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A Model-Based, Bayesian Approach to the CF4/Ar Etch of SiO2

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ABSTRACT

The design and optimization of highly nonlinear and complex processes like plasma etching is challenging and time-consuming. Significant effort has been devoted to creating plasma profile simulators to facilitate the development of etch recipes. Nevertheless, these simulators are often difficult to use in practice due to the large number of unknown parameters in the plasma discharge and surface kinetics of the etch material, the dependency of the etch rate on the evolving front profile, and the disparate length scales of the system. Here, we expand on the development of a previously published, data informed, Bayesian approach embodied in the platform RODEo (**R**ecipe **O**ptimization for **D**eposition and **E**tching). RODEo is used to predict etch rates and etch profiles over a range of powers, pressures, gas flow rates, and gas mixing ratios of an CF_4/Ar gas chemistry. Three examples are shown: (1) etch rate predictions of an unknown material "X" using simulated experiments for a CF_4/Ar chemistry, (2) etch rate predictions of SiO_2 in a Plasma-Therm 790 RIE reactor for a CF_4/Ar chemistry, and (3) profile prediction using level set methods.

Keywords: etching, design of experiment, plasma, prediction

1. INTRODUCTION

Increasing device integration and the ever-growing consumer demand for faster processors and larger memory storage are driving a growing need for bleeding-edge nanomanufacturing processes. Moore's law, or the idea that the number of transistors per chip doubles every two years, has so far been sustained by increasing the number of processing steps for double masking and etching (Figure 1).

This steadily growing demand is paralleled by the climbing difficulty of creating the complex architectures required by next-generation devices. It is becoming more and more arduous to baseline and optimize a single process recipe. In fact, some recipes are so challenging that they can take up to two years to develop, or worse, are never put into production.

For plasma processing steps, process optimization is especially challenging. Problems with selectivity, aspect ratio dependent effects, and critical dimension uniformity are all exacerbated with increasing architectural complexity. Computational modeling of the plasma and the etched surface has the potential to inexpensively and rapidly determine optimal etch process conditions for a wide range of materials, pattern layouts and plasma systems. However, etch rates and etch profiles are difficult to predict using conventional techniques. Currently, plasma recipes can have up to ten different gas chemistries meaning hundreds of reactions can take place in a single process in parallel. Adding to the complexity, plasma reactors are multiscale, operating at the length scales of the reaction chamber, wafer, die, and feature. Variations in the concentration of the species across each of these length scales and coupling the species transport processes makes it difficult and computationally expensive to predict molecular fluxes within reasonable timescales for process development in the fab. In addition, most industrial plasma systems exhibit non-Maxwellian behavior making it a challenge to determine the velocity distributions of the incoming plasma species to the wafer's surface. Finally, there is a significant lack of knowledge of the plasma parameters. These problems are compounded as technology nodes get smaller and new materials and device structures are explored making it extremely difficult to create and optimize new recipes.

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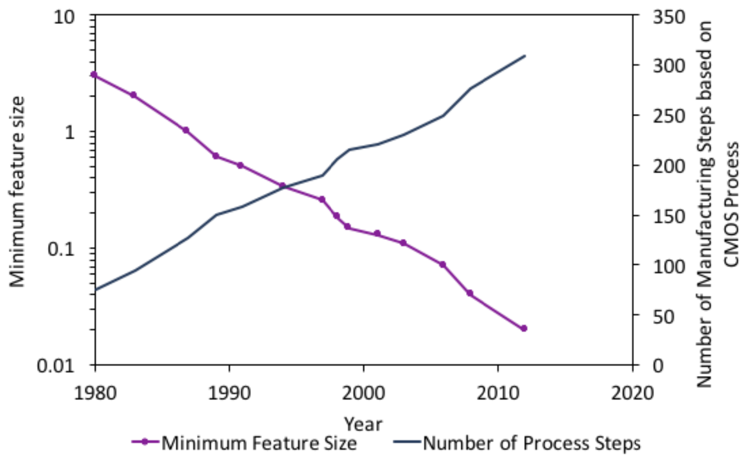

Figure 1. Growth in Number of Manufacturing Steps Required for CMOS Process[1]

1.1 Current Tools

Three distinct approaches are used today in the semiconductor industry and in academia for plasma process development: atomistic and continuum plasma-surface simulations, statistical design of experiment (DOE), the empirical iteration based on the process engineers experience (hereafter referred to as "tribal knowledge"). Each approach offers clear tradeoffs in terms of the performance of the tool at predicting etch profiles, visualization capabilities, and ease of use.

Atomistic and Continuum Plasma-Surface Simulations

Sophisticated molecular and continuum-based models already exist for plasma and surface kinetic processes.[2-6] These models can be very accurate for predicting etch profiles, but are often difficult to use in practice. Most atomistic modeling tools require significant modeling expertise and are computationally expensive. Continuum-based models have the advantage of being computationally faster, but typically lack the accuracy of more sophisticated modeling systems. For process engineers developing etch recipes, a chief barrier for the use of physics-based models is the large number of unknown or difficult to measure system and material parameters.[7, 8] Kinetic and material properties like reaction rates and sputtering yields are often unknown, difficult to measure, and have conflicting ranges as reported in literature.

Statistical Approach

In addition to physics-based models, purely statistical models formulated using design of experiment schema are possible. In this data-driven approach, regressions and surface response analyses can be used to screen for process parameter interactions. Because plasma etching and deposition are highly nonlinear processes, it is difficult to explore an entire parameter space with full factorial or fractional factorial experimental designs. Hundreds of experiments are performed while designing the process, or alternatively experiments are performed within narrow parameter windows where each parameter is assumed to be linearly independent. This assumption can lead to non-optimal process windows. Disadvantageously, statistical models are frequently limited to one use-case and cannot be applied to a new process.

Tribal Approach

Because of the stringent time demands on process development cycles, in practice most process engineers employ a "tribal approach" rather than rely on a simulation tool or long design of experiment cycle. They first start with a baseline guess of where the process should be based on their prior experience developing recipes. Then, in a usually trial and error manner, qualitative relationships based on user experience are used to adjust etch process conditions, such as pressure, power, voltage bias and chemical composition of the etch gas. In today's development flow, process engineers pick the appropriate process parameters based on their experience. They then conduct experiments and the requisite metrology to evaluate the parameters they picked. Based on these results, the process engineer iterates on the process parameters (usually one variable at a time), repeating experiments and metrology until the process metrics are met. As a result, expensive and time-consuming experiments must be conducted to determine the etch recipe.

2. METHODS

2.1 Approach

Prior research has demonstrated the success of Bayesian probability theory to estimate model parameters more precisely and to reduce the number of required experiments in a variety of fields. Examples include identifying biochemical pathways[9, 10], defining a system's chemical kinetics[11], and prediction of material properties[12], where Bayesian probability theory was used to infer unknown parameters or for model selection. Here, Bayesian probability theory is employed to rapidly calibrate existing process models using data analytics and "tribal knowledge" with the platform **R**ecipe **O**ptimization for **D**eposition and **E**tching, or "RODEo."

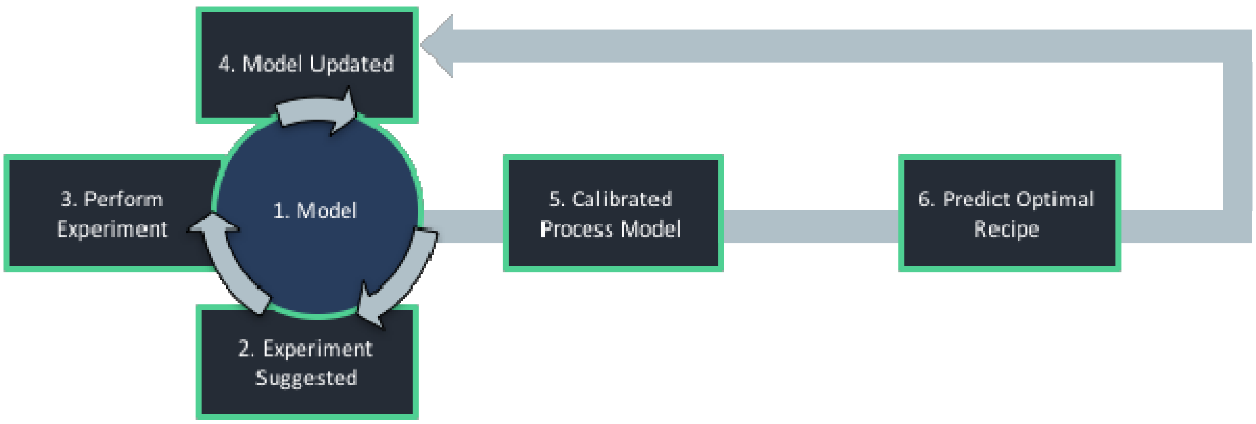

Figure 2. Schematic of the model-based Bayesian approach used in RODEo: (1) a model is inserted into engine's process module, (2) the engine suggests an experiment, (3) one or more experiments are performed, (4) the model is updated based on results of experiment, (5) the experimental cycle is completed and model is calibrated, and (6) the optimal recipe is predicted using calibrated process model.

RODEo employs Bayesian statistics and experimental data to rapidly optimize parameters for a given model and accurately predict operating conditions based on the specified process objective. RODEo first starts with a candidate model. It then selects an experiment for the engineer to perform. Once the experiment is performed, RODEo updates the input model. This approach is advantageous because it minimizes the number of calibration cycles required for the model and accommodates general probabilistic relationships among experimental outputs, model parameters, and design conditions.

RODEo has already been demonstrated on etch systems for pure O_2 and pure Ar etching systems.[13] In this study, we demonstrate RODEo's performance for the predictions of etch rates and etch profiles for a CF_4/Ar based plasma system. The following sections expand upon the models that are used as inputs into the RODEo platform.

2.2 Global Plasma Model

To model the gas chemistry, a steady state global (0-dimensional) plasma model with volume averaged plasma parameters was implemented using known reaction sets from literature[2]. Global plasma models from a variety of plasma sources have been covered significantly (including those for CF_4/Ar chemistries).[2, 3, 6, 14-20] The global plasma model is described by two principal sets of equations: a power balance and a particle balance of all species of interest.[2] It is assumed that the negative ion density vanishes at the sheath, and that the temperatures of the positive and negative ions are equal to the neutral gas temperature.[5, 6] For the CF_4/Ar plasma chemistry, the reactions in Table 1 were considered. Rate constants in the RODEo database were determined by (1) mining all reported rate equations from literature, (2) filtering out all outliers, and (3) fitting the remaining rate equations.[21]

Using the reaction set defined in Table 1, differential equations of the particle balance were defined. The differential equation of the power balance can be written as:

$$\frac{d}{dt}(en_{e0}Te) = \frac{P_{abs}}{V} - \left(eE_{C_{Ar}}K_1 n_{Ar} + eeE_{C_{CF_3}}K_1 n_{CF_3}\right) - e\left(E_e + E_{i_{Ar^+}}\right)\nu_{Ar^+}n_{Ar^+} - e\left(E_e + E_{i_{CF_3^+}}\right)\nu_{CF_3^+}n_{CF_3^+}, \quad (1)$$

where E_C represents the collisional energy losses per electron ion pair and $(E_e + E_i)$ is the energy lost to the wall per electron-ion pair. Here ν denotes the wall loss rate of positive ions such that

$$\nu = h_l u_{B,i} A/V, \quad (2)$$

where the Bohm velocity $u_{B,i}$ is calculated as $u_{B,i} = (eT_e/M_i)^{1/2}$, and h_l is the wall loss factor. Further details on the power balance and calculation of the wall loss factors can be found in literature.[2-4] Using specified fixed inputs for the plasma reactor's discharge length and diameter, the absorbed power, pressure, feed gas composition, reaction rate coefficients, and surface recombination constants, the system of equations is solved to determine species densities and electron temperatures. These results are fed as input into the plasma surface kinetics model which then outputs etch rates and the initial velocity field for the front profile propagation using level set methods.

Table 1. Set of Reactions for CF_4/Ar Global Plasma Model

N	Reaction
1	$e + Ar \rightarrow Ar^+ + 2e$
2	$e + CF_4 \rightarrow CF_3^+ + F + 2e$
3	$e + CF_3 \rightarrow CF_3^+ + 2e$
4	$e + CF_4 \rightarrow F^- + CF_3$
5	$e + CF_4 \rightarrow CF_3 + F + e$
6	$e + CF_3 \rightarrow CF_2 + F + e$
7	$CF_3^+ + F^- \rightarrow CF_3 + F$
8	$F^- + Ar^+ \rightarrow F + Ar$
9	$F + wall \rightarrow 0.5CF_4$
10	$CF_3 + wall \rightarrow 0.5CF_4$

2.3 Surface Kinetics Model of CF_4/Ar System

A Langmuir surface kinetics model was used to predict vertical and lateral etch rates. In the Langmuir model the surface of the substrate is composed of bare sites where the neutrals adsorb and sites occupied by neutrals on which bombarding ions activate chemical reactions. The etch rate, *ER*, is a function of chemical etching and physical sputtering,[15]

$$ER = (1-\theta)\gamma S\Gamma_C + (1-\theta)Y\Gamma_p, \quad (3)$$

where γ is the probability of the chemical reaction, Γ_C is the flux of the reacting species, *S* is the sticking probability, θ is the fraction of the surface covered by reaction products, *Y* is the sputtering yield, and Γ_p is the flux of the sputtering species. The plasma was assumed to be at steady state such that $\frac{d\theta}{dt} = 0$. The percentage of active sites on the surface are then balanced as

$$(1-\theta)\gamma S\Gamma_C = \theta \sum Y_{d,j}\,\Gamma_{+,j}, \quad (4)$$

where $Y_{d,j}$ and $\Gamma_{+,j}$, are the partial yields of ion-stimulated desorption and partial fluxes for the different positive ion species at the surface of the substrate.

$$Y_S = B(E^{\frac{1}{2}} - E_{0,s}^{\frac{1}{2}}) \quad (5)$$

$$Y_d = C(E^{\frac{1}{2}} - E_{0,d}^{\frac{1}{2}}) \quad (6)$$

The sputtering yield and ion stimulated desorption are functions of the square root of the ion energy. The coefficients parameters B and C depend on the type of ion and the sputtered material. E, the incident ion energy in the plasma sheath, is approximated to be 5.2 Te.[18] Material dependent parameters $E_{0,s}$ and $E_{0,d}$ are the threshold energies for sputtering and ion-stimulated desorption. Note that this surface kinetics model does not include any etch product redeposition that may be occurring by the fluorocarbon.

2.4 Profile Simulation

Level set methods were used to track motion of the interface for the etch profile simulation. In level set profile propagation, the velocity field is defined by position, time, the geometry of the interface, and the etch physics (as determined by the global plasma and surface kinetics models). The interface is represented by the zero-level set of a higher-dimensional function φ (r, t), that is φ (r, t) =0. The motion is then determined by convecting the φ(r,t) values with the normal velocity field defined by the etch rate in the surface kinetics model,[22]

$$\frac{\partial \varphi}{\partial t} + \boldsymbol{v} \cdot \nabla \varphi = 0 \tag{7}$$

Visibility of the plasma source to the etched surface was incorporated in the level set profile predictions. In order to take into account aspect ratio dependent effects based on the computed etch velocity at the surface, it was assumed that the velocity decayed normally across the surface such that

$$V_y(x, y) = V_{y0} \exp(\Delta y^2) \exp\left(\frac{5\Delta x^2}{2}\right) \tag{8}$$

where Δy and Δx are the distance of a point's coordinates from the origin of the grid.

2.5 Experiments

Experiments were performed on a Plasma-Therm 790 RIE etcher. The process space considered in all of the following examples was set by the etcher's tolerance windows. These process windows are summarized in Table 2.

Table 2. Process Window Considered on Plasma-Therm 790 Etcher

	Minimum	**Maximum**
Power (W)	50	200
Pressure (mTorr)	10	1000
Flow Rate (sccm)	14	50
Fraction of CF_4	0	1

The etch rate experiments (Example 2) were performed on a thermal oxide grown on silicon. Etch rates were measured using ellipsometry. For the pattern transfer experiments (Example 3 in the Results section), imprints were made with an Imprio®1-1100 machine using a monomat resist material on top of the thermal oxide. The imprinted resists were made up of line-space patterns with a 130-nm pitch. To perform the transfers, an Ar/O_2 etch was first used to remove the residual layer of the imprinted material and expose the underlying substrate. The CF_4/Ar etch recipes were then run at the specified process conditions for three minutes. Lastly, etch profiles were characterized on a ZEISS Neon 40 SEM. Cross-sectional SEM images were taken at 200KX and 5kV.

2.6 Validation Methodology

For the following examples, the performance of the calibrated RODEo model after a sequential experimental design was evaluated against a 3rd degree ordinary least squares regression model calibrated using two-level full-factorial design of experiment, hereafter referred to as the 2LFFD model. In a 2LFFD design of experiment, all input levels are set at two levels each (a high level and a low level) such that 2^n experiments are performed, where n is the number of process parameters available. For the CF_4/Ar system considered here n = 4 (power, pressure, total flow rate, and fraction of CF_4 in the mixture), and so 16 experiments were performed in total at the min and max process ranges specified in Table 2.

In a least squares regression, a model of the form

$$y = f(x, \beta) \tag{8}$$

is fitted to the data where β is vector of j adjustable parameters, x represents the process parameters, and y is the predicted model output. The least squares regression seeks minimize the sum S of the squared residuals,

$$S = \sum_{i=1}^{n} r_i^2 \tag{9}$$

where the residual r is defined as

$$r_i = y_i - f(x_i, \beta) \tag{10}$$

The performance of the calibrated RODEo model was assessed using two metrics: the number of experiments required to achieve a smaller square error S that is benchmarked by the 2LLFD model and the accuracy of the mapped predicted process trends.

3. RESULTS

3.1 Example 1. Etch Rate Predictions of an Unknown Material "X" Using Simulated Experiments for a CF_4/Ar Chemistry

The performance of RODEo was first evaluated synthetically using simulated experimental or "synthetic" data for etch rate predictions across the 4-dimensional process design space. To generate the synthetic data, etch rates were simulated by assigning arbitrary values to the unknown parameters in the global plasma and Langmuir surface kinetics models described in the methods section. To more closely simulate an experimental environment, the data was made noisy by adding a normally distributed error, $N(0,4)$, to the simulated etch rate. These simulated etch rates were obtained for the entire design space for a total of 6,468 process experiments. After the synthetic data was generated, the RODEo models were then reset, and a sequential experimental design was performed to calibrate the RODEo engine. A 2LFFD was constructed for comparison using the simulated data (a total of 16 calibration experiments).

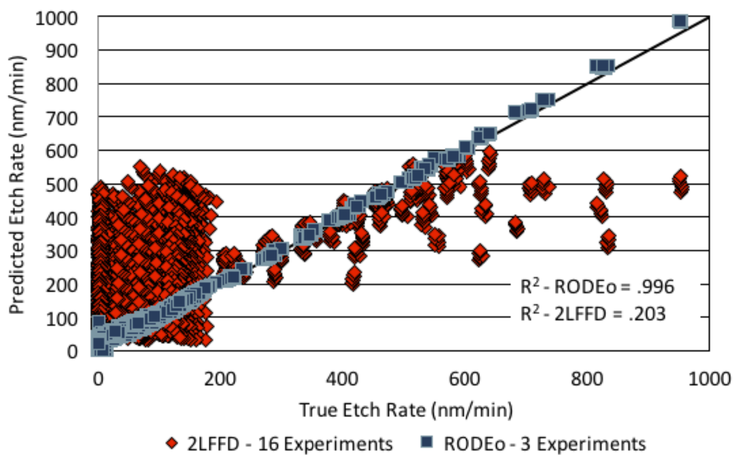

Figure 3. Comparison of etch rate predictions using RODEo after three calibration experiments versus a least square regression based on the 2LFFD model (16 experiments).

RODEo was able to accurately predict etch rates across the entire four-dimensional process space using three experiments. The 2LFFD model captured some of the trends in the etch rates but failed to capture many of the non-linear relationships in the process space. The relative process maps at a pressure of 10 mTorr and total flow rate 50 sccm are shown in Figure 3. As evidenced by the contour lines, RODEo is able to map the high etch rate regions versus the low rate regions while the 2LFFD over predicts etch rates in the high power and CF_4 fraction regions. The poor qualitative agreement of the 2LFFD compared to the experiments is due to the highly non-linear nature of the etch process.

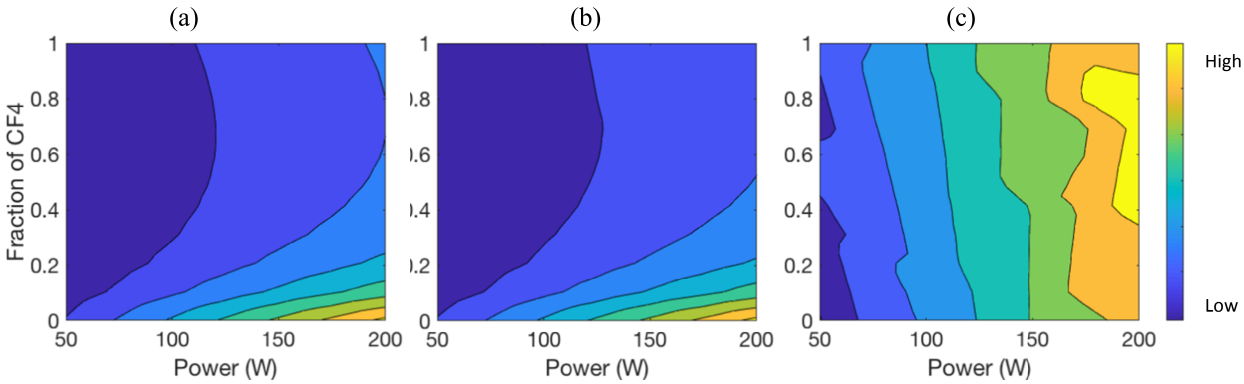

Figure 4. (a) Process map visualization of (a) experimental etch rates (b) etch rates predicted by RODEo, and (c) etch rates predicted by 2LFFD. P = 10 mTorr and Q = 50 sccm.

3.2 Example 2. Etch Rate Predictions of Sio$_2$ in a Plasma-Therm 790 RIE Reactor for a CF_4/Ar Chemistry

RODEo was next used to produce a sequential design of experiment with feedback from experimental etch rates on a blanket SiO_2 wafer. Experiments were performed on the Plasma-Therm 790 etcher and etch rates were characterized using ellipsometry. Again, RODEo's predictions were compared with the 2LFFD model (Figure 5). It is evident that similar to the simulated experiments in Example 2, the 2LFFD model severely over or under predicted etch rates in various regions of the process space while the process trends predicted by RODEo match the experimental data.

Taking a close look at the predicted data for the lower etch rate region, RODEo predicts that no etching will occur (an etch rate of 0 nm/min). This prediction behavior is a byproduct of sputtering and desorption thresholds in the Langmuir surface kinetics model. Because the surface kinetics model did not include any terms for redeposition, it is possible that the RODEo models overestimated these surface kinetics coefficients causing it to under predict these etch rates. Despite this limitation, RODEo still performs far more accurately than the 2LFFD model. After three calibration experiments, RODEo predicts the etch rate with a smaller mean square error than the 2LFFD model calibrated with sixteen experiments (Figure 6) and an R^2 value of 0.627 versus 0.103. The predicted process maps are shown in Figure 7 for fixed pressures and flow rates of 50 mTorr and 50 sccm respectively. RODEo's predicted process map qualitatively matches the experimental process map. As expected, the 2LFFD model does not capture the process trends sufficiently in the mid-range regions of power and CF_4. This inaccuracy is not surprising since the model was calibrated at the high and low levels of the process space.

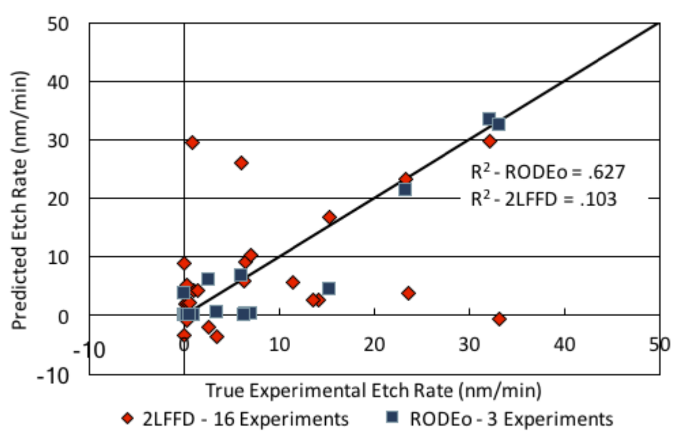

Figure 5. Experimental etch rate versus predicted etch rate for 20 test experiments. The ideal trend is plotted in black. Predictions falling closer to the ideal trend line are more accurate.

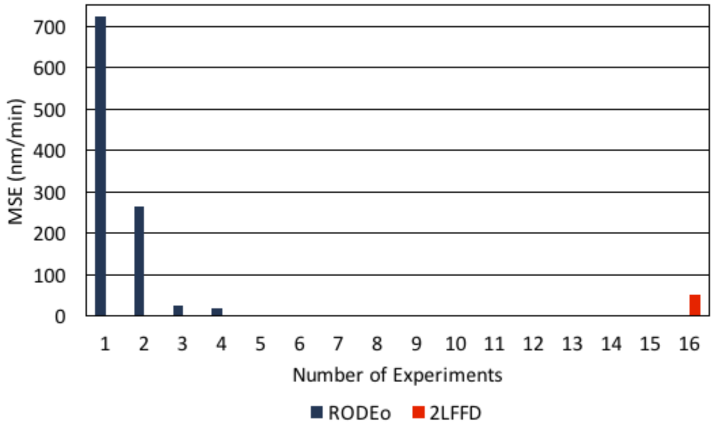

Figure 6. 2LFFD error after 16 experiments is shown in red. RODEo achieves smaller mean square error (MSE) in etch rate prediction after three experiments.

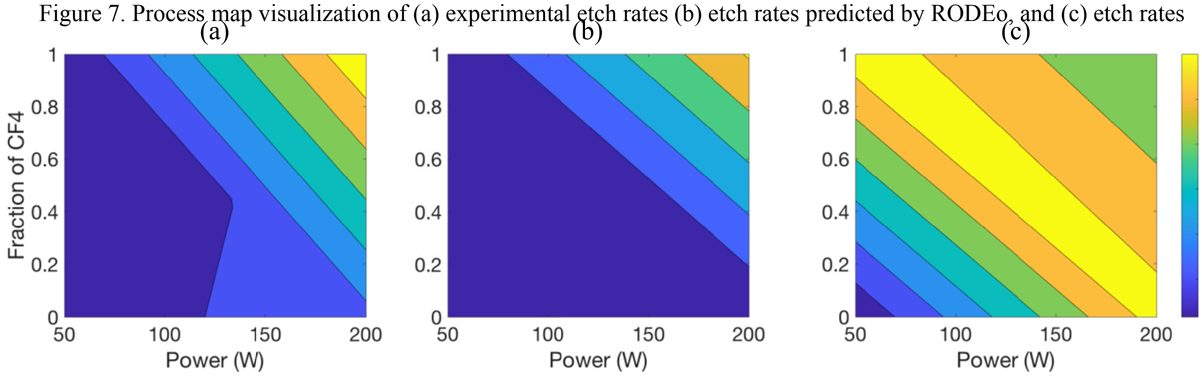

Figure 7. Process map visualization of (a) experimental etch rates (b) etch rates predicted by RODEo, and (c) etch rates predicted by 2LFFD. Pressure and flow rate are fixed at 50 mTorr and 50 sccm, respectively.

3.3 Example 3. Profile Prediction Using Level Set Methods

The calibrated RODEo model from the etch rate predictions in Example 2 was used to predict the etch profile of SiO_2 using the level set method. A pattern transfer at a pressure of 50 mTorr, power of 200W, CF_4 flow rate of 50 sccm, and CF_4 fraction of 0.8 was performed on line space patterns with a 130-nm pitch. (Figure 8).

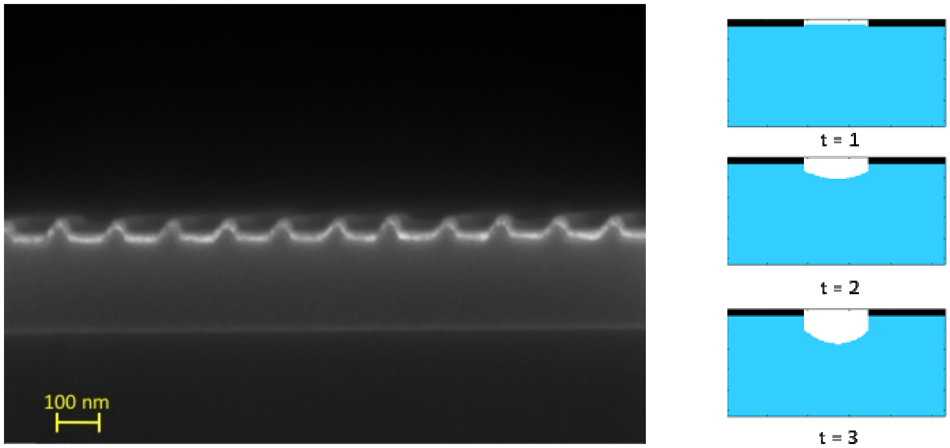

Figure 8. (a) SEM Cross-sectional profile of pattern transfer and (b) Profile predicted by RODEo engine for a pressure of 50 mTorr, power of 200W, flow rate of 50 sccm.

The heights and widths of the experimental versus predicted profiles are compared in Table 3. RODEo is able to qualitatively reproduce the etched profile and predicts the etch width with < 15% error and the etch height with less than 5% error.

Table 3. Comparison of experimental measurements with RODEo predictions.

	Experimental Measurements		RODEo Predictions	
Process Parameters	Width (nm)	Height (nm)	Width (nm)	Height (nm)
Pressure: 50 mTorr Power: 200W Flow Rate CF_4: 50 sccm	69.6	39.1	60.4	32.8

4. SUMMARY

A simplified global plasma and surface kinetics models is incorporated into the RODEo platform to map out multi-dimensional process spaces for CF_4/Ar plasma etch systems. RODEo's etch rate predictions are compared with the predictions of least squares regression models calibrated using a two-level full-factorial design of experiments. It is demonstrated that RODEo can more effectively capture many of the nonlinearities of a plasma system than a 2LLFD model. Lastly, it is shown how RODEo's front profile simulator can be used to predict an etch profile based on the results of the calibrated model.

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