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REACTION MECHANISMS AND SiO_2 PROFILE EVOLUTION IN FLUOROCARBON PLASMAS

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AGENDA

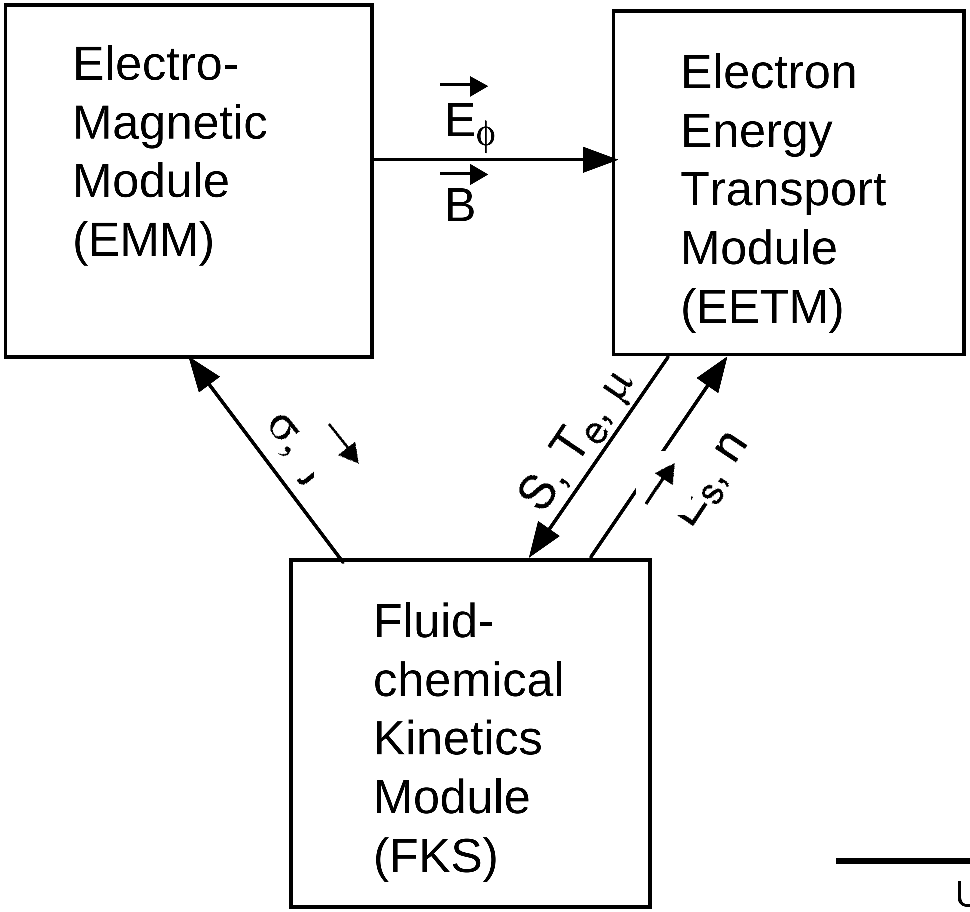
- Introduction
- Hybrid Plasma Equipment Model (HPEM)
  - Surface Kinetics Module (SKM)
  - Monte Carlo Feature Profile Module (MCFPM)
- C_2F_6 Plasma Etching of SiO_2
  - Surface Reaction Mechanism
  - Passivation and Etch Rate
  - Trench Profiles
- Summary

INTRODUCTION

- Fluorocarbon plasmas are widely used for SiO_2/Si etching due to their high etch rates and good selectivity.
- CF_x radicals passivate the wafer surface by polymeric deposition.
- Passivation-dependent surface reactions define etch rates and feature profiles.
- Our goal:
  - Develop a surface reaction mechanism
  - Model passivation dependent etching
  - Correlate etch rates and feature profiles to process parameters (e.g., bias, chemistry).

HYBRID PLASMA EQUIPMENT MODEL (HPEM)

- Modular simulation addressing low temperature, low pressure plasma processes.
- EMM calculates electromagnetic fields and magneto-static fields.
- EETM computes electron impact source functions and transport coefficients.
- FKS derives densities, momentum, and temperature or plasma species.



Electro-
Magnetic
Module
(EMM)

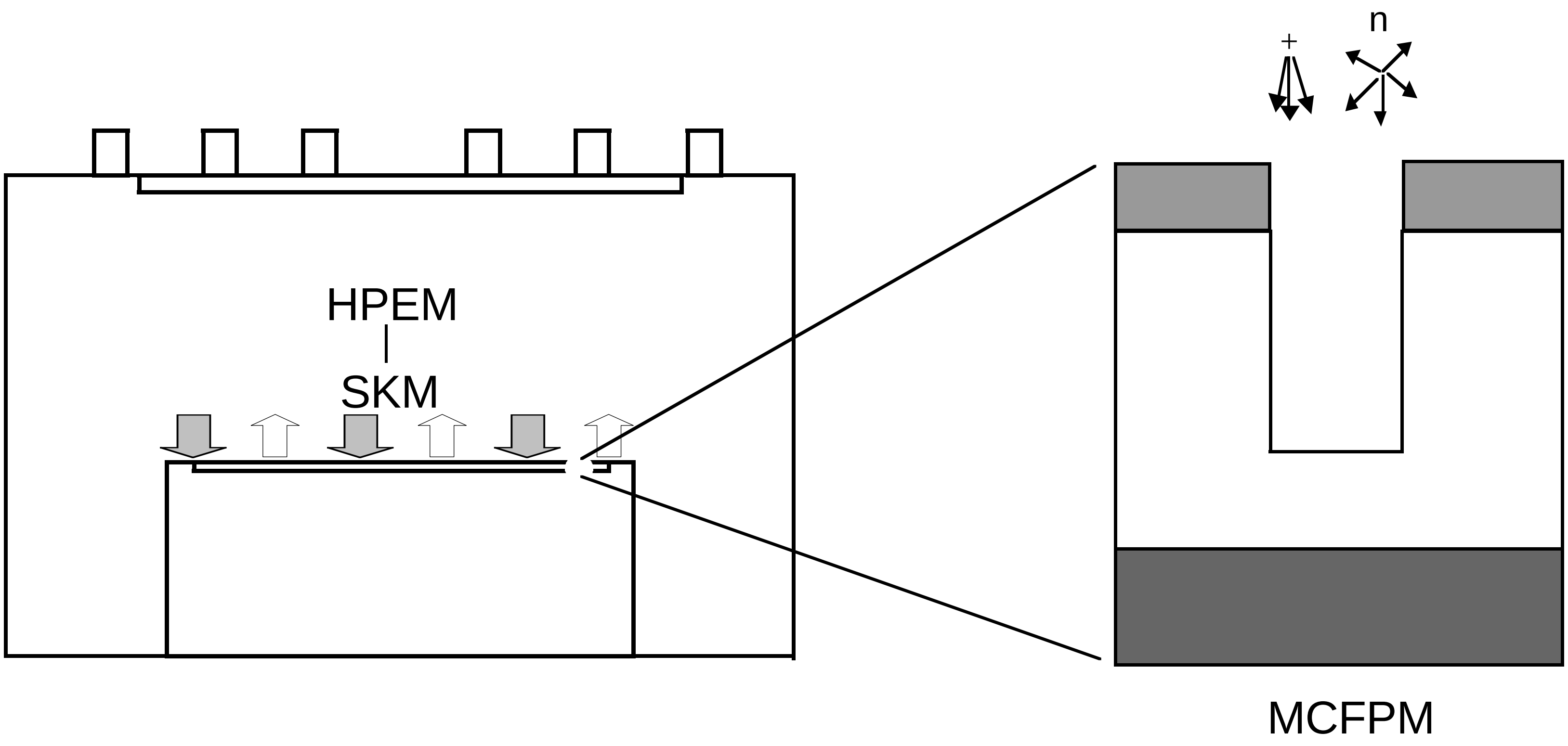
Electron
Energy
Transport
Module
(EETM)

Fluid-
chemical
Kinetics
Module
(FKS)

SURFACE MODELING: EQUIPMENT AND FEATURE SCALES

- Equipment scale: Integrating the Surface Kinetics Model (SKM) with the HPEM.
    - Coupling surface reactions to plasma properties.
    - Obtaining etch rates along the wafer.

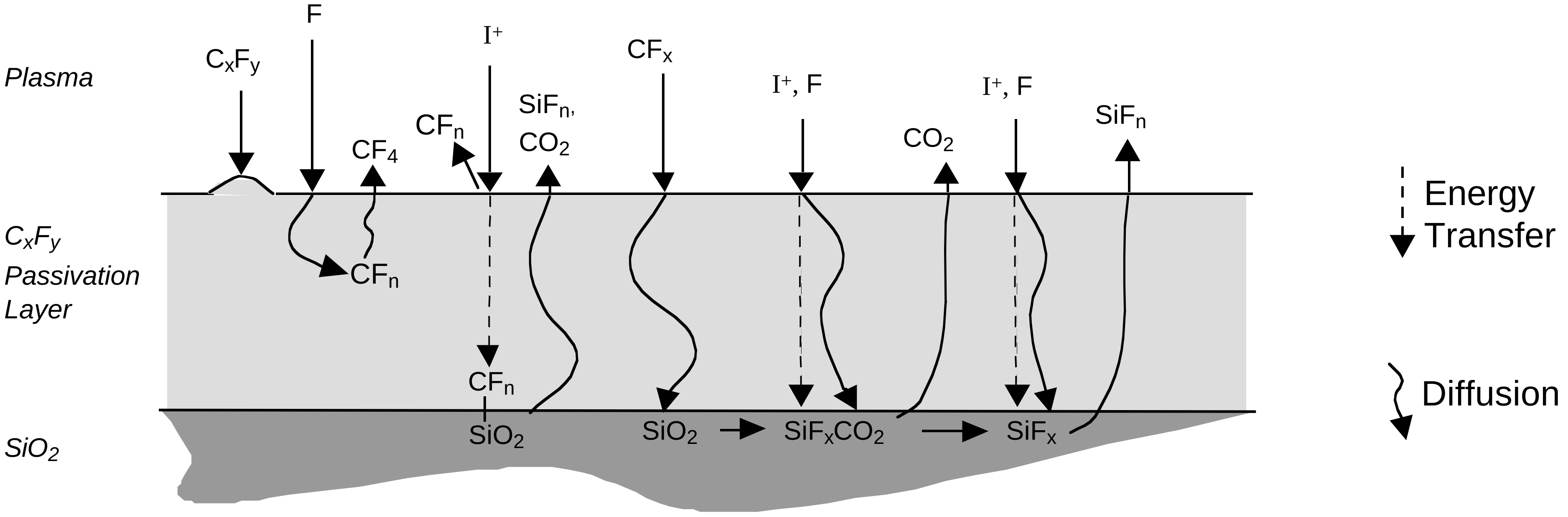
- Feature scale: Monte Carlo Feature Profile Model (MCFPM).
    - Obtaining trench profiles.



MECHANISMS FOR SiO_2 ETCHING

- Polymerization:
  - C_xF_y deposition (e.g., CF, CF_2, C_2F_3, C_2F_4)
  - F atom etching
  - Ion sputtering
  - Polymer-SiO_2 interaction

- SiO_2 etching:
  - Neutral passivation --> SiF_xCO_2 complex
  - Ion assisted desorption --> SiF_x surface sites
  - Fluorination and ion chemical sputtering -- > SiF_n volatile products



REACTOR GEOMETRY AND GAS REACTIONS

- Simulations of C_2F_6 etching of SiO_2 in an ICP reactor were performed.

- Representative gas phase reactions:

$e + C_2F_6 \rightarrow CF_3^+ + CF_3 + e + e$

$e + C_2F_6 \rightarrow CF_3 + CF_3 + e$

$e + CF_4 \rightarrow CF_2 + F + F + e$

$e + CF_4 \rightarrow CF_3^+ + F + e + e$

$e + CF_3 \rightarrow CF_2 + F + e$

$e + CF_3 \rightarrow CF_2 + F + F^-$

$e + CF_2 \rightarrow CF_2^+ + e + e$

$e + CF_2 \rightarrow CF + F + e$

$F + F + M \rightarrow F_2 + M$

$CF_3 + CF_3 + M \rightarrow C_2F_6 + M$

$CF_2 + F_2 \rightarrow CF_3 + F$

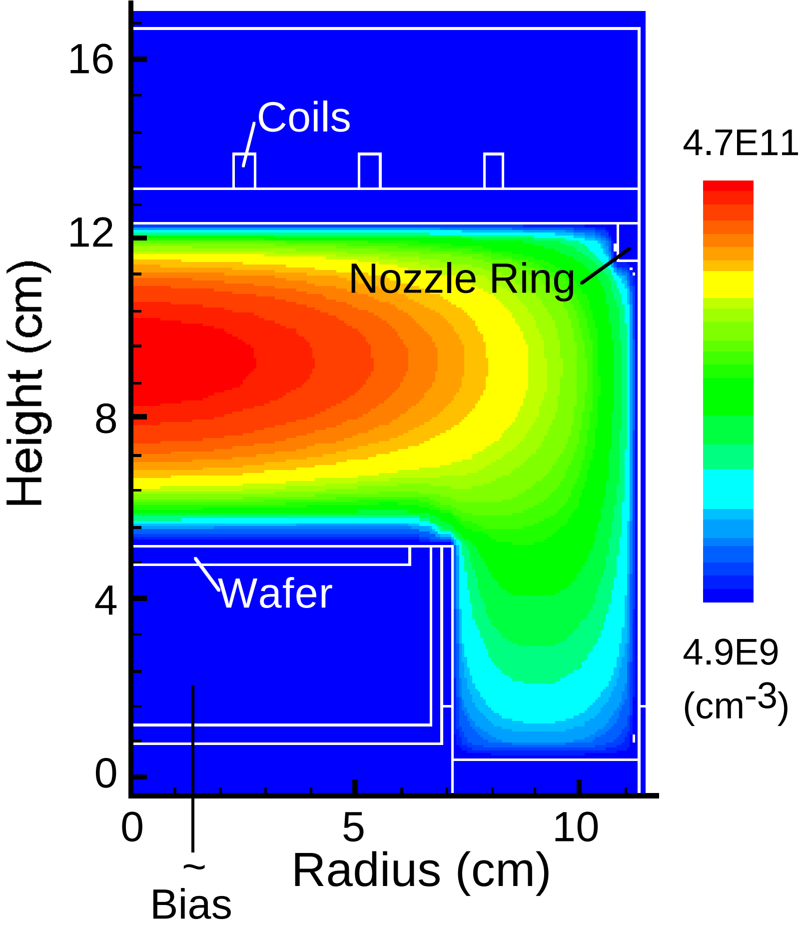
$CF_3 + F_2 \rightarrow CF_4 + F$

$C_2F_5 + F \rightarrow CF_3 + CF_3$

$CF_3 + F \rightarrow CF_4$

$CF_2 + F \rightarrow CF_3$

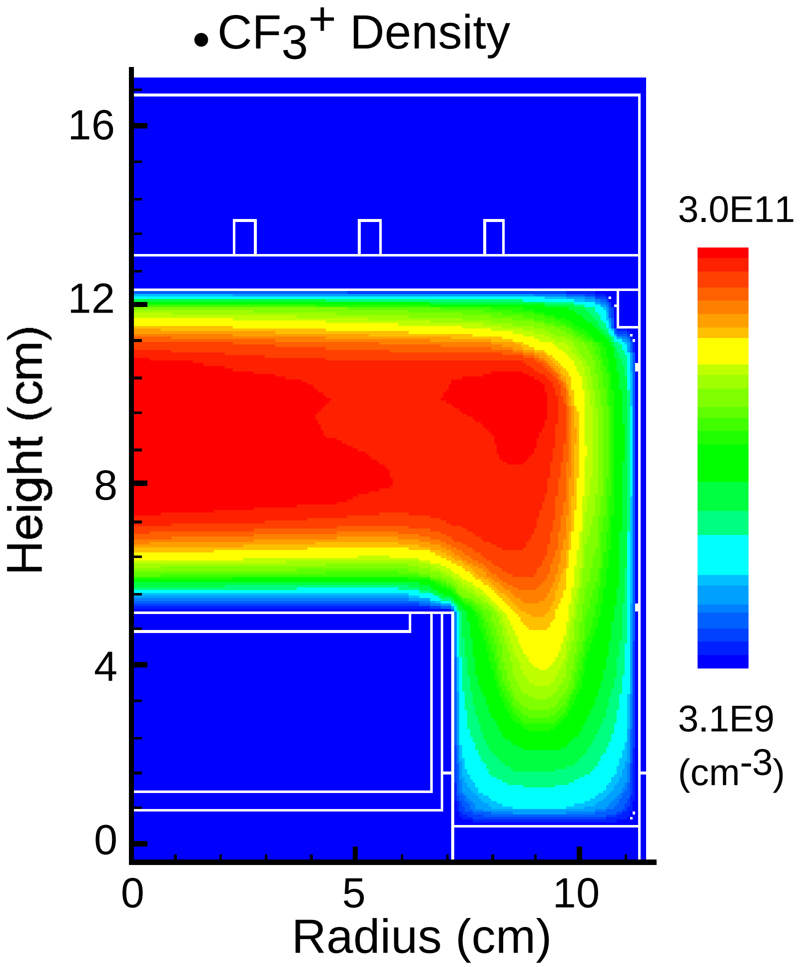
- Electron Density



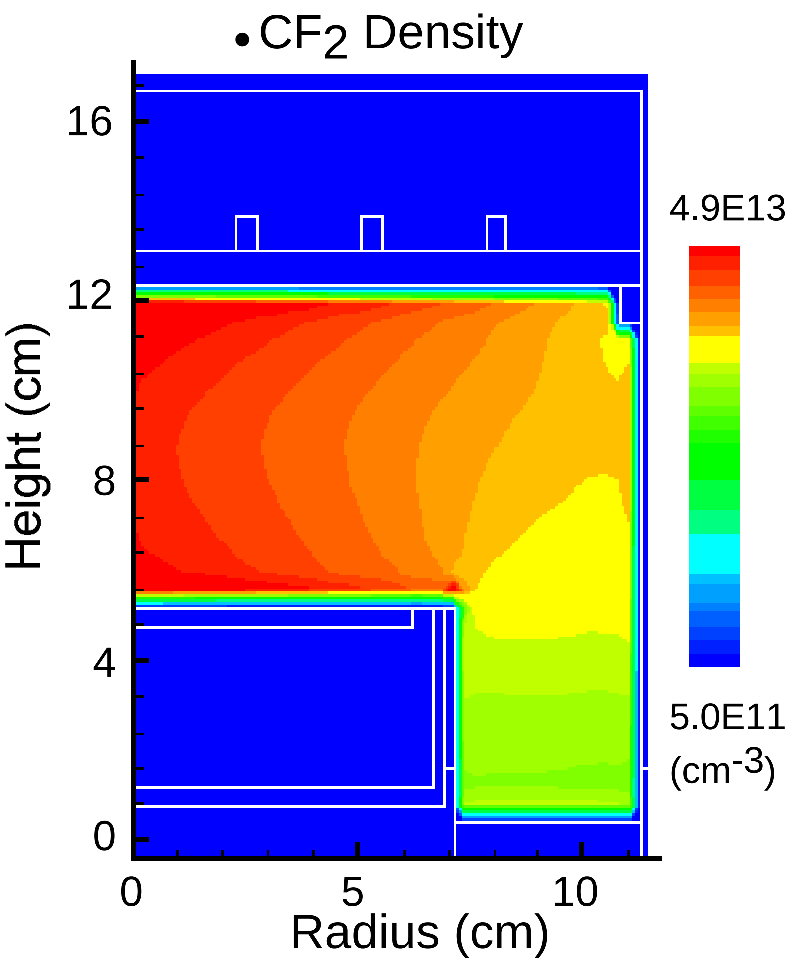
- C_2F_6, 6 mTorr, 40 sccm, 1400 W ICP, 100 V bias.

DENSITY DISTRIBUTIONS: BASE CASE

- The high power, low pressure process produces large and uniform densities of ions and radicals.



- CF_3^+ Density



- CF_2 Density

- C_2F_6, 6 mTorr, 40 sccm, 1400 W ICP, 100 V bias.

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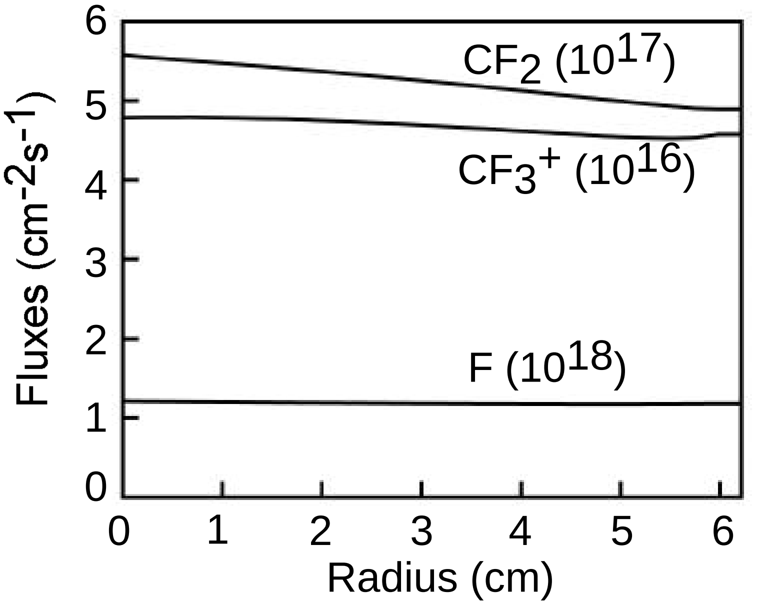
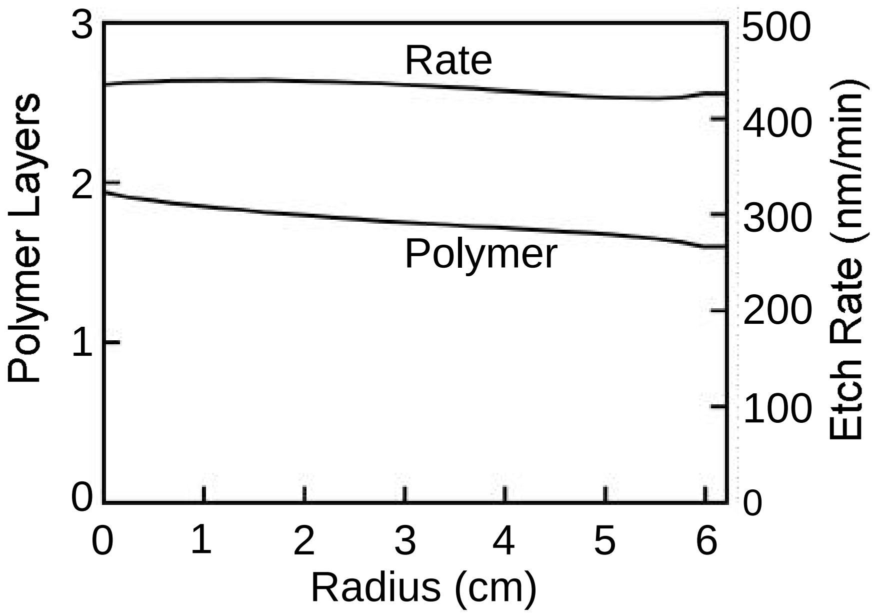
FLUXES AND ETCH RATE

- Radial distributions of wafer fluxes are uniform as a consequence of the density distributions.

- Polymer thickness and etch rate are uniform along the wafer surface.

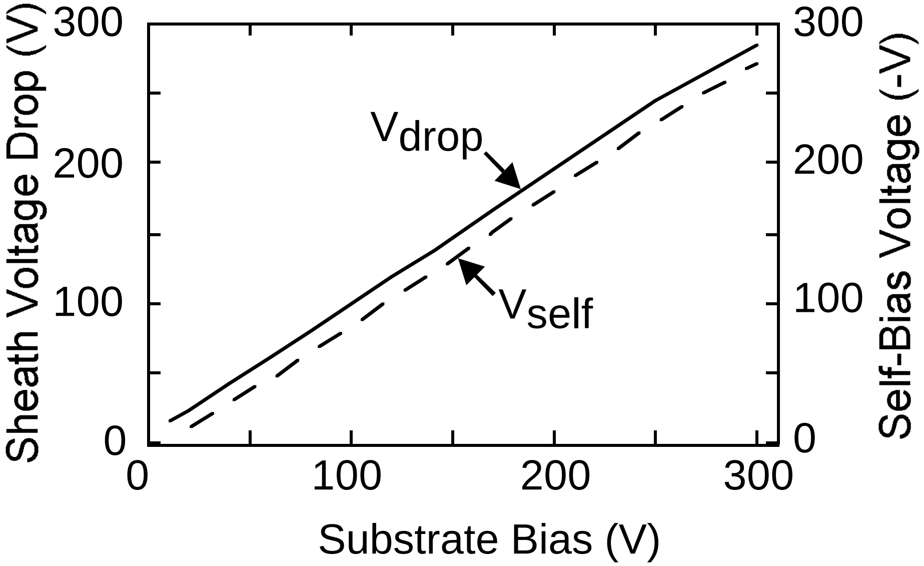


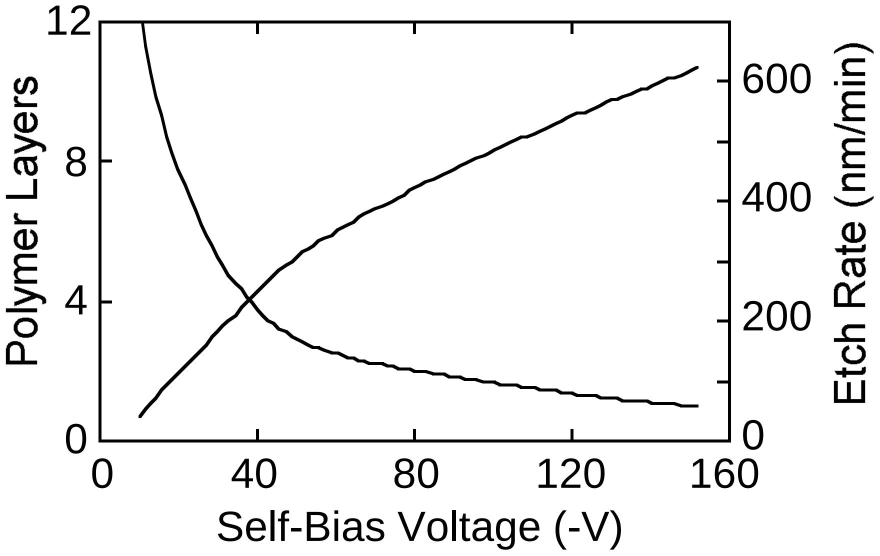


- C_2F_6, 6 mTorr, 40 sccm, 1400 W ICP, 100 V bias.

SUBSTRATE BIAS

- With increasing bias, the ion energy increases due to increasing sheath voltage.
- The polymer thickness decreases with increasing bias because of increasing ion sputtering consumption. Consequently the etch rate increases.
- Low-energy-ion activation of surface sites for polymerization produces thick passivation at low biases.





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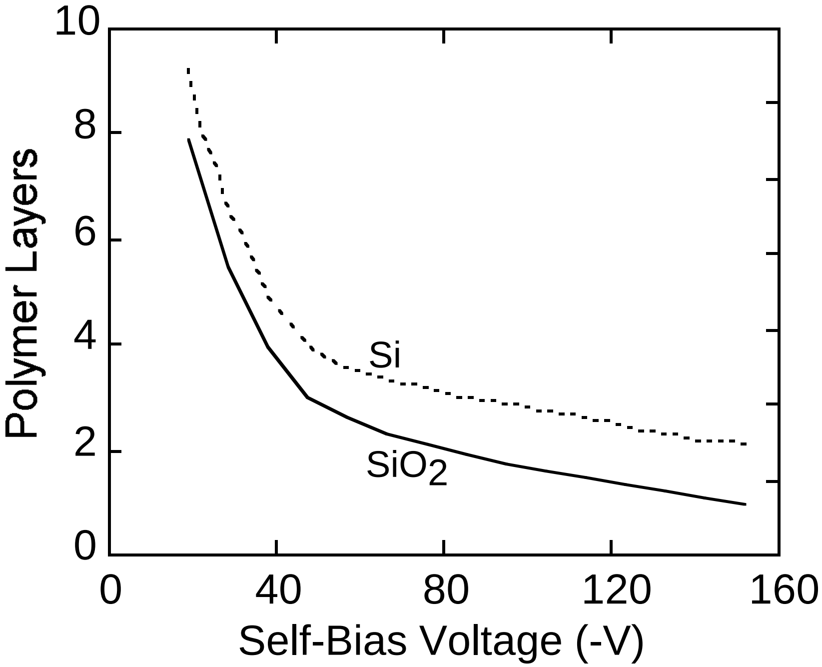
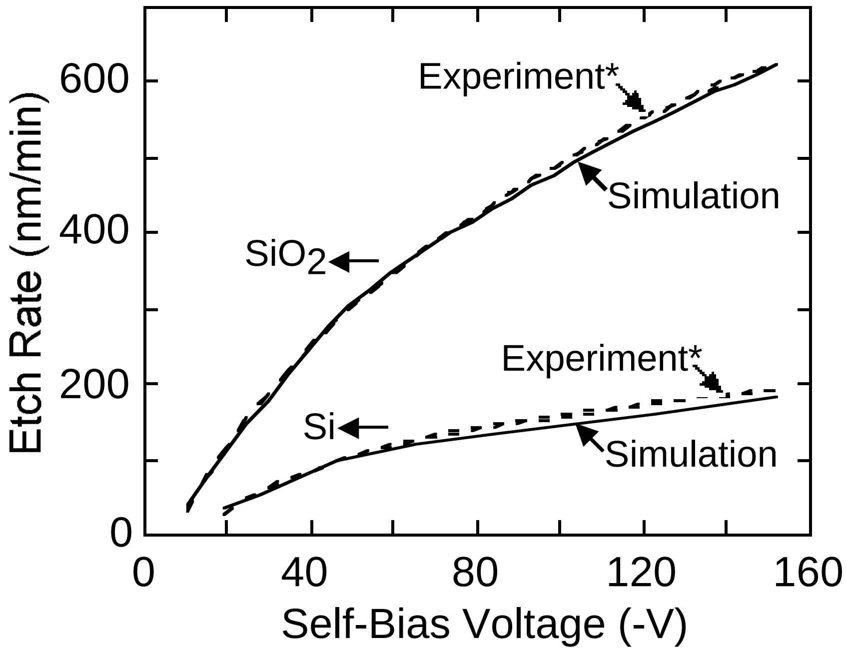
SiO_2 AND Si ETCHING

- The polymer thickness is larger on Si than on SiO_2 at same process conditions due to the lack of polymer consumption by the substrate oxygen in Si etching.
- The etch rates of SiO_2 are larger than those of Si at the same process conditions.
- Simulations agree well with experiments.

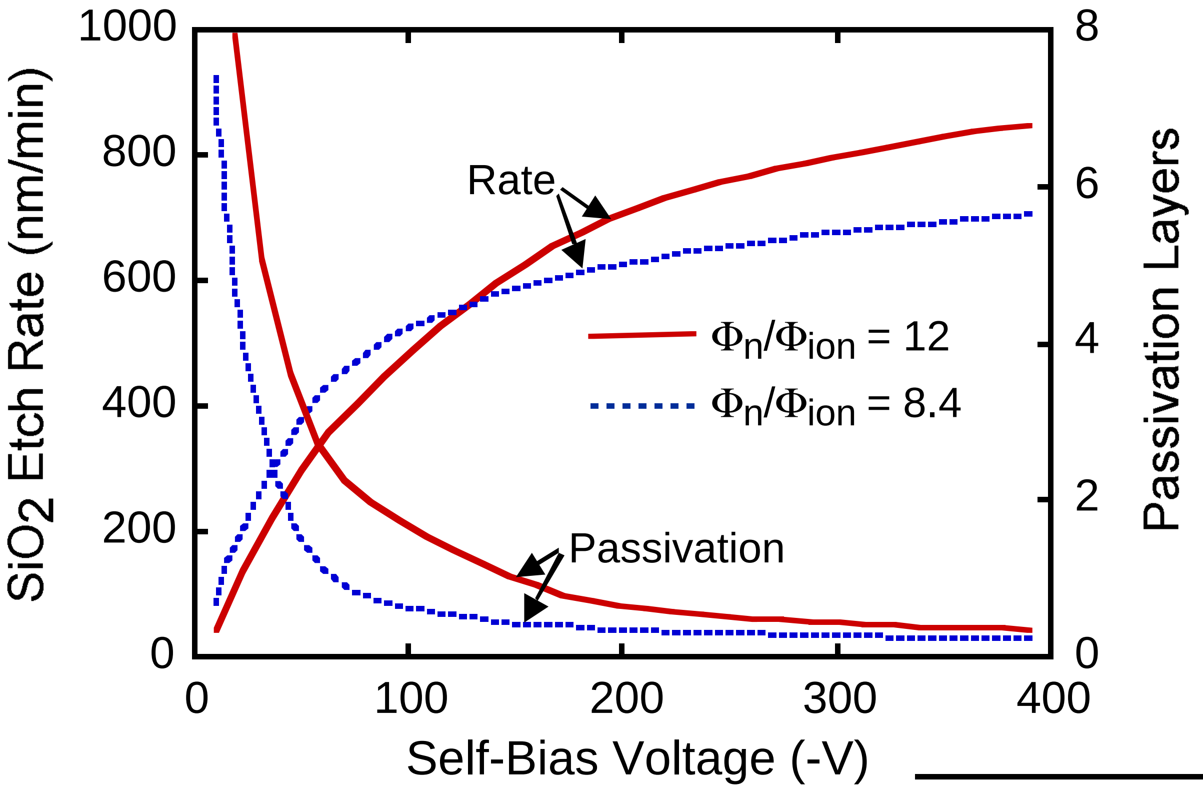




* G. S. Oehrlein et al., J. Vac. Sci. Technol. A 17, 26 (1999).

PASSIVATING NEUTRAL TO ION FLUX RATIO

- The passivation thickness increases with increasing passivating neutral to ion flux ratio (Φ_n/Φ_{ion}).
- At low biases, the passivation is thick. The etch rate decreases with increasing Φ_n/Φ_{ion} due to decreasing energy and species transfer through the polymer.
- At high biases, the etch rate saturates due to starvation of passivation. Increasing Φ_n/Φ_{ion} leads to increasing etch rate.



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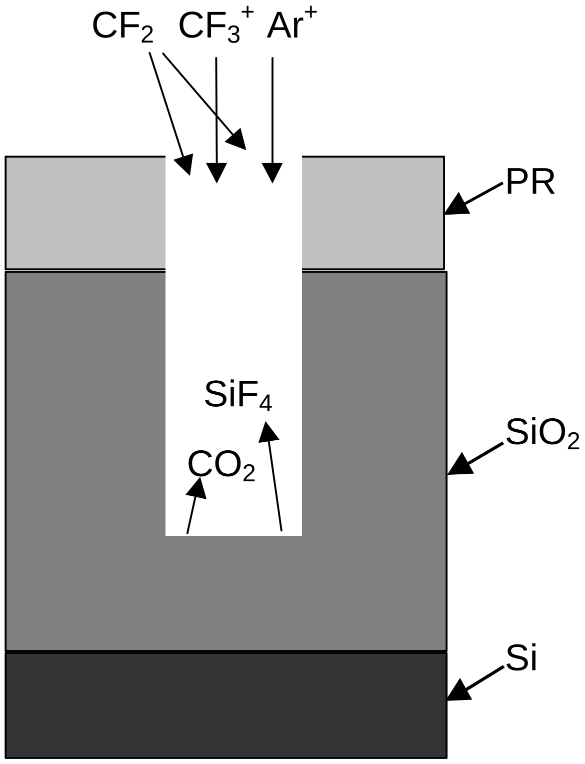
MONTE CARLO FEATURE PROFILE MODEL (MCFPM)

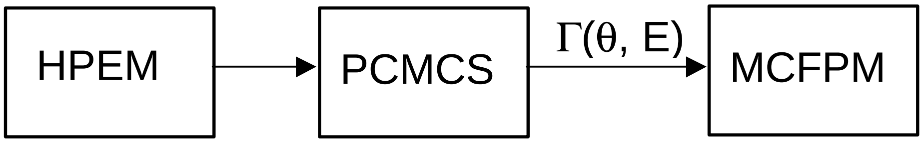
- Profiles of SiO_2 in C_2F_6/Ar plasma etching were investigated with the MCFPM.

- The MCFPM model predicts the time and spatially dependent microscale processes which produce etch profiles.



- The Plasma Chemistry Monte Carlo Simulation (PCMCS) uses HPEM results to produce reactive fluxes (energy and angle) to the surface.

- The MCFPM uses these fluxes to implement a user defined reaction mechanism.

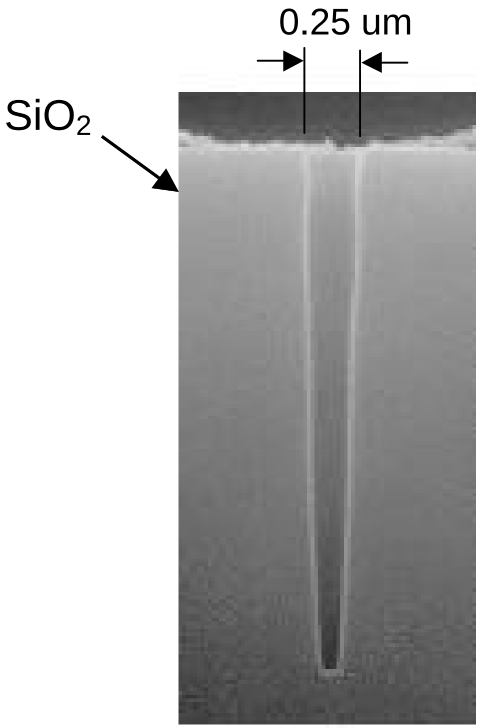

HPEM $\rightarrow$ PCMCS $\xrightarrow{\Gamma(\theta, E)}$ MCFPM

TAPERING OF PROFILES

- In high aspect ratio (AR) etching of SiO_2 by fluorocarbon plasmas, the sidewall of trenches are passivated by C_xF_y neutrals due to the broad angular distributions of neutral fluxes.

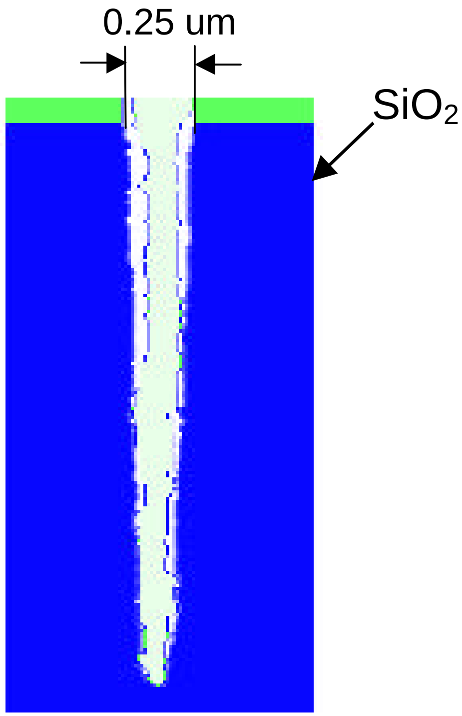
- Tapered trench profiles are produced when the passivation/ion flux ratio is large.

Experiment
(Similar Process Conditions)



AR = 10:1
(C. Cui, AMAT)

Simulation



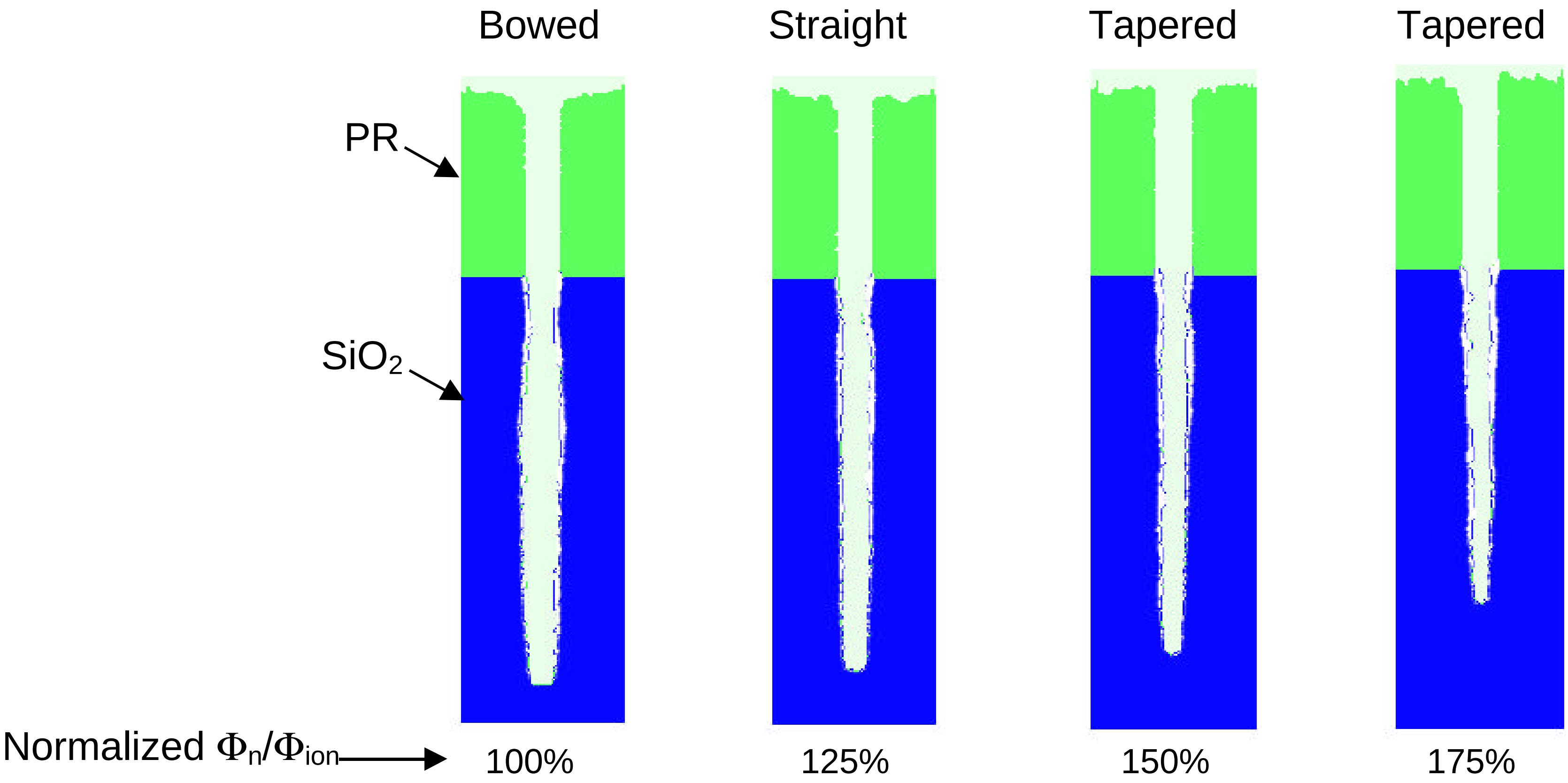
AR = 10:1

- The critical dimension shrinks from the top to the bottom of the trench.

PASSIVATION/ION FLUX RATIO

- Increasing passivating neutral to ion flux ratio (Φ_n/Φ_{ion}) leads to more tapered profiles due to increasing sidewall passivation.

- When the passivating neutral flux is too small, insufficient sidewall protection by the passivation layer leads to a bowed profile.



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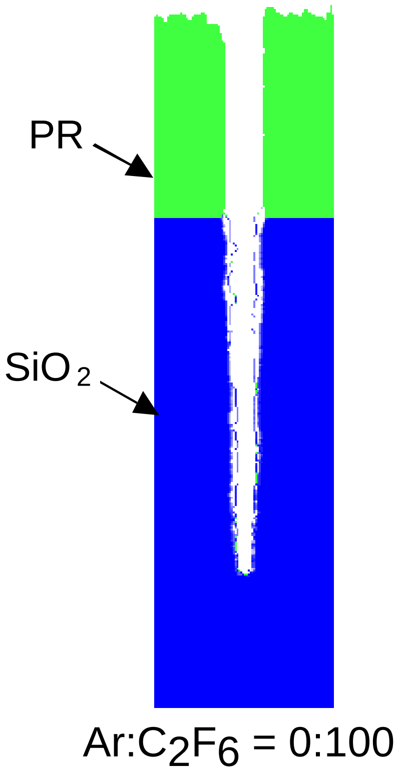
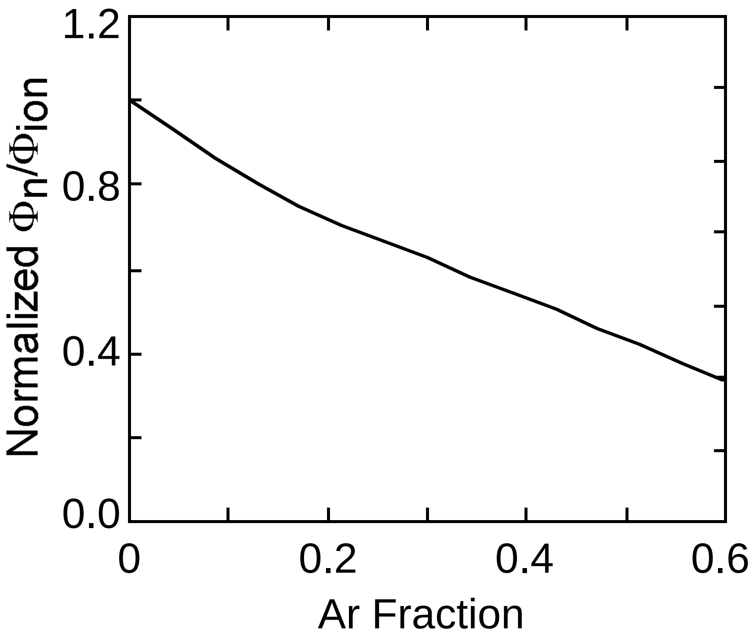
INFLUENCE OF AR MIXTURE

- The passivating neutral to ion flux ratio (Φ_n/Φ_{ion}) decreases with increasing Ar fraction in the Ar/C2F6 feedstock gas.

- A tapered trench transitions to a straight and a bowed profile with increasing Ar fraction.

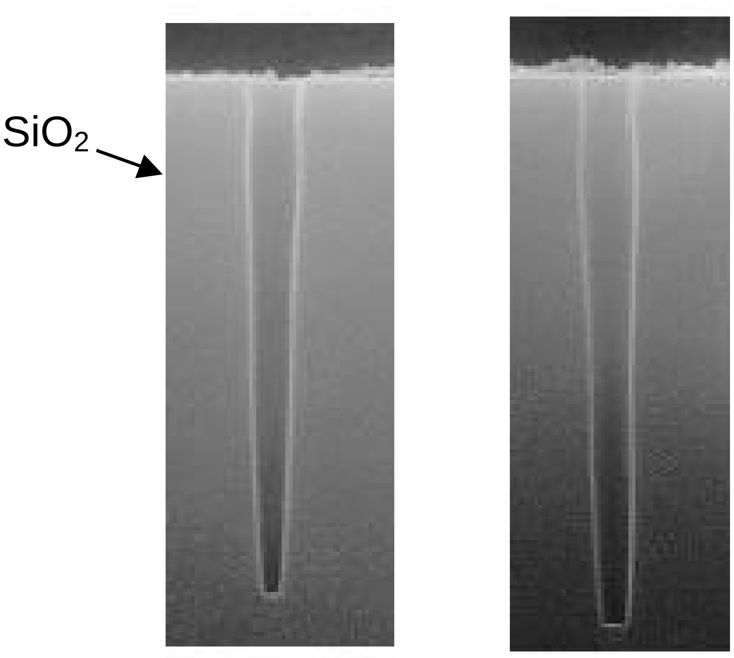




INFLUENCE OF ION ENERGY

- With increasing ion energy, the increasing ion sputtering yield of the sidewall passivation layer produces a less tapered profile.
- The etch rate also increases due to decreasing (but sufficient) passivation.
- Simulations and experiments obtained similar trends.

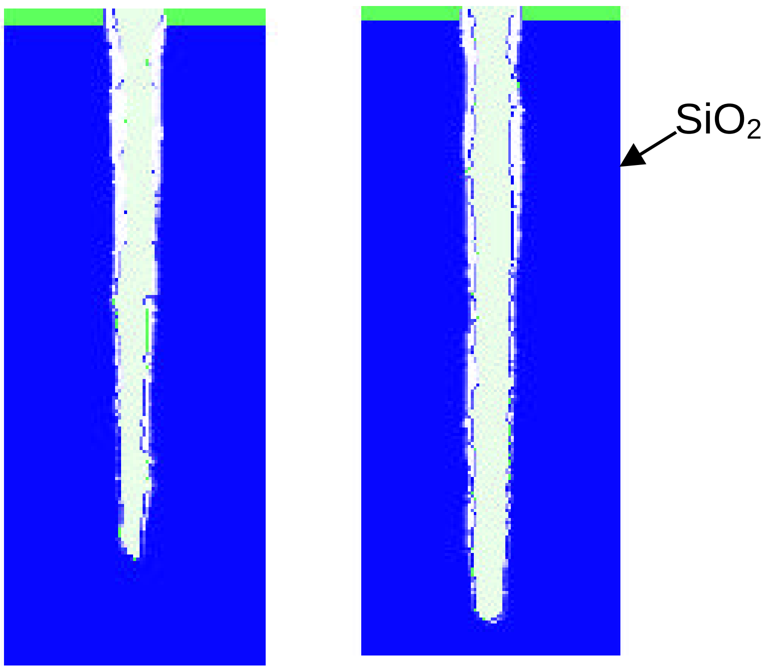
Experiments
(Similar Proccess



800 W 1000 W

Bias Power
(C. Cui, AMAT)

Simulations



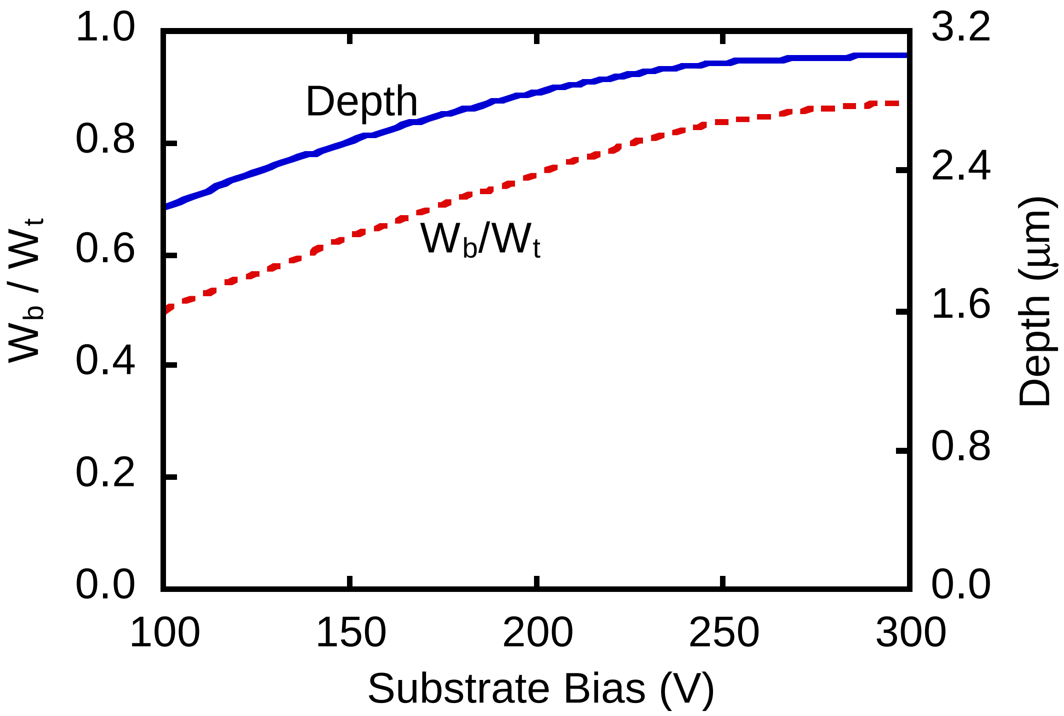
100 V 160 V

Bias Voltage

INFLUENCE OF ION ENERGY (cont.)

- When the ion energy is high, the SiO_2 etching is limited by the passivation instead of the ion sputtering yield.

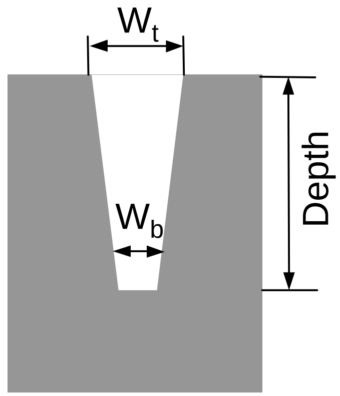
- The etch rate and the bottom width of the trench are saturated at high ion energies.



W_b: Trench width 0.5 µm above the bottom.

W_t: Trench width at the top.

Depth: Trench depth after equal etch times.



SUMMARY

- In C_2F_6 etching of SiO_2, a polymer is grown on the surface by C_xF_y deposition. The polymer influences etching by limiting diffusion and dissipating ion bombarding energy

- With increasing substrate bias, the polymer thickness decreases due to increasing ion sputtering, resulting in increasing etch rates and less tapered profiles. The etch rate saturates at high biases due to insufficient neutral passivation.

- The etch selectivity of SiO_2 over Si is attributed to the polymer consumption by oxygen atoms in the SiO_2 film.

- Processes with high passivating neutral to ion flux ratios produce tapered profiles. The bottom critical dimension of the trench decreases with increasing ratio of passivating neutral to ion fluxes.