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# INVESTIGATION of Si and $SiO_2$ ETCH MECHANISMS USING an INTEGRATED SURFACE KINETICS MODEL

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# AGENDA

- Introduction
- Description of the Model
  - Hybrid Plasma Equipment Model (HPEM)
  - Surface Kinetics Module (SKM)
- $C_2F_6$ etching of Si
  - Reactor wall temperature
- $C_2F_6$ etching of $SiO_2$
  - Substrate bias
- Summary



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# INTRODUCTION

- Fluorocarbon ($C_mF_n$) plasmas are widely used for Si/$SiO_2$ etching due to their favorable kinetic properties and high 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 goal:

    - Develop a surface reaction model
    - Couple the surface model with the bulk plasma simulator - HPEM
    - Quantitatively investigate the surface reaction mechanisms
    - Optimize the processes



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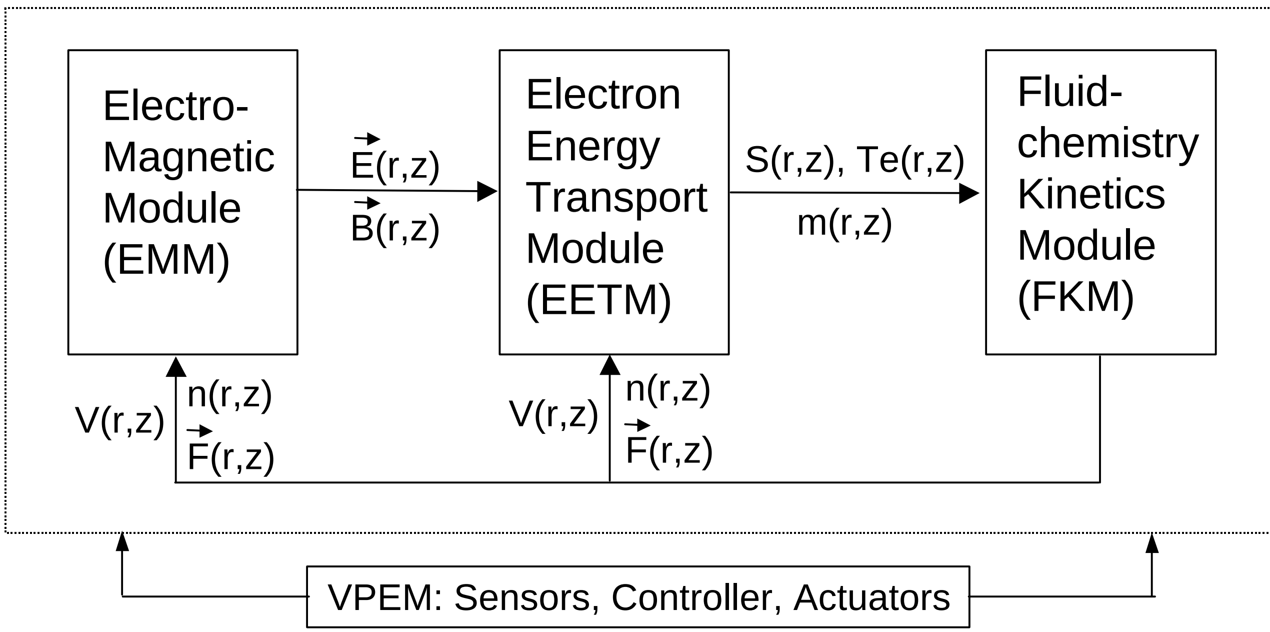
# HYBRID PLASMA EQUIPMENT MODEL (HPEM)

- 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.



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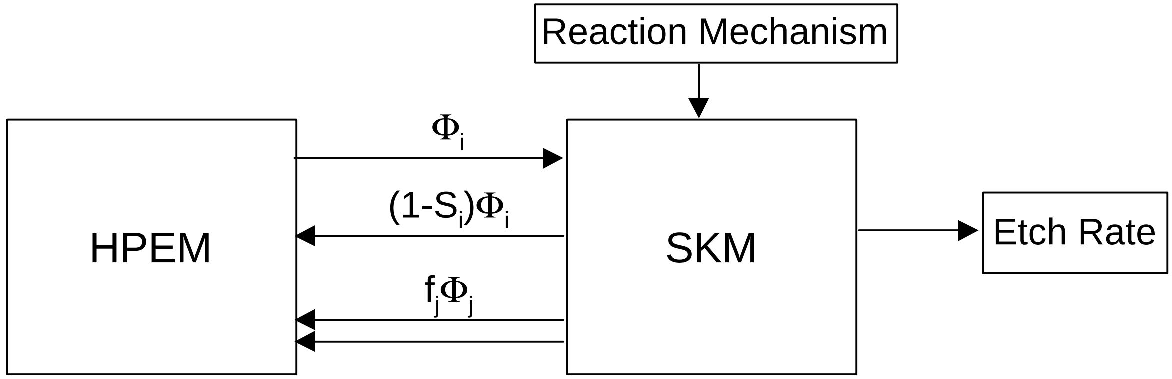
# SURFACE KINETICS MODEL (SKM)

- 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 etch rates




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



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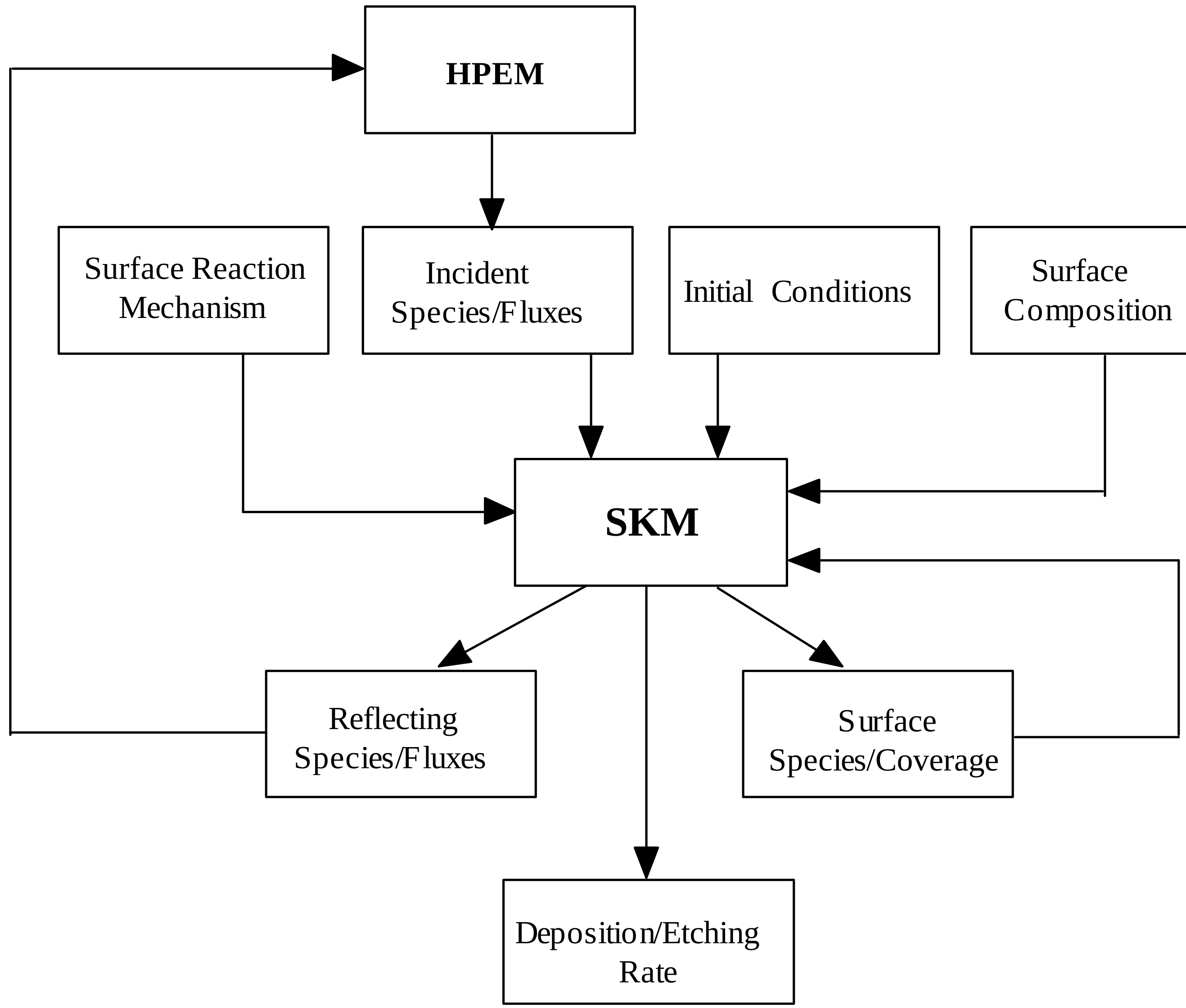
# $C_mF_n$ PLASMA: SURFACE REACTIONS

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## ENERGY DEPENDENCE OF REACTION PROBABILITY

- All surface reactions involving ion reactants in the SKM allow for ion energy dependence.
- Ions are accelerated to the surface through the sheath, arriving on the surface with energy of

$$E_{ion} = Q\ f(r)\ V_{sh}(r)$$

where

Q: Ion charge.

f(r): Ratio of ion mean free path to sheath thickness.

$V_{sh}(r)$: Sheath voltage drop.

- Surface reactions have a general energy dependence given by

$$K = K_0\ (E_{ion}^n - E_{th}^n) / (E_{ref}^n - E_{th}^n)$$

where

$E_{ion}$: Incident ion energy.

$K_0$: Etching yield or reaction probability for ion with energy $E_{ref}$.

$E_{th}$: Threshold energy for the process.

n: Energy dependence (1/2 for this work).



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# POLYMER LAYER PASSIVATION

- During Si/$SiO_2$ etching by fluorocarbon plasmas, a $C_mF_n$ polymer layer will simultaneously deposit on the surface of the wafer and the reactor wall.

- The SKM allows the growth of the passivation layer by $CF_x$ radical polymerization on the surface. F atoms etching and energetic ion sputtering can consume the layer.

- The steady state passivation thickness is reached when the film generation and consumption rates are balanced.

- SKM uses passivation thickness dependent rates for mass and energy transfers through the layer.



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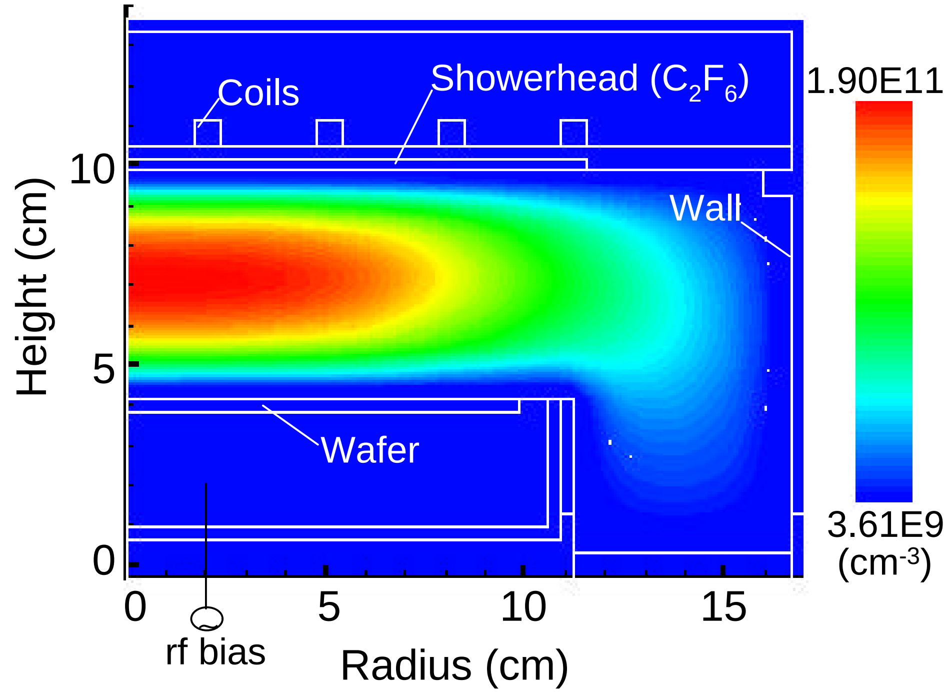
# $C_2F_6$ ETCHING of Si

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

| | | |
|---|---|---|
| $e + C_2F_6$ | $\rightarrow$ | $CF_3^+ + CF_3 + e + e$ |
| $e + C_2F_6$ | $\rightarrow$ | $CF_3 + CF_3 + e$ |
| $e + CF_3$ | $\rightarrow$ | $CF_2 + F + e$ |
| $e + CF_3$ | $\rightarrow$ | $CF_2 + F + F^-$ |
| $e + CF_4$ | $\rightarrow$ | $CF_2 + F + F + e$ |
| $e + CF_4$ | $\rightarrow$ | $CF_3^+ + F + e + e$ |
| $F + F + M$ | $\rightarrow$ | $F_2 + M$ |
| $CF_3 + CF_3 + M$ | $\rightarrow$ | $C_2F_6 + M$ |
| $CF_2 + F_2$ | $\rightarrow$ | $CF_3 + F$ |
| $CF_3 + F_2$ | $\rightarrow$ | $CF_4 + F$ |
| $CF_2 + CF_3$ | $\rightarrow$ | $C_2F_5$ |
| $C_2F_5 + F$ | $\rightarrow$ | $CF_3 + CF_3$ |
| $CF_3 + F$ | $\rightarrow$ | $CF_4$ |
| $CF_2 + F$ | $\rightarrow$ | $CF_3$ |

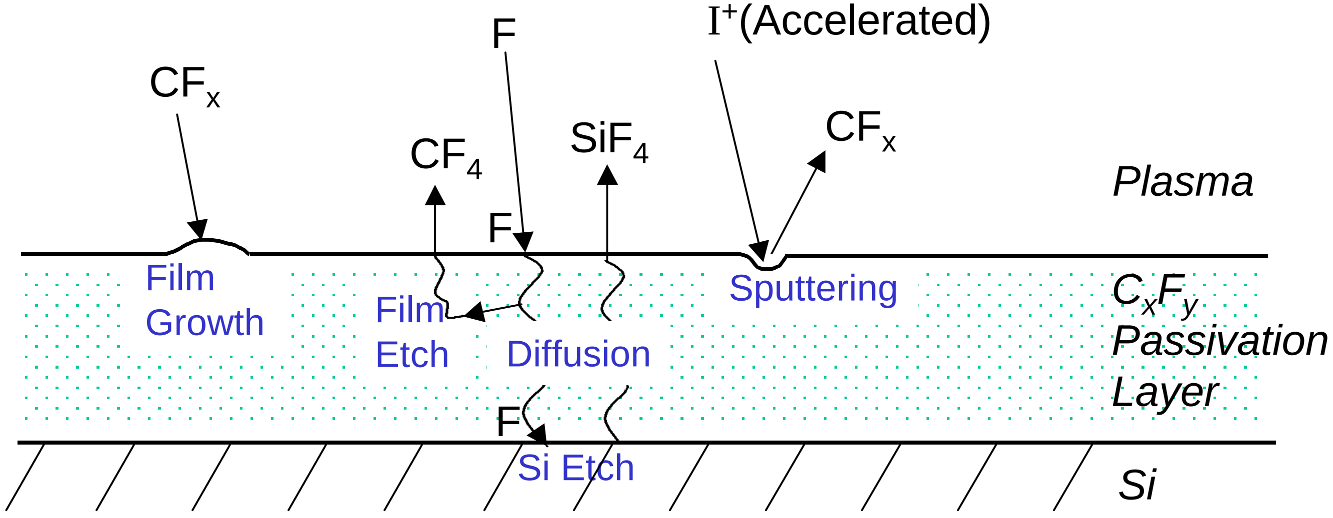
- Electron Density




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

# REACTION MECHANISM FOR $C_2F_6$ ETCHING OF Si

- The reaction mechanism was based on the work of G. S. Oehrlein *et al* *.
- A $C_xF_y$ polymer layer is formed on the Si surface in coincidence with Si etching. The steady state passivation layer thickness is a balance of $CF_x$ deposition, ion sputtering and F etching of the layer.
- Si etching precursor (F) needs to diffuse through the passivation layer.




* T.E.F.M. Standert, M.Scharkens, N.R.Rueger, P.G.M. Sebel, and G.S. Oehrlein, J. Vac. Sci. Technol. A 16(1), 239 (1998)



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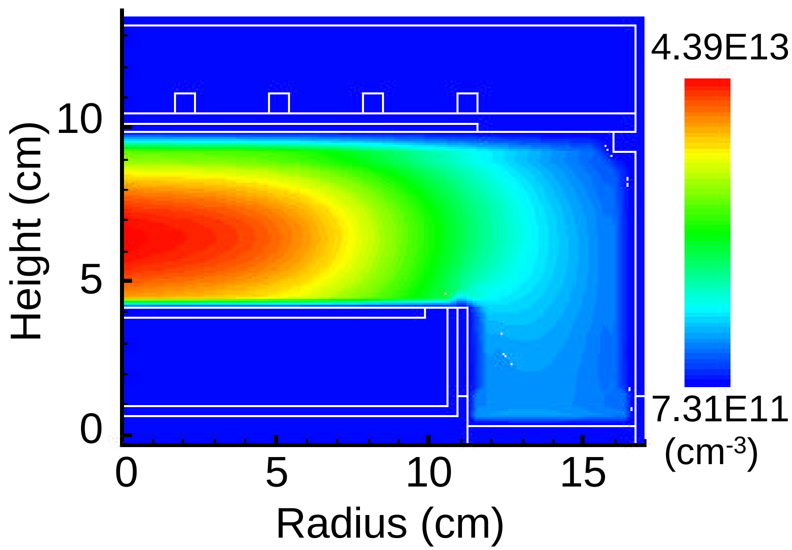
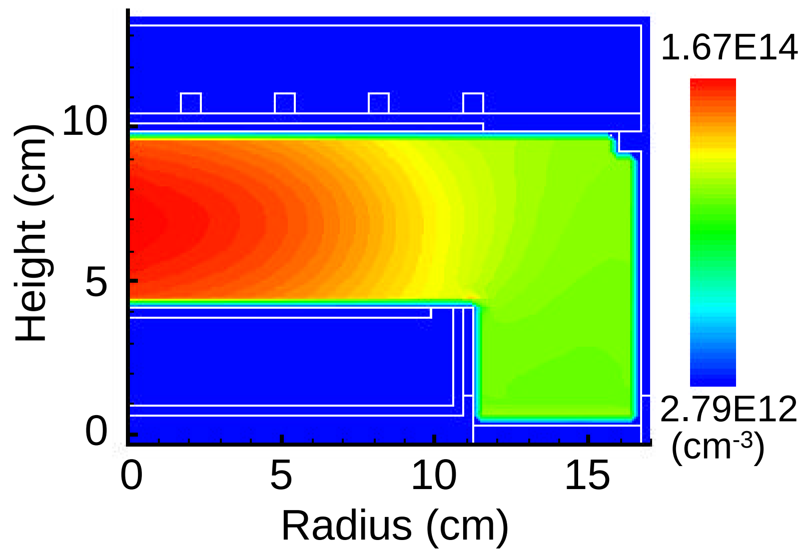
# RADICAL DENSITIES: BASE CASE

- Radical densities peak on the axis.
- The less uniform $CF_2$ density distribution is 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.



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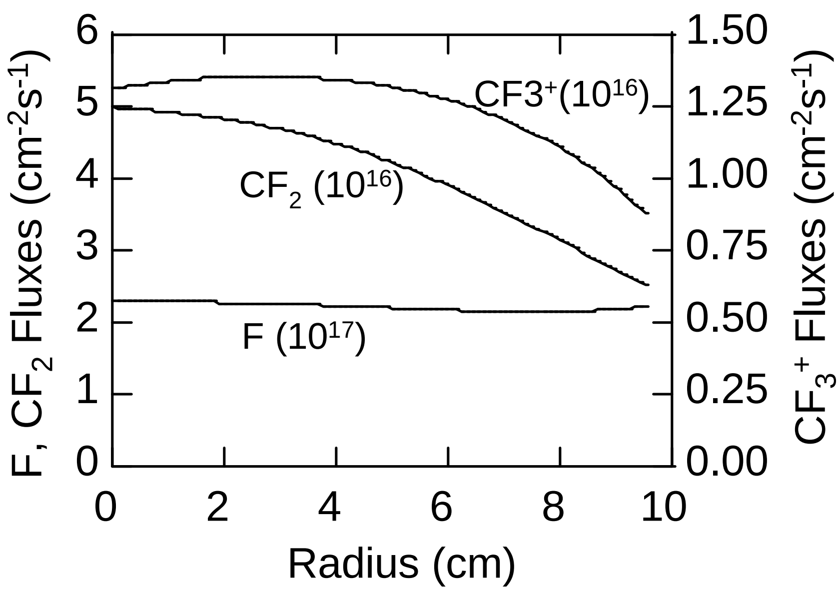
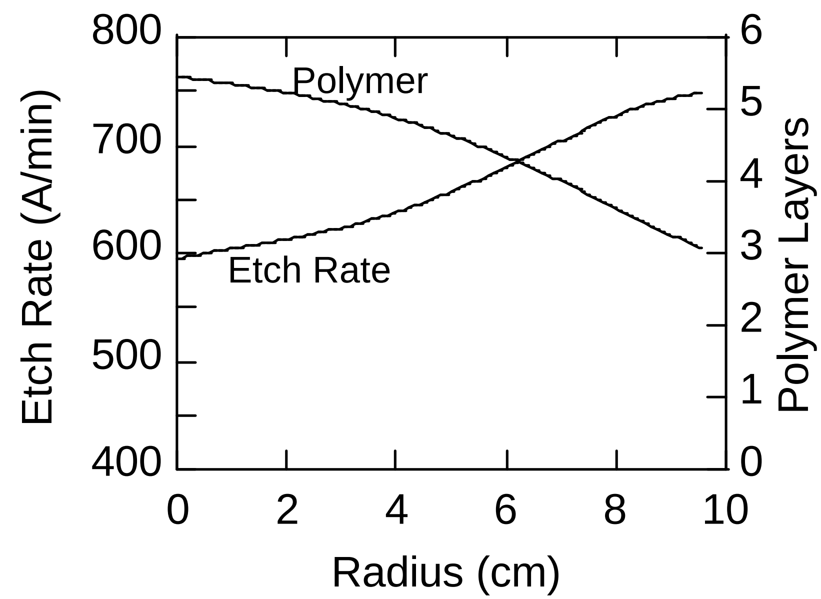
# RADIAL DISTRIBUTIONS: FLUXES & ETCH RATE

- Radial flux distribution of $CF_2$ is less uniform than that for F as a consequence of the low sticking coefficient for F.
- Polymer thickness follows the $CF_2$ flux for this case.
- Etch rate increases in the radial direction, inversely to the polymer thickness due to F atom diffusion.



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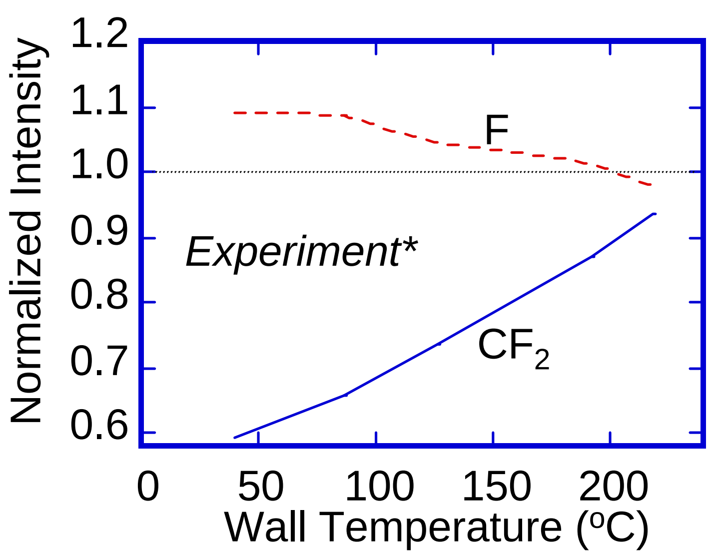
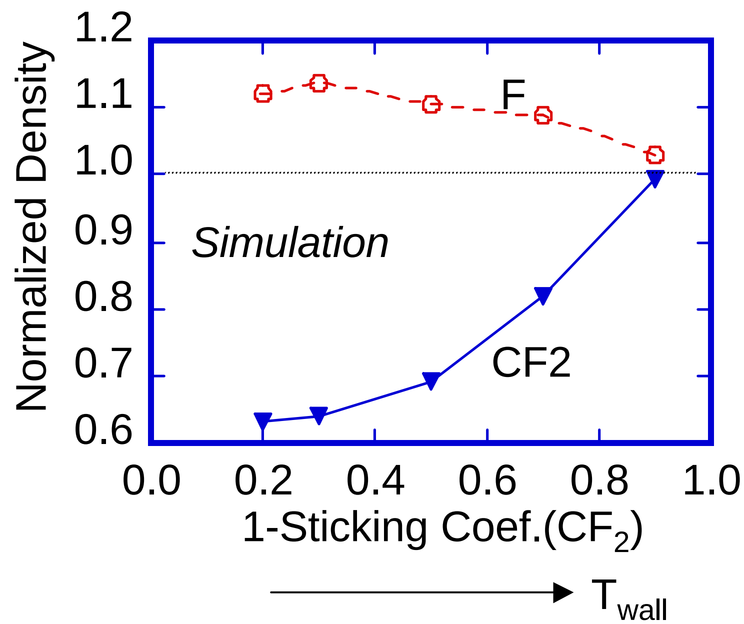
# INFLUENCE OF WALL TEMPERATURE

- Experiments showed a variation of radical densities vs. $T_{wall}$.* We simulated the consequence of varying $T_{wall}$ by modifying the sticking coefficient of $CF_2$ to the wall.
- With increasing $T_{wall}$, the $CF_2$ loss rate is smaller due to the lower sticking coefficient, which produces an increase of $CF_2$ density in the bulk plasma.
- The resulting gas chemistry favors consumption of F atoms. So F density drops.

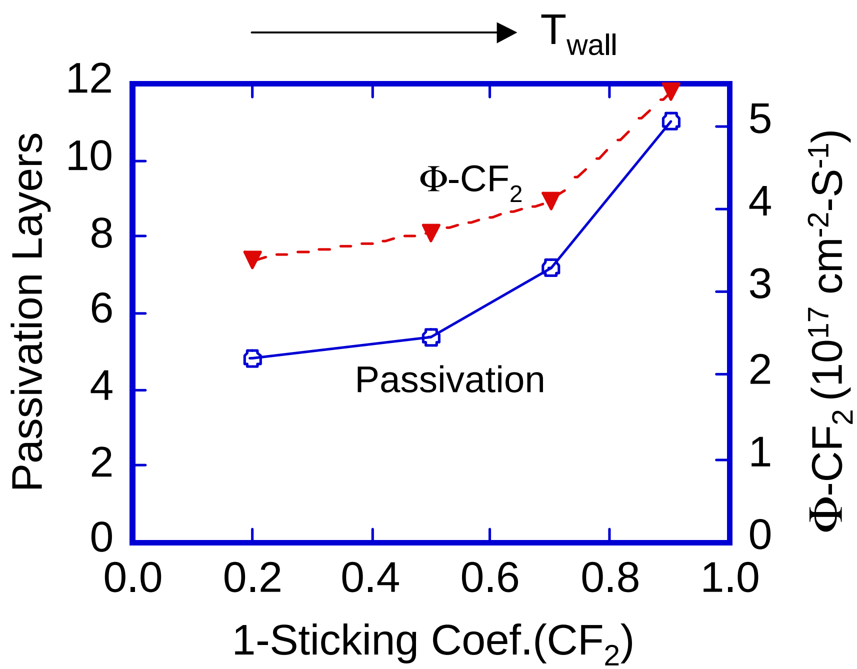


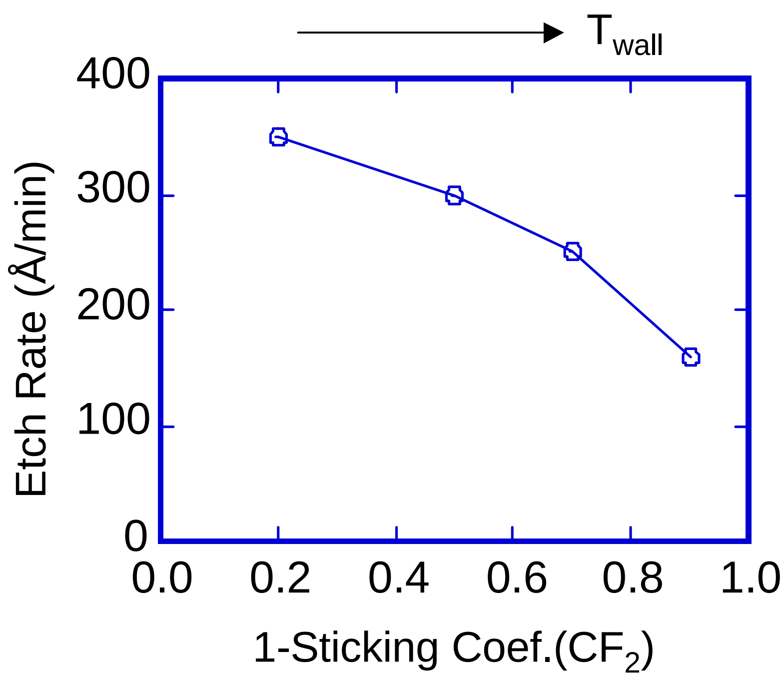




* M.Scharkens, R.C.M. Bosch, and G.S. Oehrlein, J. Vac. Sci. Technol. A 16(1), 239 (1998)

# PASSIVATION LAYER AND ETCH RATE

- As wall temperature increases, the increased $CF_2$ density produces larger fluxes to the wafer. This leads to a thicker passivation layer.
- The diffusion flux of the Si etching precursor (F) through the passivation layer decreases with increasing passivation, so the etch rate drops.



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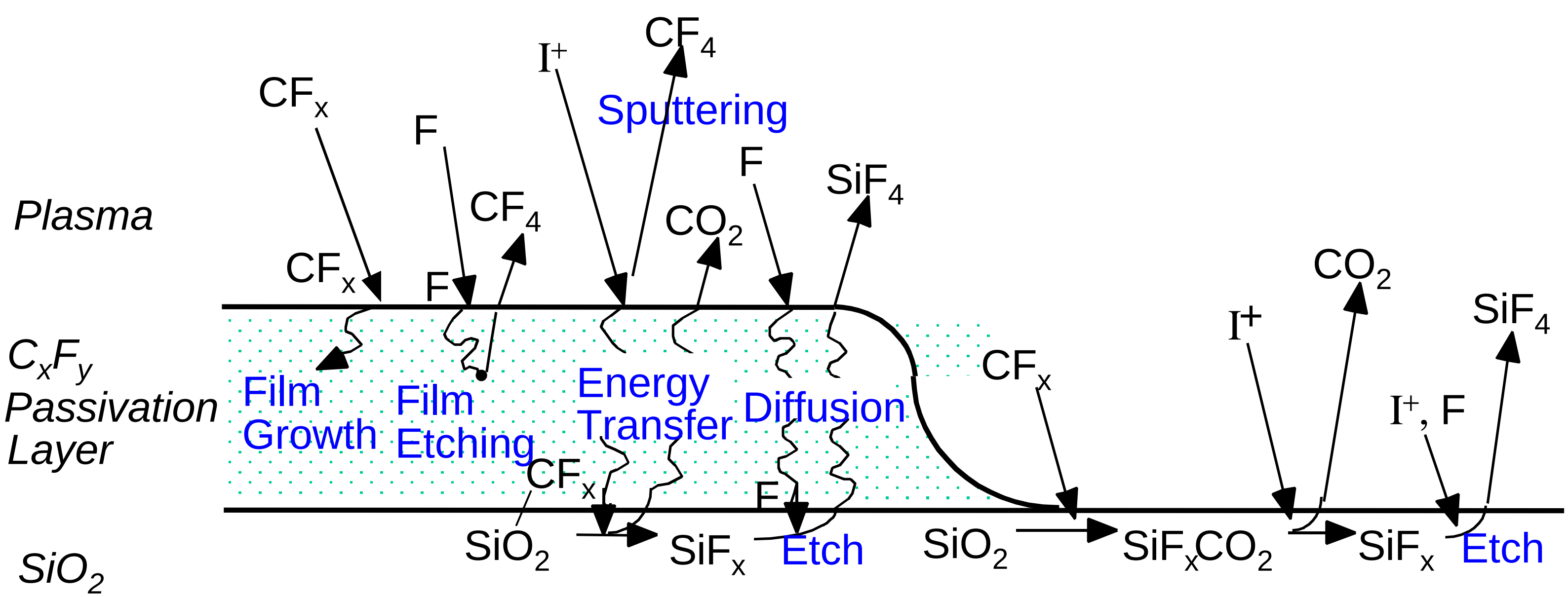
# REACTION MECHANISM FOR $C_2F_6$ ETCHING OF $SiO_2$

- 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.



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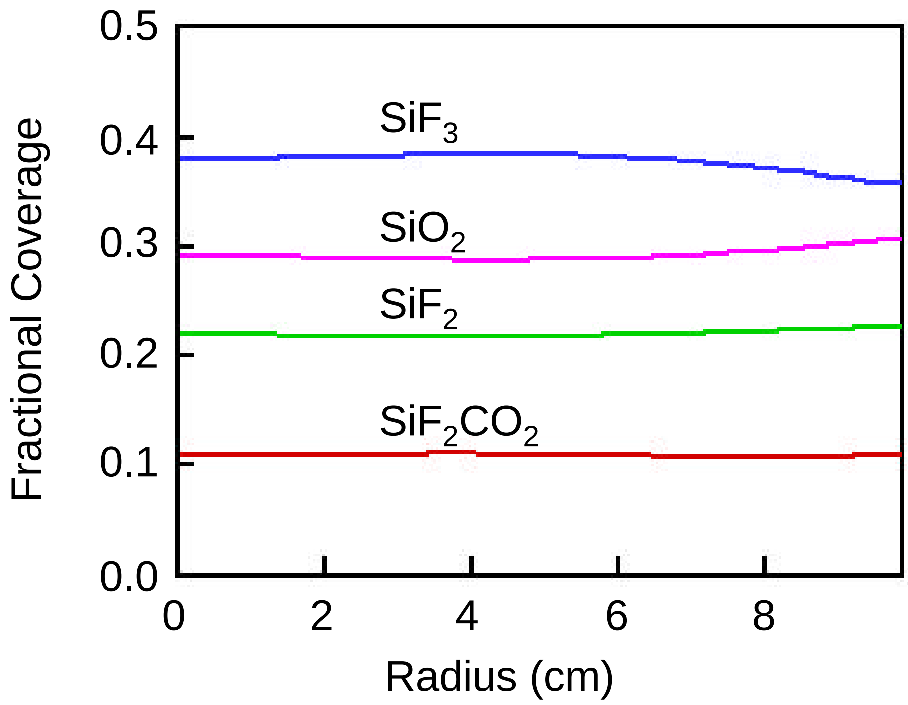
# SURFACE COVERAGE

- The wafer surface sites are occupied by several surface species.
- The surface coverages at steady state depend on the relative rates of
  - complex formation
  - F atom etching
  - Ion activation
  - Sputtering




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



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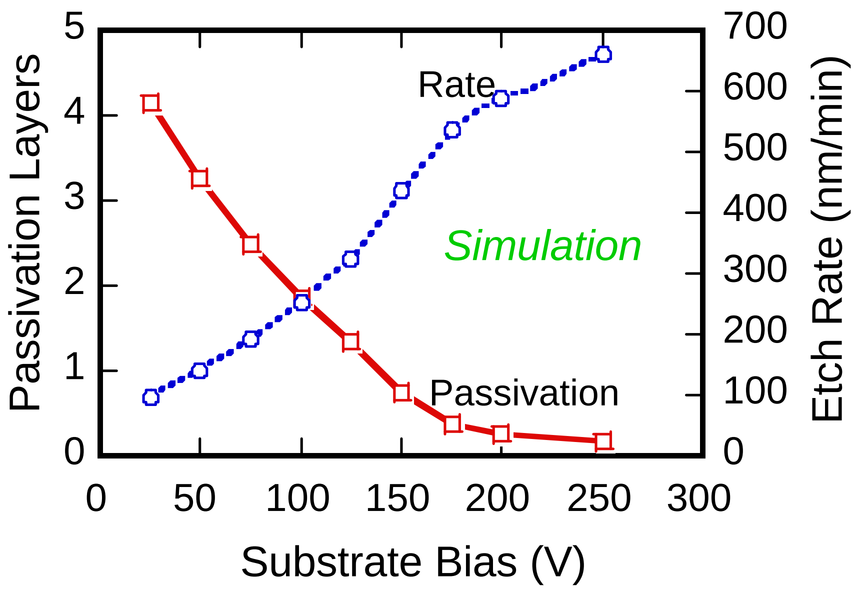
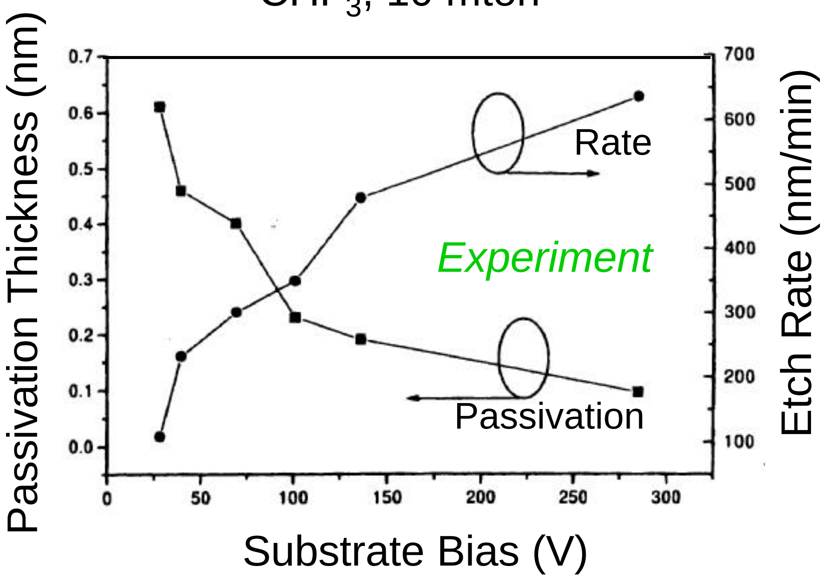
# SUBSTRATE BIAS

- With increasing substrate bias, the passivation layer thickness decreases and the etch rate increases.
- Simulations and experiments obtained similar trends.

• $C_2F_6$, 10 mtorr




• $CHF_3$, 10 mtorr *




*N.R. Rueger, G.S. Oehrlein et al, J. Vac. Sci. Technol. A 15, 1881 (1997)

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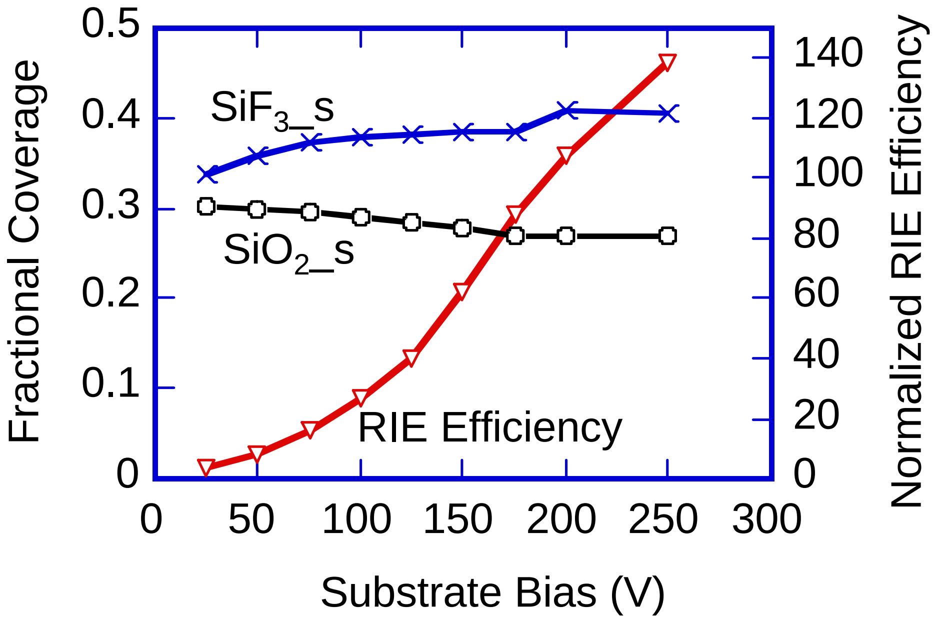
# SUBSTRATE BIAS

- With increasing bias, the variation in surface coverage is not big when the processes are not limited by the F atom diffusion.
- The normalized reactive ion etch efficiency increases with increasing substrate bias due to the increase in sheath voltage and decrease in passivation thickness.




Normalized RIE Efficiency

$$\propto \frac{V_{sheath}}{(1+0.3\times[P\_s])^2}$$



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# SUMMARY

- The Surface Kinetics Model (SKM) has been coupled with the HPEM to simulate surface interactions and their influences on the bulk plasma.

- In Si etching, higher loss of $CF_2$ on reactor walls leads to lower $CF_2$ density in the gas phase. This produces thinner passivation layers and higher etch rates.

- Consumption of $C_xF_y$ at the polymer-$SiO_2$ interface during the $SiO_2$ etching leads to thinner passivation compared with Si etching.

- In $SiO_2$ etching, with increasing substrate bias, the surface coverages change little when the process is not limited by F diffusion.

- Increasing bias leads to higher sheath voltage and thinner passivation, so higher RIE efficiency. The etch rate increases accordingly.