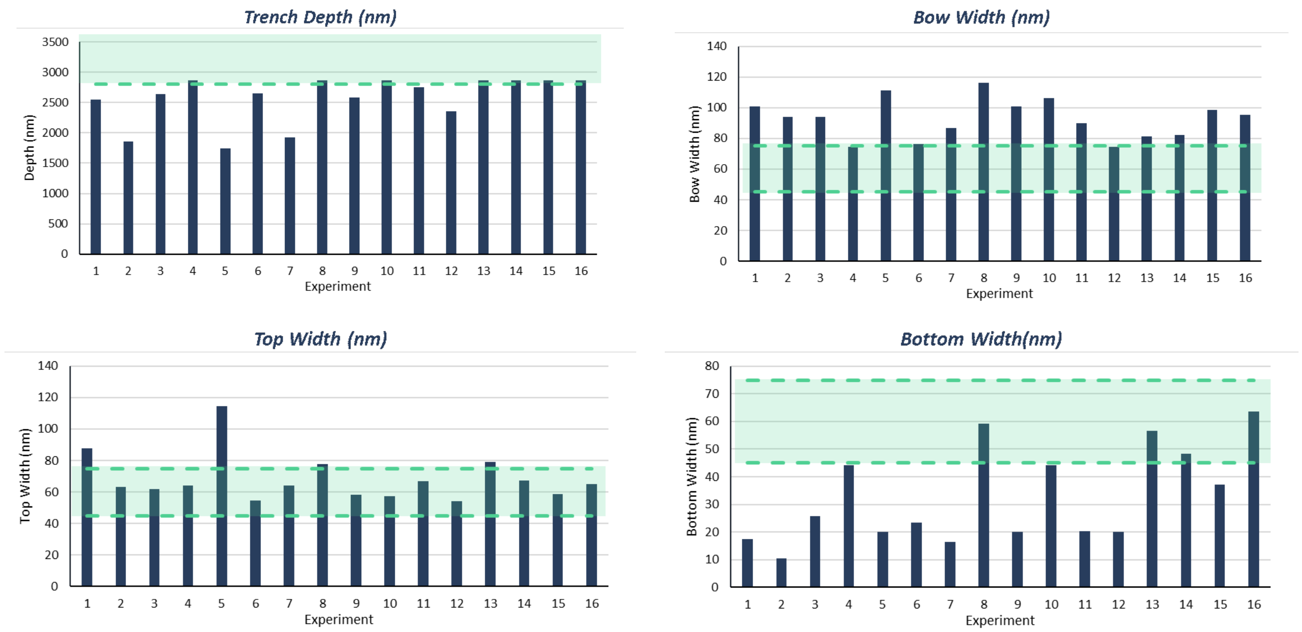

Figure 4. Synthetic experimental results for the depth, bow width, top width, bow width. The green blocks delineate the ranges of the target CDs.

4. AUTOMATED IDENTIFICATION OF ETCH RECIPE

4.1 Automated model build

The first step is the model build. Here the process engineer provides the initial stack to be etched (Fig. 5) and the etch profiles of the 16 synthetic experiments in this example. SandBox Studio™ AI then uses this information in a pre-analysis of the many reduced-order physics-based models available and predicts their probability of being the best model. Such a ranked table is illustrated in Fig. 5. The top ranked model is predicted to have a 75% probability of being the best model for the available data. The next closest model has a probability of 24% and the remaining models have probabilities of less than 1% each of being correct. The automation then selects the first model for calibration.

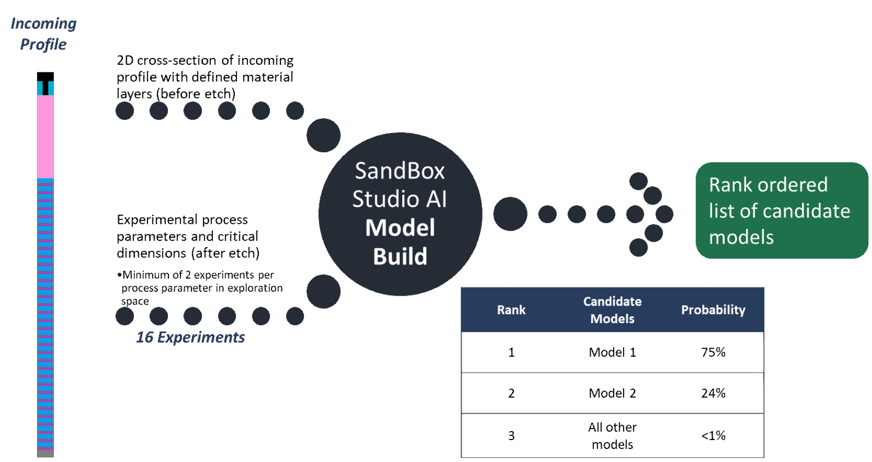

Figure 5. Schematic of the automated model build. In the diagram is a table of the rankings of each potential model in order of the probability it is correct.

4.2 Automated model calibration

Once the model has been selected, the model is calibrated to best fit the experimental etch profiles. Fig. 6 illustrates a couple of examples of the etch profiles predicted by the calibrated model compared to the synthetic experiments. The qualitative agreement is obviously good. The goodness of the fit is quantitatively presented in Fig. 7, which are parity plots of the predicted depth, bow width, top width, and bottom width versus the experimental measurements. The agreement is excellent.

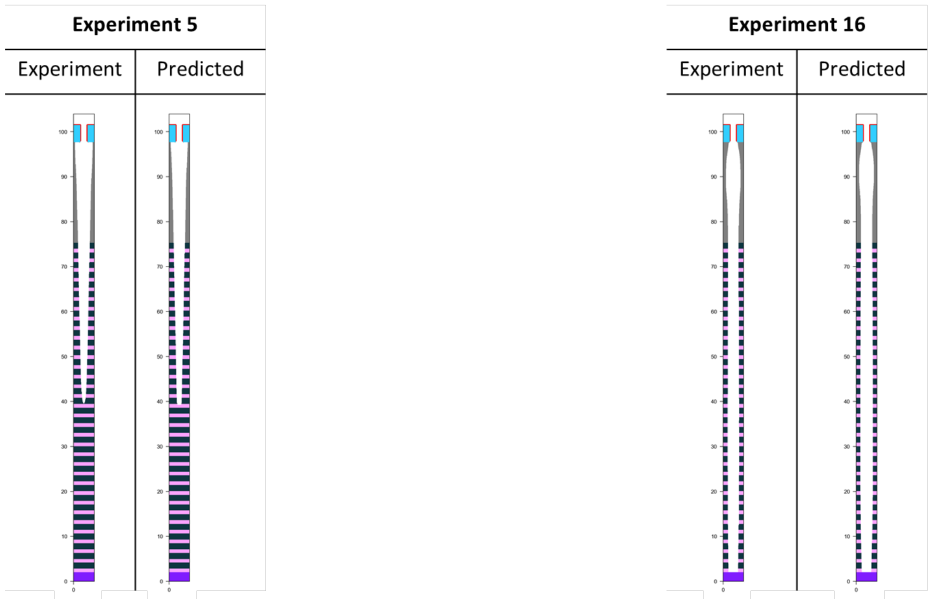

Figure 6. Example images of the experimental and predicted etch profiles for experiments 5 and 16 illustrating the accuracy of the calibrated model.

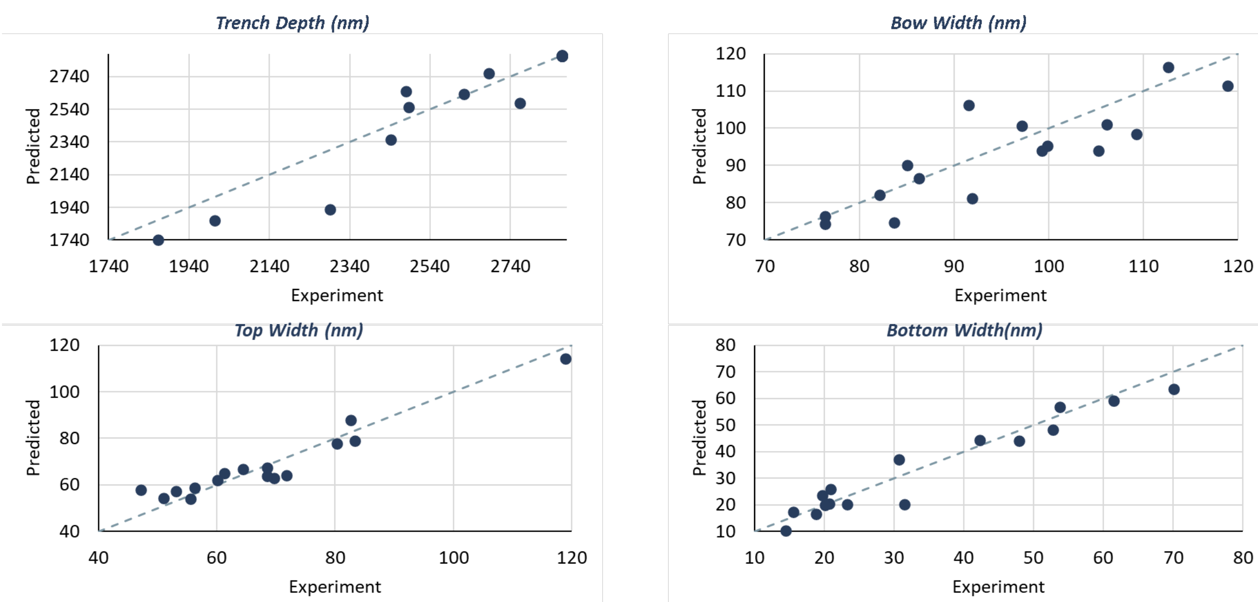

Figure 7. Parity plots of the predicted target CDs from the calibrated model versus the experimental values of the target CDs.

4.3 Automation of AI model

One could use the calibrated physics-based model to explore the six-dimensional process parameter space to identify the process windows to achieve the target CDs. However, these simulations are very time consuming. Instead, an AI model is automatically trained based on the physics-based model. Parity plots of the predicted depth, bow width, top width, and bottom width from the AI model versus the training and test data from the physics-based model are shown in Fig. 8. The bow width is overpredicted at its lowest value, and there is a cluster of underpredictions of the bottom width at its larger values. The prediction of the depth and top width are near perfect. Overall, the agreement is excellent.

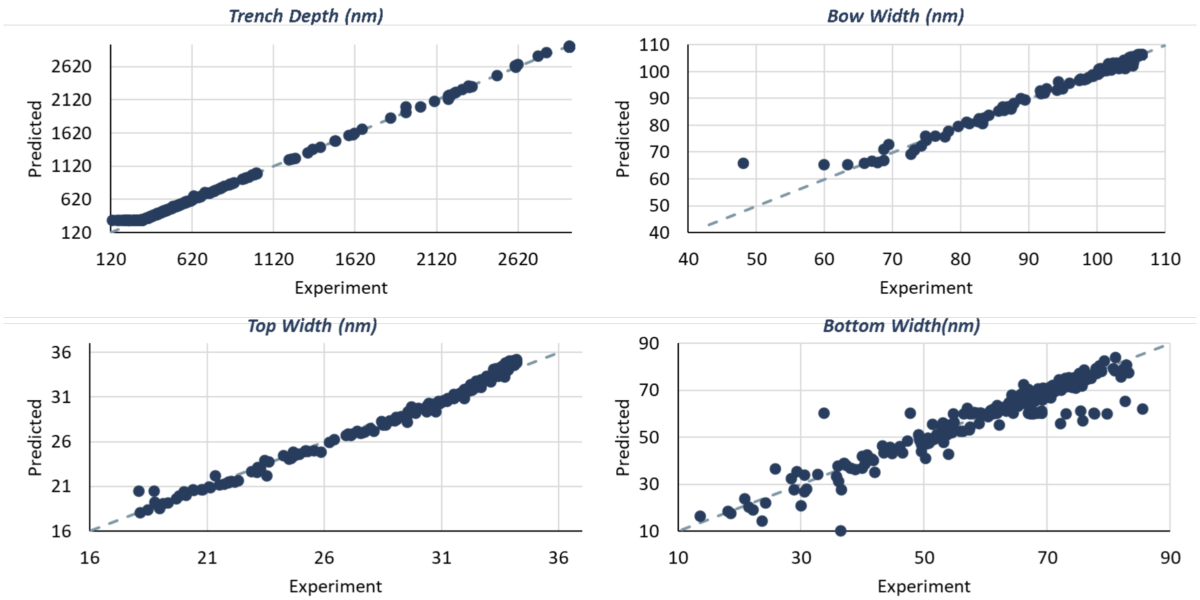

Figure 8. Parity plots of the predicted target CDs from the AI model versus experimental values generated from the calibrated model.

4.4 Visualization of multidimensional process parameter space

With the calibrated model the process parameters of G1 and G2 flow rates, pressure, power, bias, and temperature can be explored. For example, one can probe any of the critical dimensions (top, bow, and bottom width and etch depth) as a function of the six process parameters. For a given critical dimension, the six-dimensional space can be conveniently flattened in the form of the patent-pending Quilt™ process map generated using the SandBox Studio™ software tool.

The variation of the bow width as a function of process parameters is shown in Fig. 9. This type of figure provides a convenient way for the etch engineer to visualize the available process space. Moderate to high pressures and low to moderate times favor achieving the target bow width CD. The target bow CD is quickly identified as the blue regions. The bow CD can be minimized at low P2 and high P4.

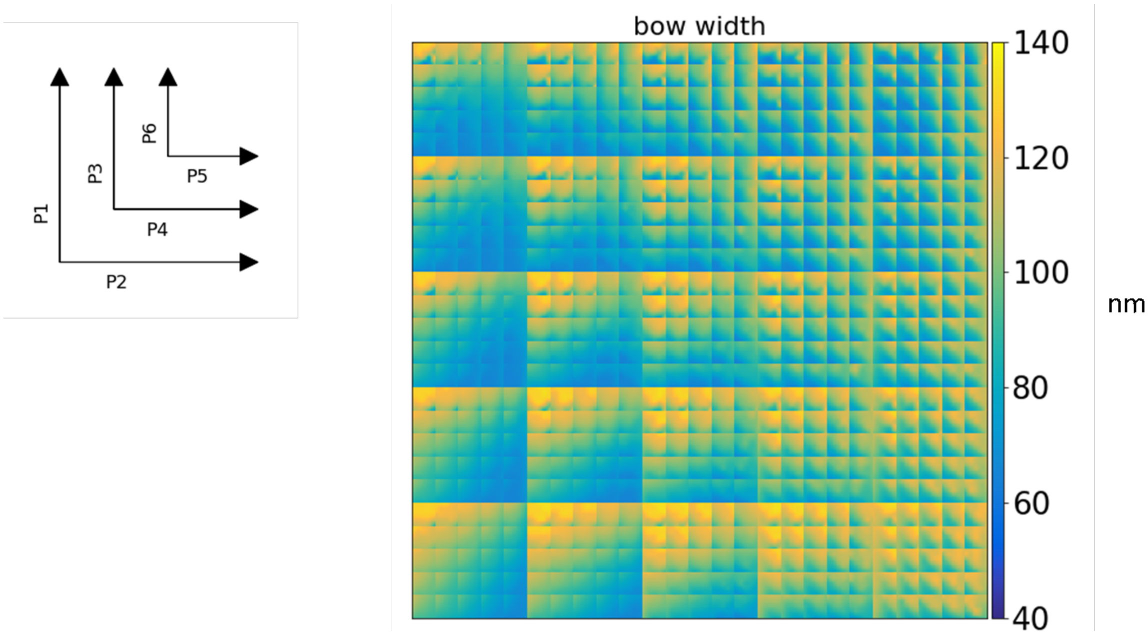

Figure 9. Quilt™ plot for the bow width generated by the AI model.

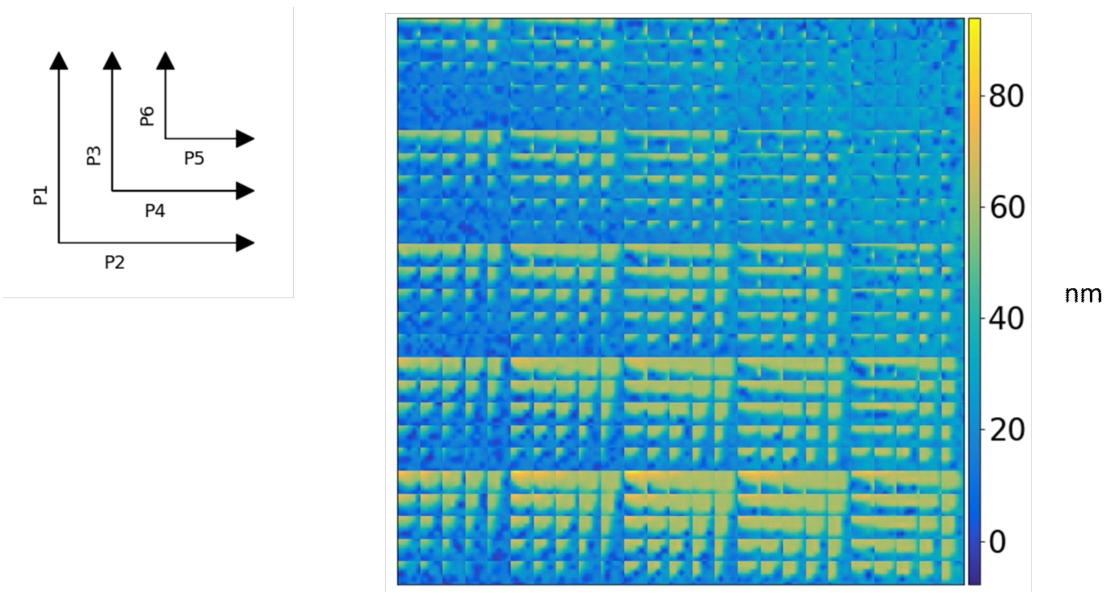

Figure 10. Quilt™ plot for the bottom width generated by the AI model.

Fig. 10 presents the Quilt™ for the bottom width. Here the target bottom width is achieved at low P1 and high P3. Comparing Figs. 9 and 10, it is apparent that there are conflicting trends that will narrow the process window. Of course, a Quilt™ for each of the critical dimensions can be constructed. In the next section the synthesis of all of these is discussed to identify the process window and optimal etch recipe.

4.5 Optimal etch recipe

If we require all the target CDs to be satisfied, we can construct a pass-fail Quilt™. This is illustrated in Fig. 11, where green indicates the process windows where the all the target CDs are achieved. The largest volume pass region is a small area encircled by the white box. Considering its size, the identification of this process window would be extremely challenging with experimentation alone. The resulting experimental profile at the optimal process conditions is shown on the right. The produced trench is highly uniform with a minimal bow and taper.

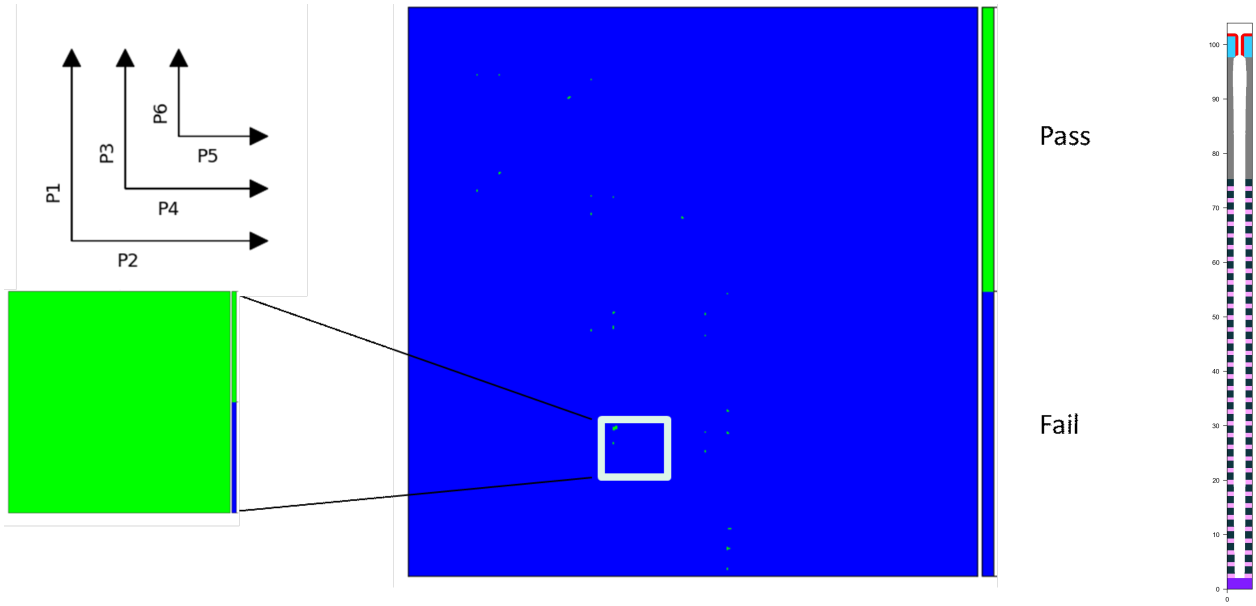

Figure 11. Pass-fail Quilt™ for all the target CDs after model calibration with 16 experiments. The green regions of moderate pressure and long times determine the predicted operating windows for a successful etch. The resulting experimental profile (right) shows a uniform channel.

The process parameters for the optimal process window are listed in Table 3. Table 4 shows quantitatively that all the targeted etch CDs are achieved. This underscores the value of a model as tool to organize and leverage precious experimental data to identify where best to conduct the next experiments. In a traditional 2 level full factorial design, 2^6 or 64 experiments would have been performed just to characterize the process space. Here, an optimal recipe is found with just 17 experiments—nearly a 4X improvement in time and materials required for the recipe's development.

Table 3. Range of process parameters of the largest process window from the pass-fail Quilt™ in Fig. 11.

	Min	**Optimal Point**	**Max**
P1	0.04	0.25	0.26
P2	0.24	0.25	0.26
P3	0.24	0.25	0.26
P4	0.99	1.00	1.00
P5	0.00	0.00	0.01
P6	0.45	0.46	0.47

Table 4. Twenty-six targets and predicted CDs, all of which meet the pass criteria using the recipe predicted by the largest process window of the pass-fail Quilt™.

Critical Dimension	**Target Value (nm)**	**Experimental Value (nm)**	**PASS/FAIL**
Bow width	60 ± 15	74	PASS
Bottom width	60 ± 15	54	PASS
Top width	60 ± 15	63	PASS
Depth	>2800	2869	PASS

5. CONCLUDING REMARKS

We have successfully demonstrated the automated development of an etch model for a 3D NAND channel etch using SandBox Studio™ AI. The automated steps include identifying a candidate model with 75% probability of success, calibrating the model with high accuracy, and determining the optimal process parameters by efficient search of the six-dimensional parameter space. The first recommended recipe from SandBox Studio™ AI met all target criteria. All the SandBox Studio™ AI steps were self-contained and completely automated requiring the process engineer to only enter the initial stack to be etched and the etch profiles from the experiments. Automated model development using SandBox Studio™ AI eliminates many of the obstacles facing model-driven manufacturing optimization. For this specific example with a computer with six nodes, all the automated steps were completed in three days. This computational time investment is competitive with the weeks and months often take for solely empirical etch recipe development.

ACKNOWLEDGMENTS

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