27th IEEE International Conference on Plasma Science
New Orleans, Louisiana
June 4 - 7, 2000

SURFACE AND GAS PHASE REACTIONS FOR FLUOROCARBON PLASMA ETCHING OF SiO_2

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†Work supported by SRC, NSF, and Applied Materials.

AGENDA

- Introduction

- Description of the Model
  - Hybrid Plasma Equipment Model (HPEM)
  - Surface Kinetics Module (SKM)

- Surface Reaction Mechanisms in C_2F_6 etching of SiO_2
  - Surface Passivation
  - Substrate Bias

- Profile Simulations for C_2F_6 Etching of SiO_2
  - Monte Carlo Feature Profile Model (MCFPM)
  - Ion to Neutral Flux Ratio
  - Ion Energy

- Summary

INTRODUCTION

- Fluorocarbon (C_mF_n) plasmas are widely used for SiO_2/Si etching due to their high rate and good selectivity.

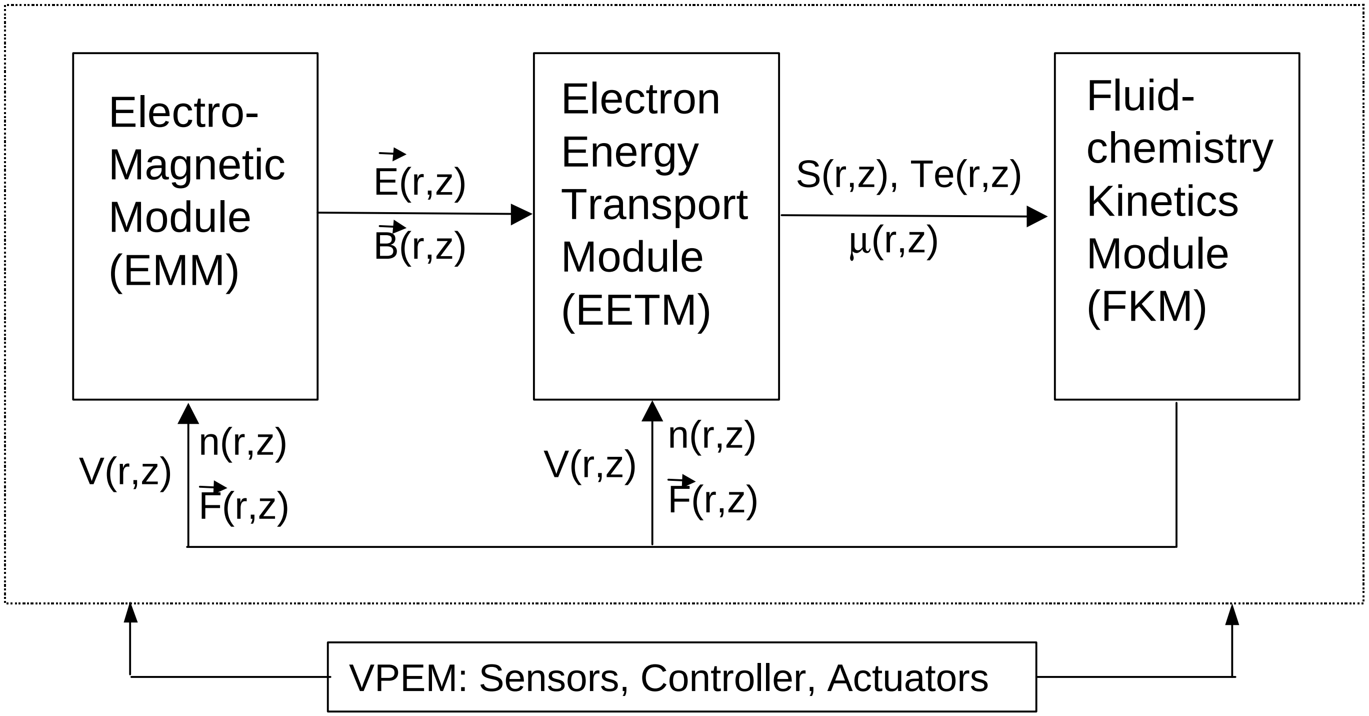
- CF_x radicals passivate the wafer surface and so influence etching behavior.

- The passivation thickness depends on wafer materials, plasma-wall interactions, and processing parameters.

- Our goals:
    - Develop a surface reaction mechanism
    - Model passivation dependent etching
    - Investigate influences of process parameters (e.g., bias, chemistry).

HYBRID PLASMA EQUIPMENT MODEL (HPEM)

- Modular simulator addressing low temperature, low pressure plasmas.
- EMM calculates electromagnetic fields and magneto-static fields.
- EETM computes electron impact source functions and transport coefficients.
- FKM derives the densities, momentum and temperature of plasma species.
- VPEM shell can be added to HPEM for process control.



Electro-Magnetic Module (EMM)

$\vec{E}(r,z)$

$\vec{B}(r,z)$

Electron Energy Transport Module (EETM)

S(r,z), Te(r,z)

$\mu(r,z)$

Fluid-chemistry Kinetics Module (FKM)

V(r,z)

n(r,z)

$\vec{F}(r,z)$

V(r,z)

n(r,z)

$\vec{F}(r,z)$

VPEM: Sensors, Controller, Actuators

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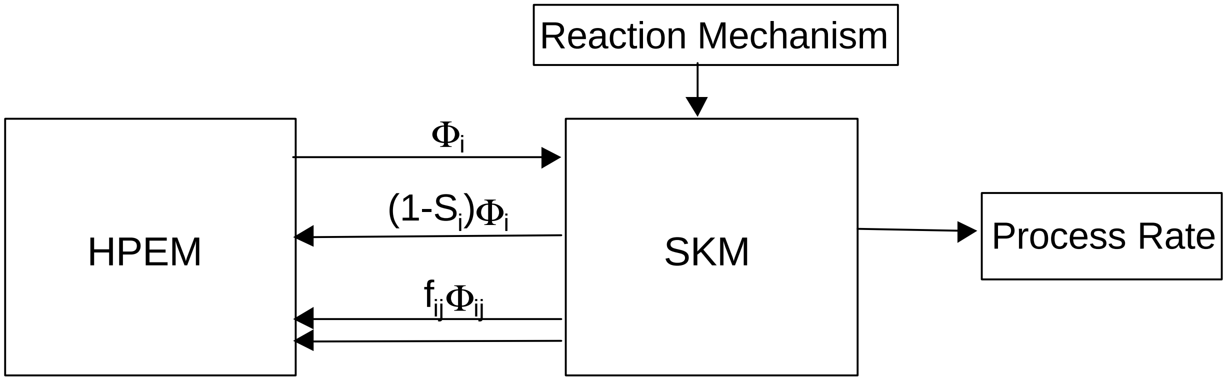
SURFACE KINETICS MODEL (SKM)

- The Surface Kinetics Model (SKM) is an integrated module of the HPEM.

- The SKM
  - Uses reactant fluxes from the HPEM
  - Applies a user defined reaction mechanism
  - Updates surface sticking and product reflection coefficient for the HPEM
  - Calculates surface coverages and process rates



Reaction Mechanism

HPEM

Φ_i

$(1-S_i)\Phi_i$

$f_{ij}\Phi_{ij}$

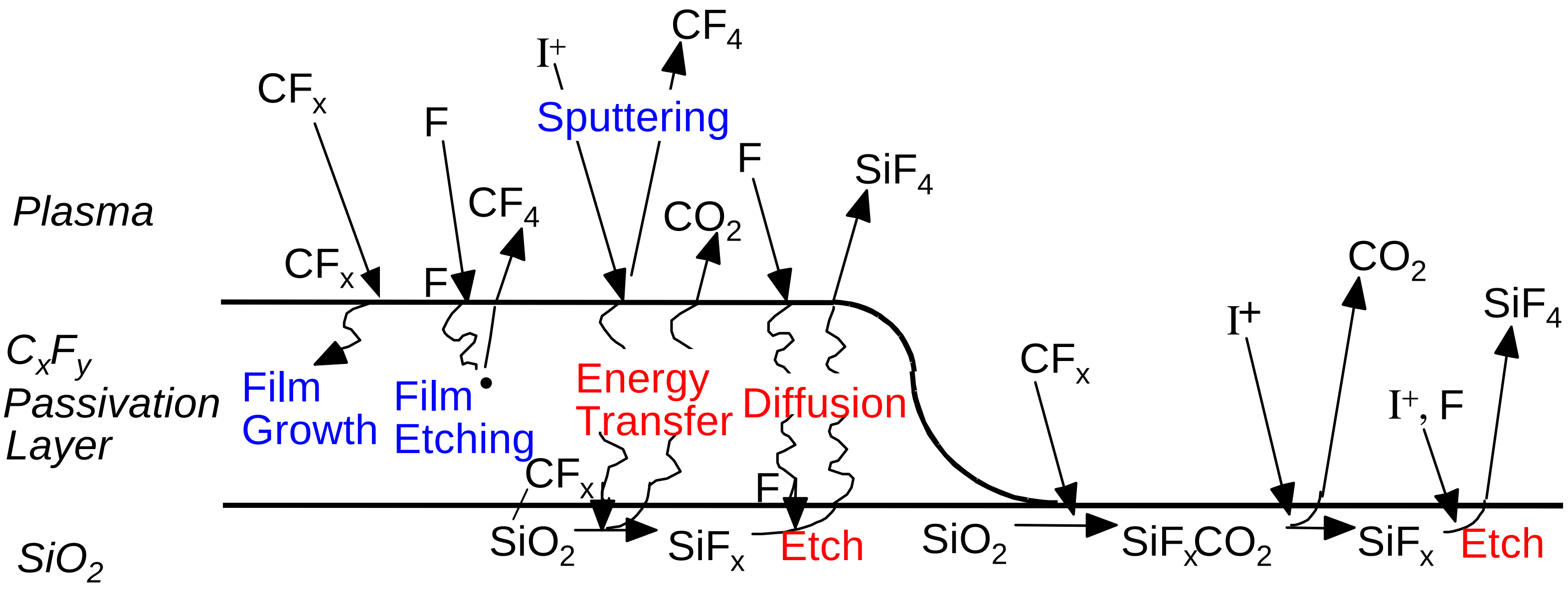
SKM

Process Rate

- The SKM uses a multi-layer surface site balance model at every mesh point along the plasma-surface boundary.

C_2F_6 PLASMA ETCHING OF SiO_2

- The reaction mechanism for SiO_2 etching is based on:
  - Growth of C_xF_y passivation layer (balance of deposition and consumption).
  - Formation of complex at the interface between oxide and passivation layer resulting from chemisorption of CF_x.
  - Ion activated (through passivation layer) etching of complex. Rate of activation scales inversely with passivation layer thickness.
  - Diffusion of etch precursor and etch product.



SiO_2 ETCH REACTION MECHANISM

- Simulations of C_2F_6 etching of SiO_2 in an ICP reactor were performed.
- Representative gas phase reactions:

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

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

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

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

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

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

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

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

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

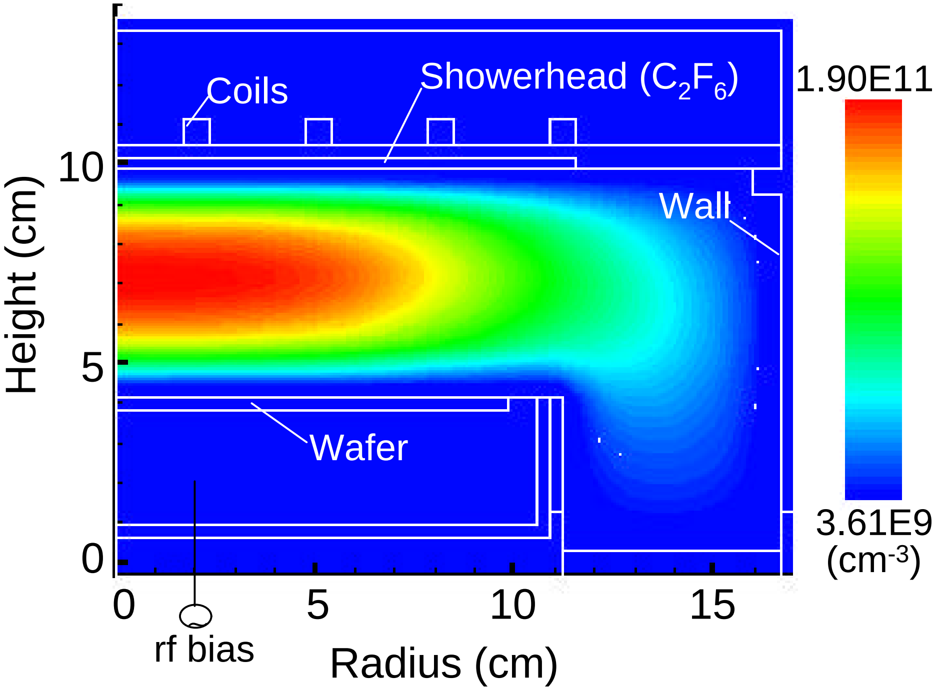
$CF_2 + F_2 \rightarrow CF_3 + F$

$CF_3 + F_2 \rightarrow CF_4 + F$

$CF_2 + CF_3 \rightarrow C_2 F_5$

$C_2F_5 + F \rightarrow CF_3 + CF_3$

- Electron Density

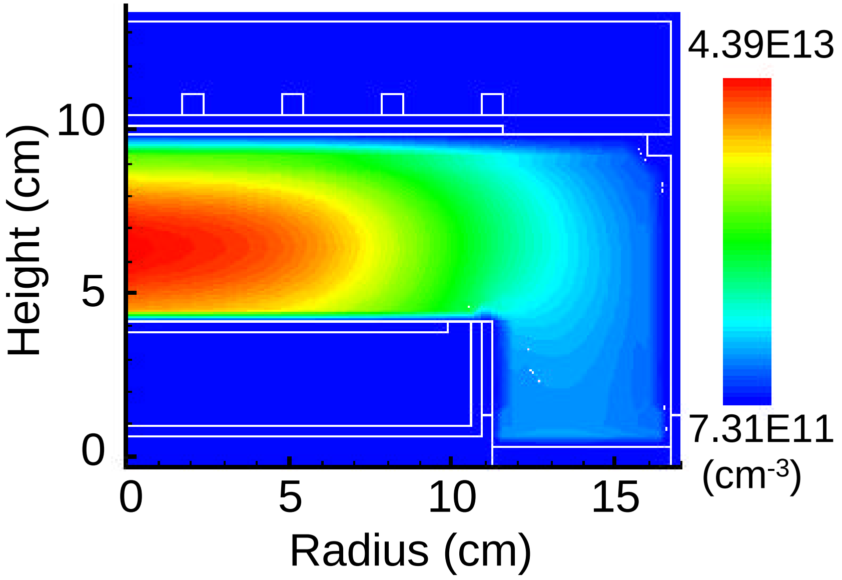


- C_2F_6, 10 mtorr, 200 sccm, 650 W ICP, 100 V bias

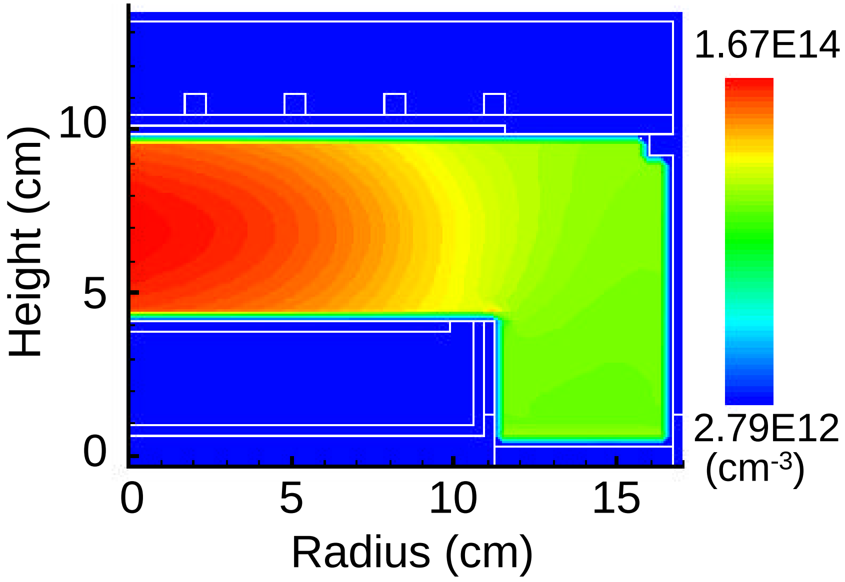
RADICAL DENSITIES

- Less uniform CF_2 density distribution due to its higher loss rate at the reactor wall.

- CF_2 Density



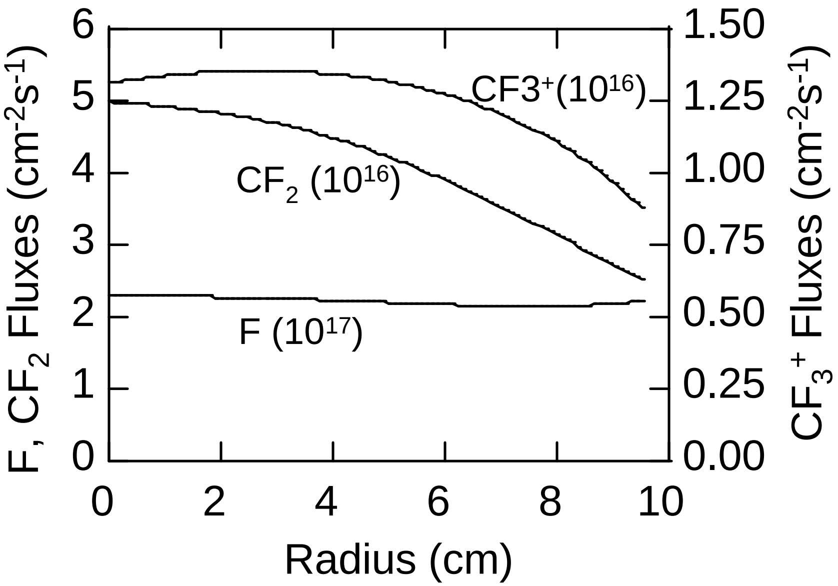
- F Density

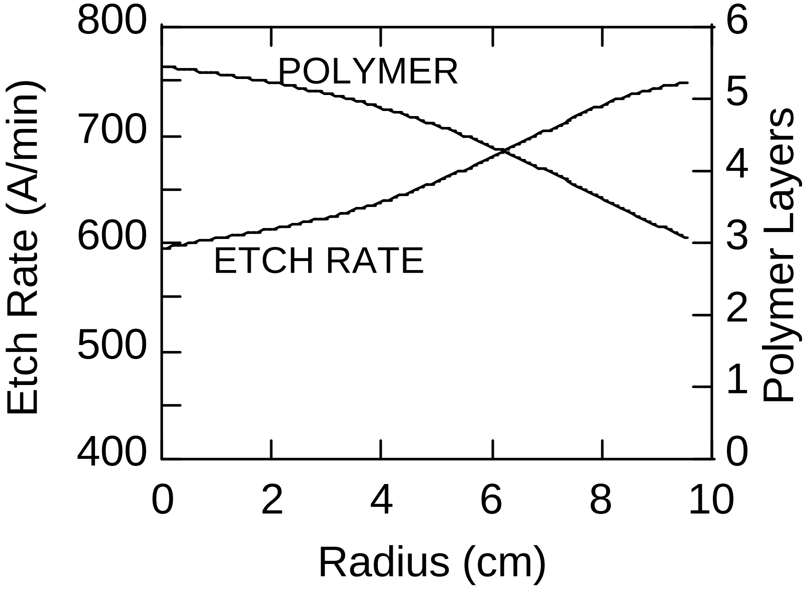


- C_2F_6, 10 mtorr, 200 sccm, 650 W ICP, 100 V bias.

RADIAL DISTRIBUTIONS

- Radial flux distribution of CF_2 is less uniform than that of F as a consequence of the of the density distributions.
- Polymer distribution follows the CF_2 flux distribution for this case.
- Etch rate increases in the radial direction, inverse to the behavior of polymer distribution.



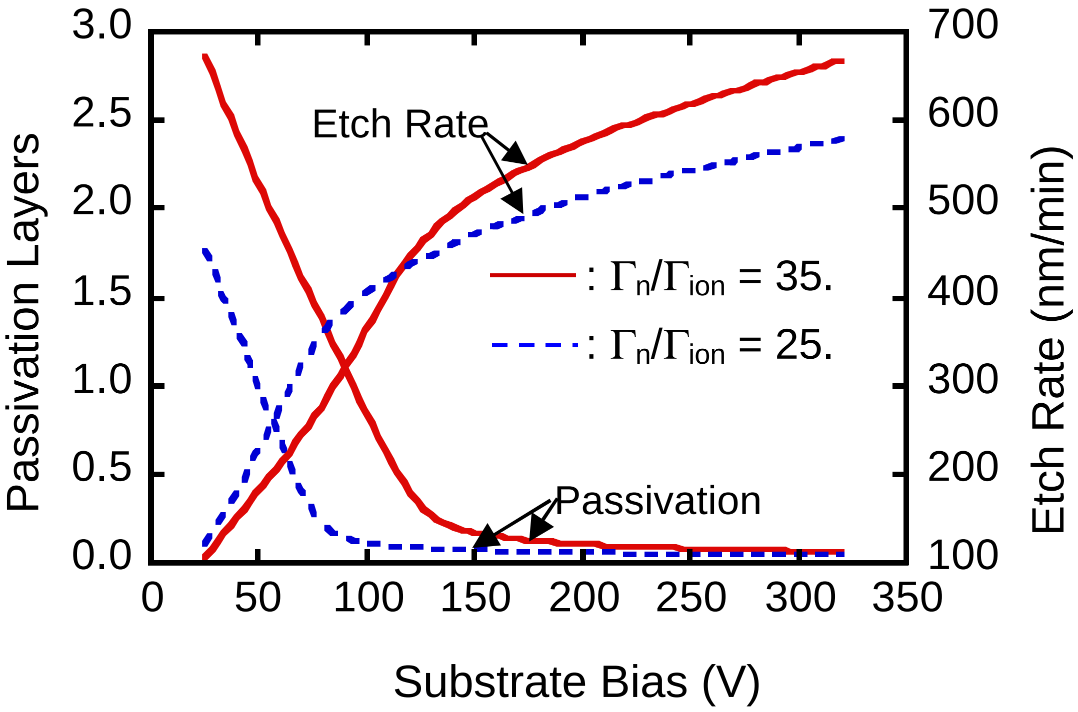


- C_2F_6, 10 mtorr, 200 sccm, 650 W ICP, 100 V bias.

SUBSTRATE BIAS

- At low biases, the passivation layer thickness decreases with increasing bias due to increasing ion sputtering of the polymer, and the etch rate increases.

- At high biases, the passivation is starved and the etch rate goes to saturation. More passivating neutral flux (CF_x, $x \leq 2$) is required to increase the etch rate.



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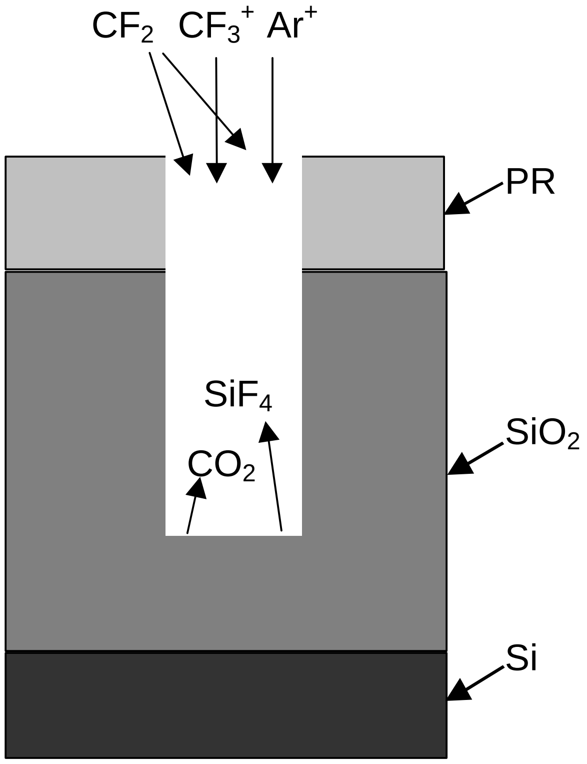
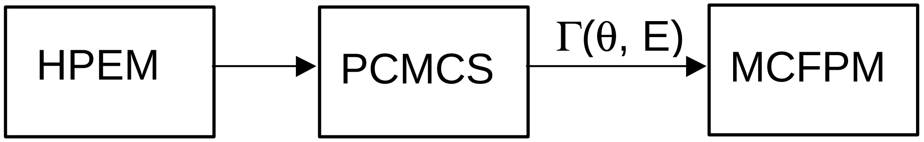
MONTE CARLO FEATURE PROFILE MODEL (MCFPM)

- 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 Model (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.

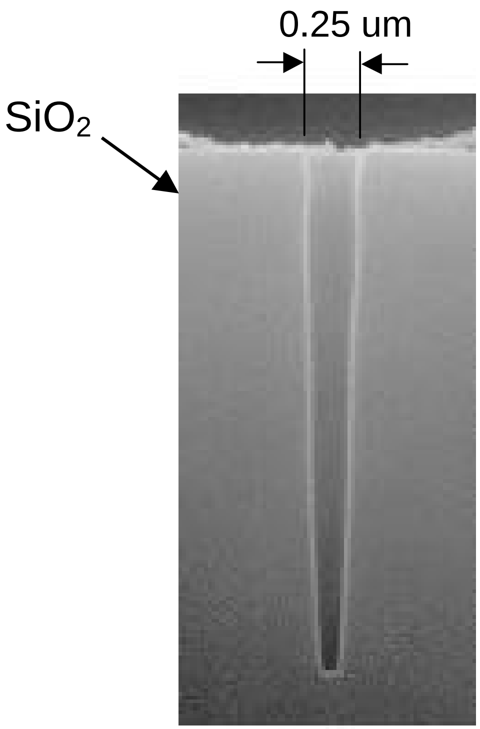


TAPERING OF PROFILES

- In high aspect ratio (AR) etching of SiO_2 by fluorocarbon plasmas, the sidewall of trenches are passivated by neutrals (CF_x, $x \leq 2$) due to the broad angular distributions of neutral fluxes.

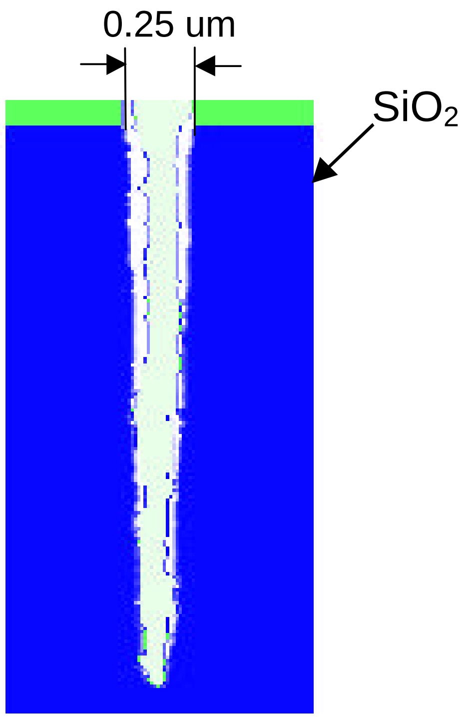
- Tapered trench profiles are produced when the passivation/ion flux ratio is large.

Experiment



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

Simulation



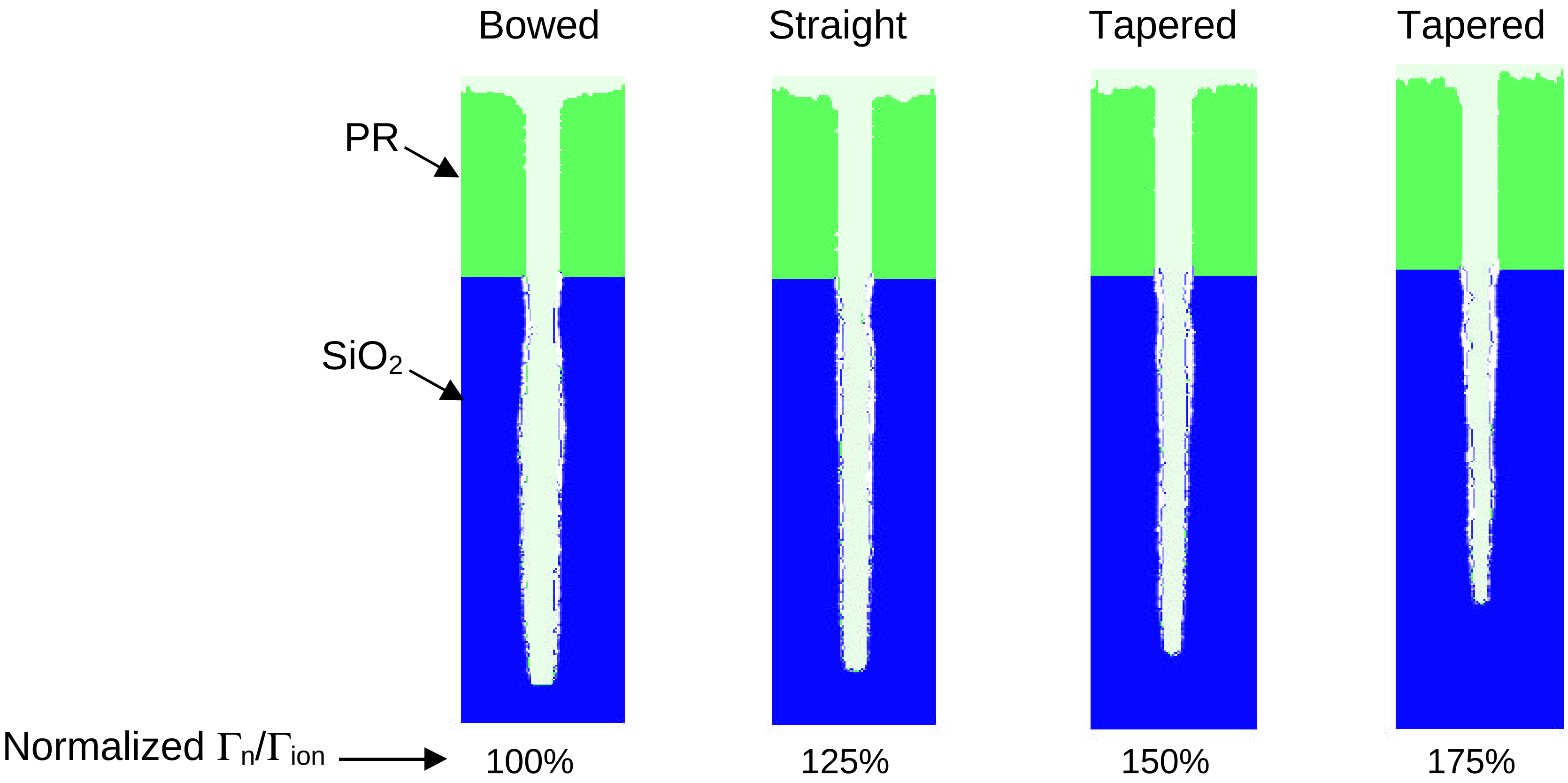
AR = 10:1

- Ar/C_2F_6 = 20/80.
- 1000 W ICP power, 150 V bias.
- 10 mTorr.
- Radial location: 3 cm.

PASSIVATION/ION FLUX RATIO

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

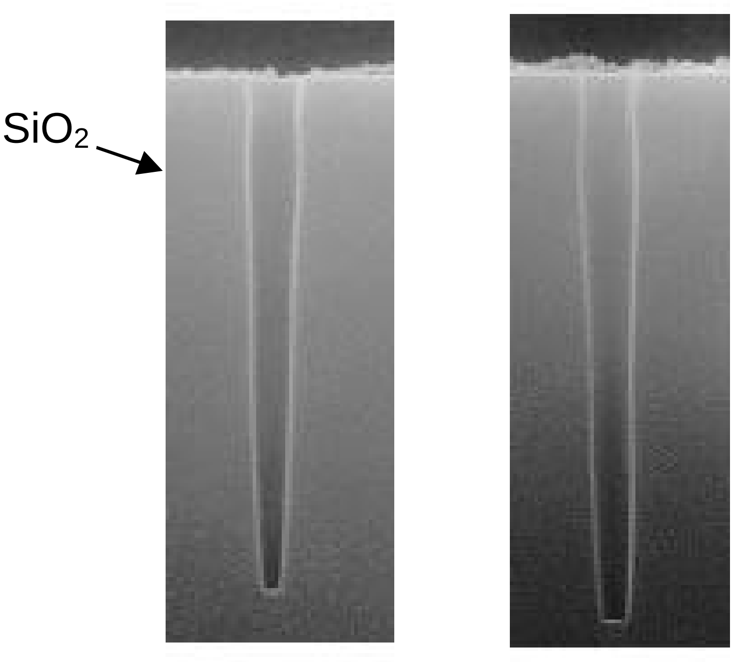
- When the passivating neutral flux is too small, insufficient sidewall protection by the passivation layer leads to a bowed profile.



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 with increasing ion energy due to decreasing (but sufficient) passivation.
- Simulations and experiments obtained similar trends.

Experiments

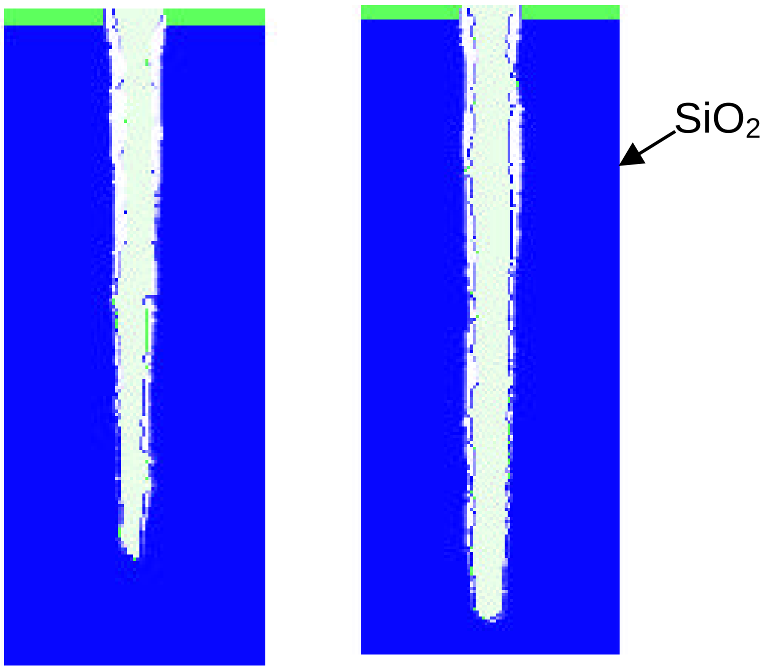


800 W　　1000 W

Bias Power

(C. Cui, AMAT)

Simulations

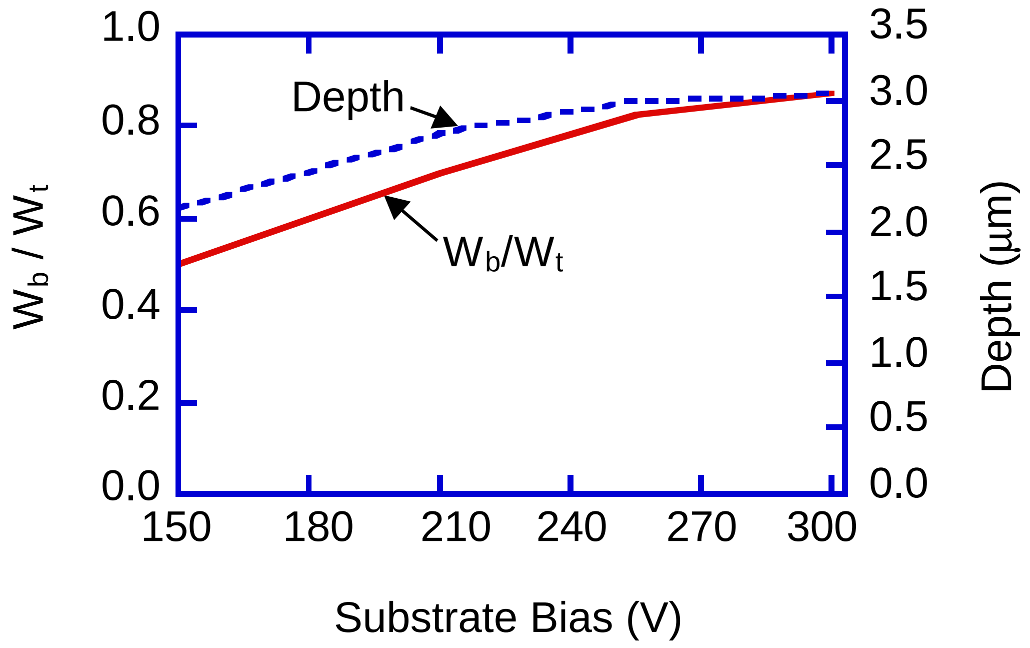


150 V　　180 V

Bias Voltage

INFLUENCE OF ION ENERGY (cont.)

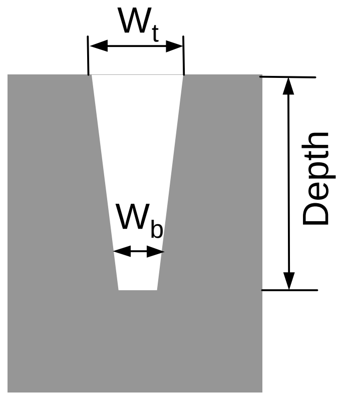
- When the ion energy is very high, the SiO_2 etching is limited by the passivation instead of the ion sputtering yield.
- The etch rate and the bottom width of the trench are saturated at high ion energies.



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

- The polymeric passivation at the surface in fluorocarbon plasma etching of SiO_2 strongly influences the process kinetics and feature profiles.

- With increasing substrate bias, the passivation thickness on the wafer decreases due to increasing ion sputtering, resulting in increasing etch rates and less tapered profiles.

- At high ion energies, sufficient passivation is required for the wafer etching.

- Processes with high passivating neutral to ion flux ratios produce tapered profiles. Both the bottom critical dimension and the etch rate decrease with increasing ratio of passivating neutral to ion fluxes.