A Cellular Automata Simulation of Atomic Layer Etching

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## Atomic Layer Etching

<table>
<thead>
<tr>
<th>Start</th>
<th>Reaction A</th>
<th>Switch Steps</th>
<th>Reaction B</th>
<th>End/Repeat</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Modification</td>
<td>Self-Limiting</td>
<td>Self-Limiting</td>
<td>Film Removed</td>
</tr>
<tr>
<td></td>
<td>Chlorination</td>
<td></td>
<td>Ion Bombardment</td>
<td></td>
</tr>
</tbody>
</table>

### Generic ALE:

- **Si Surface**

### Example Si ALE:

- **Si Surface**

From Kanarik et al. *JVST A* 2015

## Advantages
- Atomic scale precision
- Selective

## Challenges
- Processing time
- Throughput
Fast Model for Simulating ALE

GOAL: Build a fast, cellular automata or rule based model for fast simulation and optimization of ALE

METHOD
• Build on full plasma and MD simulations of ALE (e.g. Agarwal and Kushner, JVST A 2009; Ranjan et al. JVST A 2016)
• Remove atoms by experimentally and theoretically supported probability based rules

Agarwal & Kushner JVST A 2009
Fast Model for Simulating ALE

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METHOD

• Build on full plasma and MD simulations of ALE (e.g. Agarwal and Kushner, JVST A 2009; Ranjan et al. JVST A 2016)

• Remove atoms by experimentally and theoretically supported probability based rules

• Assume the self-limiting modification or chemical activation of surface atoms is complete

• Include sputtering effects due to increased ion bombardment
Rule Based Model for ALE

<table>
<thead>
<tr>
<th>Configurations</th>
<th>Configuration 1</th>
<th>Configuration 2</th>
<th>Configuration 3</th>
<th>Configuration 4</th>
<th>Configuration 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Probabilities - Set 1 (no sputter)</td>
<td>85%</td>
<td>100%</td>
<td>92.5%</td>
<td>70%</td>
<td>72.5%</td>
</tr>
<tr>
<td>Probabilities - Set 2</td>
<td>100%</td>
<td>100%</td>
<td>100%</td>
<td>85%</td>
<td>93%</td>
</tr>
<tr>
<td>Sputter Probabilities - Set 2</td>
<td>15%</td>
<td>25%</td>
<td>20%</td>
<td>5%</td>
<td>10%</td>
</tr>
<tr>
<td>Probabilities - Set 3</td>
<td>100%</td>
<td>100%</td>
<td>100%</td>
<td>100%</td>
<td>100%</td>
</tr>
<tr>
<td>Sputter Probabilities - Set 3</td>
<td>25%</td>
<td>35%</td>
<td>30%</td>
<td>15%</td>
<td>20%</td>
</tr>
</tbody>
</table>

Evolution of a Flat Surface

Probability Set 1 (No secondary removal)

Etch Cycle

0

4

10

14

Average etch rate (layers per etch cycle) reaches steady-state immediately
Evolution of a Flat Surface

Etch Cycle

Probability Set 1 (No secondary removal)

0

4

10

14

Roughness increases and reaches steady-state at around 10-12 etch cycles
Effect of Increased Ion Energy

Etch Cycle

13

20

Probability Set 2

Probability Set 3

- Etch rate reaches steady-state immediately
- Etch rate faster for probability set 3, which has higher primary and secondary probabilities of removal
Effect of Increased Ion Energy

- Roughness larger for higher secondary etch rate
- Larger number of cycles needed to reach steady-state
Smoothing of Initial Rough Surfaces

- Etch rate independent of initial surface
- Initial surface variations persist for many etch cycles
- Rough surfaces smoothed by etch
Long Time Evolution of Roughness

Initially Flat - Probability Set 2
3 Realizations

Initially Sinusoidal - Probability Set 2
3 Realizations

- Variability among realizations
- Many etch cycles required to approach steady-state
- Slower approach to steady-state for non-smooth surfaces
# Etch Rate per Cycle

Layers etched per cycle for different probability sets and initial configurations of the surface and predictions based on probability averages

<table>
<thead>
<tr>
<th>Initial Surface</th>
<th>Probability Set 1</th>
<th>Pred. Set 1</th>
<th>Probability Set 2</th>
<th>Pred. Set 2</th>
<th>Probability Set 3</th>
<th>Pred. Set 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flat</td>
<td>0.87</td>
<td>0.84</td>
<td>1.14</td>
<td>1.11</td>
<td>1.27</td>
<td>1.25</td>
</tr>
<tr>
<td>Sinusoidal</td>
<td>0.89</td>
<td>0.84</td>
<td>1.16</td>
<td>1.11</td>
<td>1.28</td>
<td>1.25</td>
</tr>
<tr>
<td>Square Wave</td>
<td>0.89</td>
<td>0.84</td>
<td>1.16</td>
<td>1.11</td>
<td>1.28</td>
<td>1.25</td>
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- Etch rate is determined by the averages of the probabilities for Set 1

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**Avg 84%**
Etch Rate per Cycle

Layers etched per cycle for different probability sets and initial configurations of the surface and predictions based on probability averages

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<th>Avg Set 1</th>
<th>Probability Set 2</th>
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<th>Probability Set 3</th>
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Etch rate is determined by the sum of the averages of the two probabilities Sets 2 and 3.

<table>
<thead>
<tr>
<th>Probabilities - Set 2</th>
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Avg 95.6% → 111%

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Etch Rate versus Roughness

- Etch rate and roughness both increases Ar bombardment/plasma power
- Etch rate and long-time roughness independent of initial surface roughness
- More layers etched per cycle leads to greater roughness
- Tradeoff of low speed for smoother surface
Conclusions

• Fast cellular automata model with few parameters for simulation of atomic layer etching (ALE).

• The etch rate and etch roughness depends only on the probability sets used and not on the initial configurations of the surface, whether they be flat, sinusoidal or square patterned.

• The roughness correlates strongly with the etch rate and so there is a trade-off between desirable higher etch rates and undesirable roughness.