A MODEL-BASED, BAYESIAN APPROACH TO THE CF$_4$/Ar ETCH OF SiO$_2$

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THE PROBLEM

The research, development, and optimization of advanced chemical processes requires significant time and dollar investment.

CHALLENGES FOR ETCH DEVELOPMENT

Expensive and Limited Materials

Costly Equipment Use

Requires High levels of Technical Expertise

Identifying and optimizing process windows for plasma etching severely lengthens time to market by months and sometimes years across industries. Some processes are never even completed.
THE PROBLEM

Process Development and Optimization of Etch Recipes Requires Significant Time and $$$

System Behavior is Very Challenging to Predict
• Large and multidimensional process space
• Nonlinear relationships between process parameters

Current Chemical Process Tools Have Limitations
• Difficult to calibrate models
• Cannot capture tool drifts
• Lengthy simulation times
• Limited empirical models
PLASMA ETCHING PROCESS CONSIDERATIONS

Process Tradeoffs Make Optimization of Parameters Very Difficult

Profile
(Critical Dimensions, Line Edge Roughness, etc.)

(More) By-products
Manage by Chemistry

(More) Radical Flux
High Pressure/Rich

Aspect Ratio Dependent Etching
(Iso-Nested Bias)
Ion Limited

(More) Ion Energy
Manage by Power

Selectivity
Reduced Damage

“Plasma etch challenges for next-generation semiconductor manufacturing,” Rastogi et al, SPIE 2017
Engineer uses tribal knowledge to pick etch process parameters.

Etch experiments are performed.

Etches are characterized. Process metrics met?

Yes

Recipe completed and process data is stored.

No

Process "knobs" are tweaked.
1. A model is inserted into engine’s process module.
2. Engine suggests an experiment.
3. Experiment is performed.
4. Model is updated based on results of experiment.
5. Experimental cycle is completed and model is calibrated.
6. Optimal recipe is predicted using calibrated process model.

This step is modular. Any model can be inserted into it to optimize for a given process objective.
Engineer uses tribal knowledge to pick etch process parameters.

Etch experiments are performed.

Etches are characterized. Process metrics met?

No

Process "knobs" are tweaked.

Produce optimal experiment design for given process space

Yes

Recipe completed and process data is stored.

SandBox Studio helps engineer use stored process data to pick starting etch process parameters.

- Take advantage of past data to pick better starting points
- Minimize number of experiments required

Initial data indicates that SandBox Studio:

- reduces time to develop recipe by 3X
- reduces total recipe development costs by 3X
- increases quality of recipe through high accuracy process windows
**MODEL SYSTEM**

**Reactor dimensions**

**Kinetic parameters**
1. Reaction sets
2. Ion/neutral cross-sections
3. Gas temperature

**Process Parameters**
1. Pressure
2. Flow Rate
3. Power

**Global Plasma Model:**
Mass balances and energy balances for electrons

**Inputs**
1. Fluxes of neutrals and charged species
2. Electron temperature

**Outputs**
- Langmuir surface kinetics model
- Etch rates and etch profile
EVALUATION METHODOLOGY

(1) Define Experimental Goal

- Etch Rate Predictions for Ar/CF₄ system
- 4 process knobs: power, pressure, flow rate, fraction of CF₄
- Substrate Material

(2) Run Process Optimization Cycles

- SandBox Studio Sequential Design
- Regression Model fit with experiments based on a 2 level full factorial design (2LFFD)

(3) Compare results of Process Optimization Cycles

- Visualize predicted process maps.
- Predict etch rates
CALIBRATION CYCLES

Three Examples Are Shown in Order of Increasing Complexity

1. “Synthetic” Calibration and Validation Cycles for Ar/CF$_4$ Etch Rate Predictions

2. Experimental Calibration and Validation Cycles for Ar/CF$_4$ Etch Rate Predictions

3. Profile Predictions Using Level Set methods
EXAMPLE 1. SIMULATED ETCH RATE PREDICTIONS OF SiO₂ IN A PLASMA-THERM 790 RIE REACTOR USING CF₄/Ar
**EXAMPLE 1**

**Methodology**

1. Calibrated SandBox Studio with 3 sequential experiments selected by SandBox Studio.
2. Performed 2LFFD (16 experiments)
3. Evaluated predicted results over entire process space (6,400 synthetic experiments in total).

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<thead>
<tr>
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<th>Minimum</th>
<th>Maximum</th>
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<tbody>
<tr>
<td>Power (W)</td>
<td>50</td>
<td>200</td>
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<tr>
<td>Pressure (mTorr)</td>
<td>10</td>
<td>1000</td>
</tr>
<tr>
<td>Flow Rate (sccm)</td>
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<td>50</td>
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<tr>
<td>Fraction of CF$_4$</td>
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<td>1</td>
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EXAMPLE 1

2LFFD calibrated with 16 experiments while SandBox Studio was calibrated with 3 experiments.

SandBox Studio is 300X more accurate at predicting etch rates.
EXAMPLE 1

Comparison of Predicted Process Maps for etch rates (nm/min) at P=10 mTorr and Flow Rate=50 sccm

SandBox Studio accurately reproduces the process space after 3 calibration experiments.
EXAMPLE 2. EXPERIMENTAL ETCH RATE PREDICTIONS OF $\text{SiO}_2$ IN A PLASMA-THERM 790 RIE REACTOR USING $\text{CF}_4/\text{Ar}$
EXAMPLE 2

Methodology

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1. Calibrated SandBox Studio with 3 sequential experiments selected by SandBox Studio.
2. Performed 2LFFD (16 experiments)
3. Evaluated predicted results over entire process space (20 etch rate experiment total)
EXAMPLE 2

2LFFD calibrated with 16 experiments while SandBox Studio was calibrated with 3 experiments.
Similar to simulated experiments, SandBox Studio accurately reproduces the process space after 3 calibration experiments.
**EXAMPLE 2**

**Number of Calibration Experiments Required**

Sequential design approach minimizes square error in 5X fewer experiments.
EXAMPLE 3. PROFILE PREDICTIONS USING LEVEL SET METHODS
PROFILE PREDICTION USING LEVEL SET METHODS

SandBox Studio Profile Predictions for a Pressure of 50 mTorr, power of 200W, and CF$_4$ flow rate of 50 sccm.

After 3 calibration experiments, SandBox Studio qualitatively reproduces the etched profile at each time step and predicts the etch width with < 15% error and the etch height with less than 5% error.

Cross-sectional SEM Profile at 200KX and 5kV

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<th>SandBox Studio Predictions</th>
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<tr>
<td>Width</td>
<td>69.6</td>
<td>60.4</td>
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<tr>
<td>Height</td>
<td>39.1</td>
<td>32.8</td>
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SandBox Studio Profile Predictions after Each Time Step (min)
SUMMARY

- Combining physical models and Bayesian statistics produces faster model calibration and process optimization.
- SandBox Studio platform calibrates predictive models 5X faster than full factorial designs.
- SandBox Studio captures nonlinearities more effectively than a regression model based on 2LFFD.
- Calibrated SandBox Studio model accurately capture experimental etch profiles.
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