45th AVS International Symposium
Baltimore, Maryland
2-6 November, 1998

AN INTEGRATED SURFACE KINETICS-PLASMA EQUIPMENT MODEL FOR ETCHING†

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† Work supported by SRC and NSF.

AGENDA

- **Introduction**
- **Description of the Integrated Surface-Plasma Model**
- **C_2F_6 etching of Si**
    - **Dependence on wall temperature**
    - **Dependence on substrate bias**
- **Cl_2 etching of p-Si**
    - **Radical and Ion fluxes**
    - **Etch rate**
- **Conclusion**

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INTRODUCTION: PlASMA-SURFACE INTERACTION

- In plasma etching, reactant fluxes interact with both the substrate and the wall of the reactor. The reaction products from these surfaces return to the plasma to modify the gas composition and thus plasma properties, and ultimately fluxes back to the surfaces.

- Since the walls of the reactor have a larger area than the wafer, the plasma-reactor wall interaction is very important for determining the plasma composition.

- Our goal is to develop a self-consistent accounting of surface chemistry combined with a plasma model to address the omni-surface reactions, to investigate surface reaction mechanisms.

- This was accomplished by developing a Surface-Kinetics-Module for the Hybrid Plasma Equipment Model.

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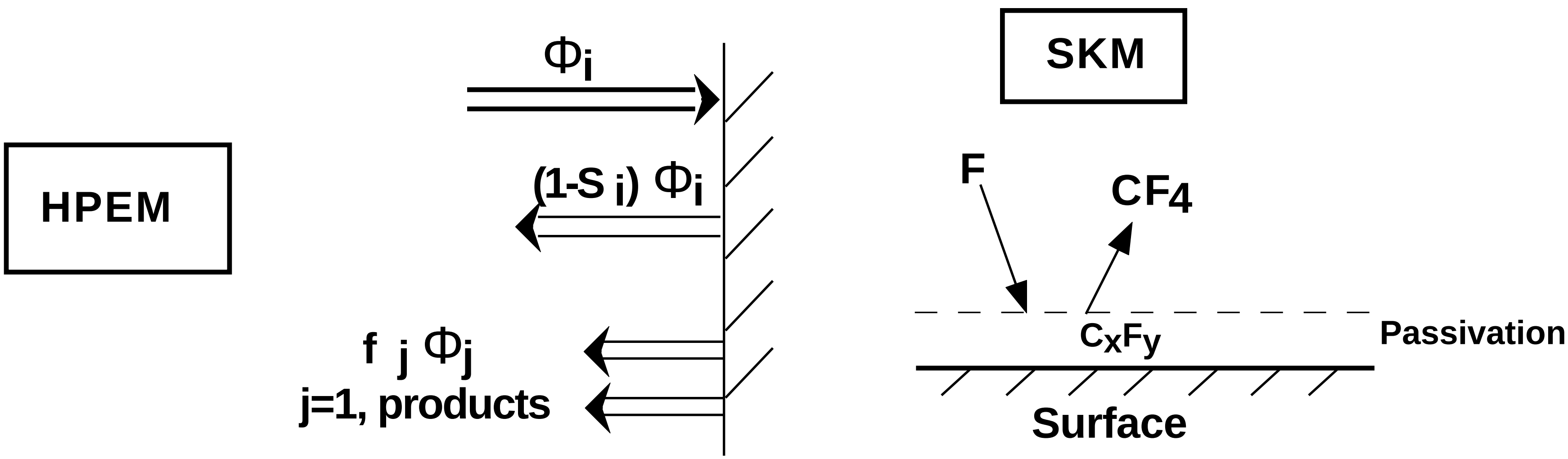
DESCRIPTION OF THE SURFACE-KINETICS-MODULE

- The Surface-Kinetics-Module (SKM) is an integrated module of the Hybrid Plasma Equipment Model (HPEM).
- Using reactant fluxes to surfaces from the HPEM, the SKM updates the surface sticking and product reflection coefficients used as surface boundary conditions in the HPEM.



- This is accomplished by formulating a multi-layer surface site balance model at every mesh point along the plasma-surface boundary.

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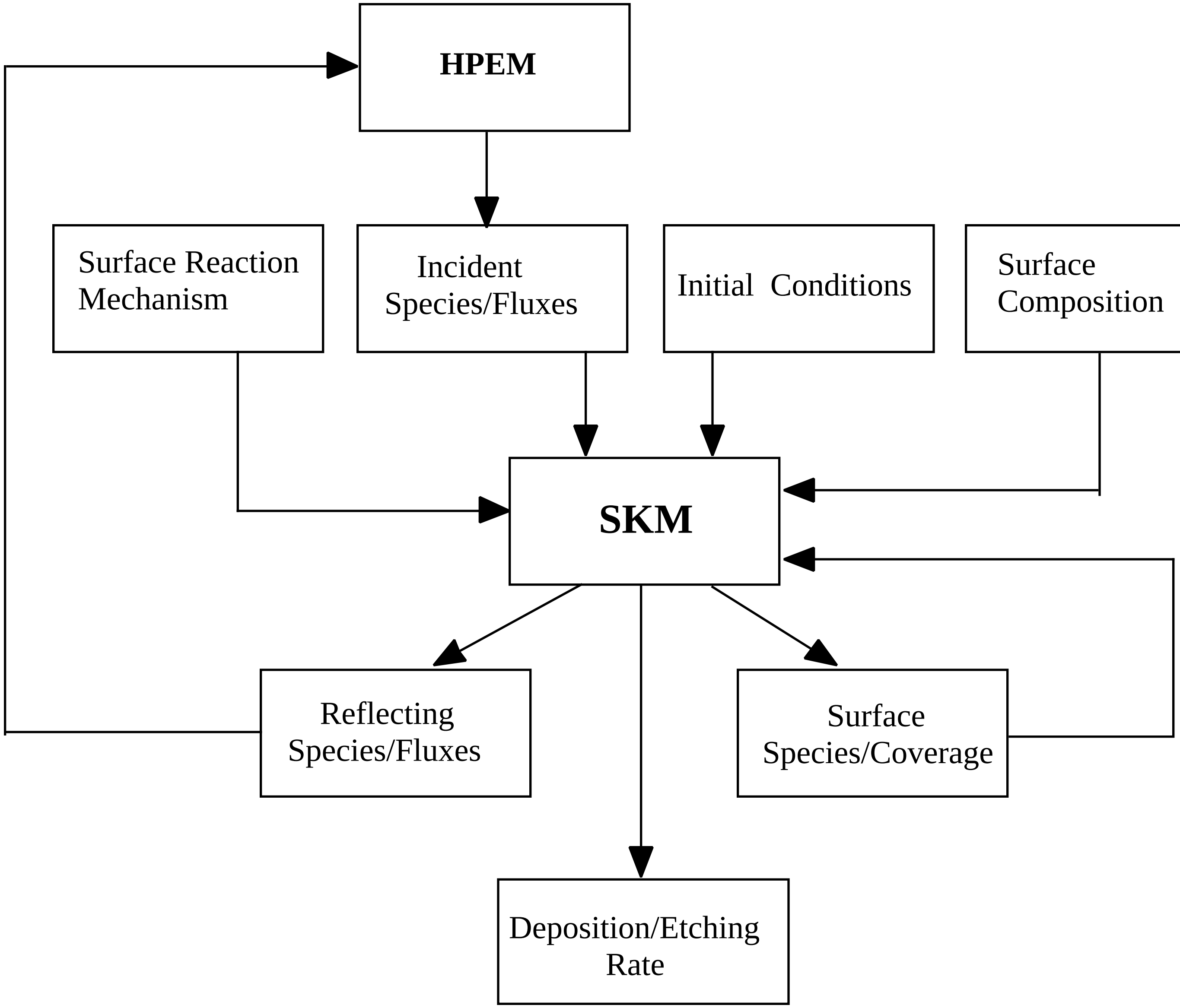
SCHEMATIC OF THE SURFACE-KINETICS-MODULE



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ENERGY DEPENDENCE OF REACTIONS

- All surface reactions 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 (function of location)

$V_{sh}(r)$ = Sheath voltage drop (function of location)

- Surface reactions have a general energy dependence given by

$$K = k_0 \left(E_{ion}^n - E_{th}^n\right) / \left(E_{ref}^n - E_{th}^n\right)$$

where

k_0 = Etching yield on reaction probability for ion with energy E_{ref} .

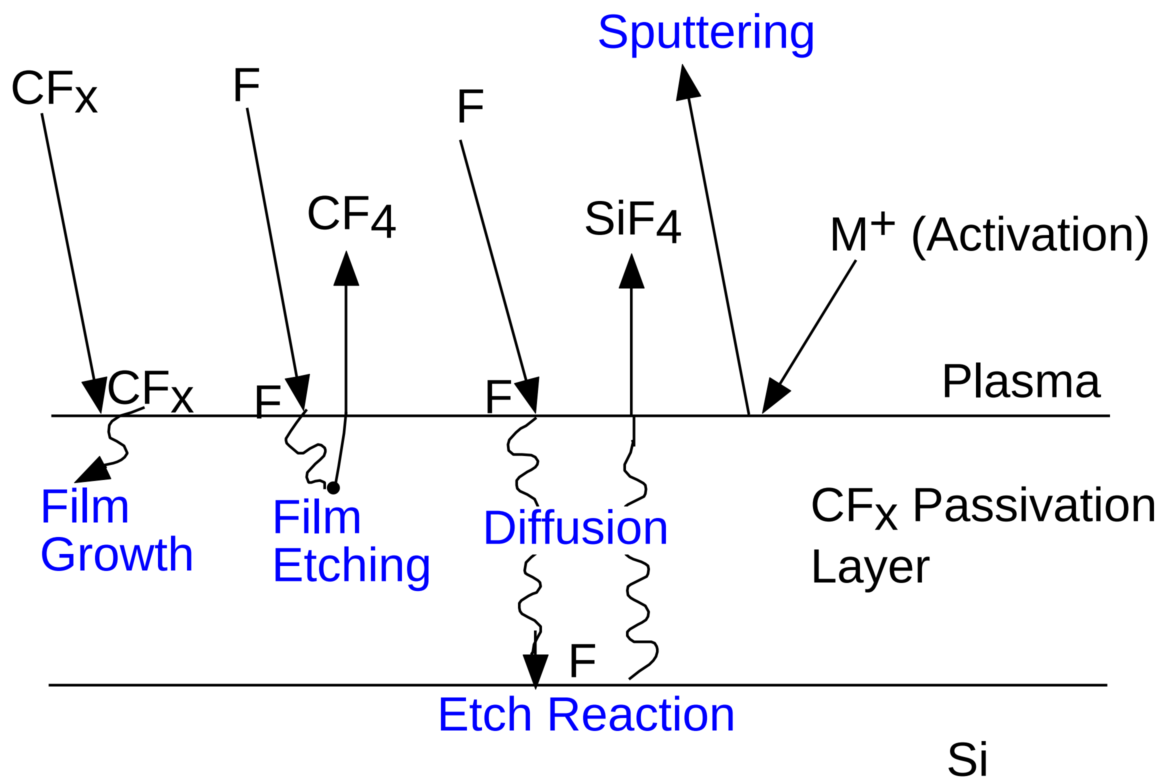
E_{th} = Threshold energy for process.

n = Energy dependence (1/2 for all etching process in this work)

REACTION MECHANISM FOR C_2F_6 ETCHING OF Si

- **C_2F_6 etching of Si in an ICP reactor has been investigated.**
- **The reaction mechanism is based on the works of T.E.F.M. Standert et. al *.**
- **Representative surface reactions ("_s" denotes surface species)**
  W: Reactor wall, P: Passivation layer

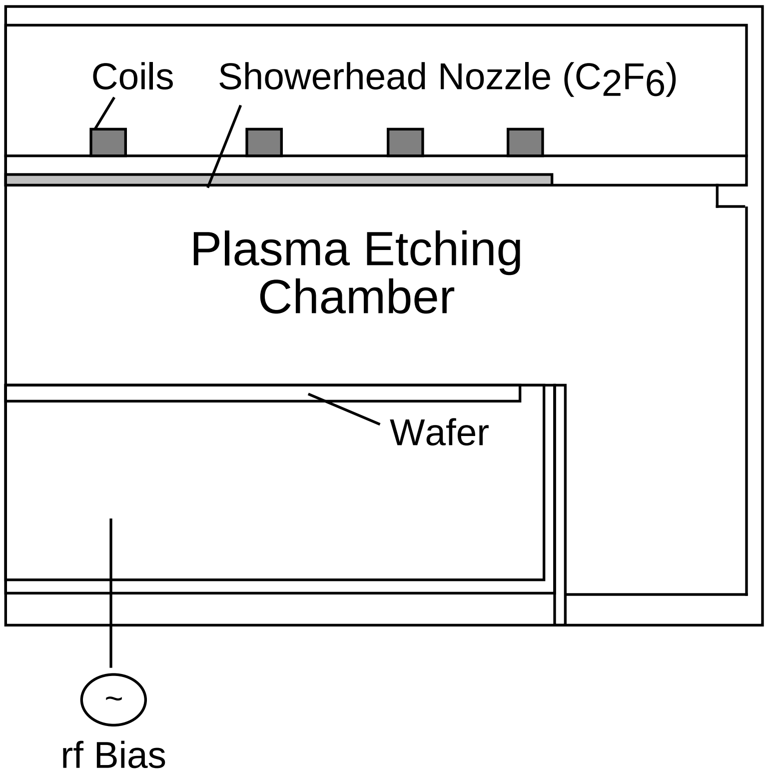
CF_2	--> P
CF_3^+ + P	--> CF_4
F + P	--> F_t
F_t	--> F_i
F_i + Si_s	--> SiF_s
F_i + SiF_s	--> SiF_2_s
F_i + SiF_2_s	--> SiF_3_s
F_i + SiF_3_s	--> SiF_4
CF_2 + W	--> W



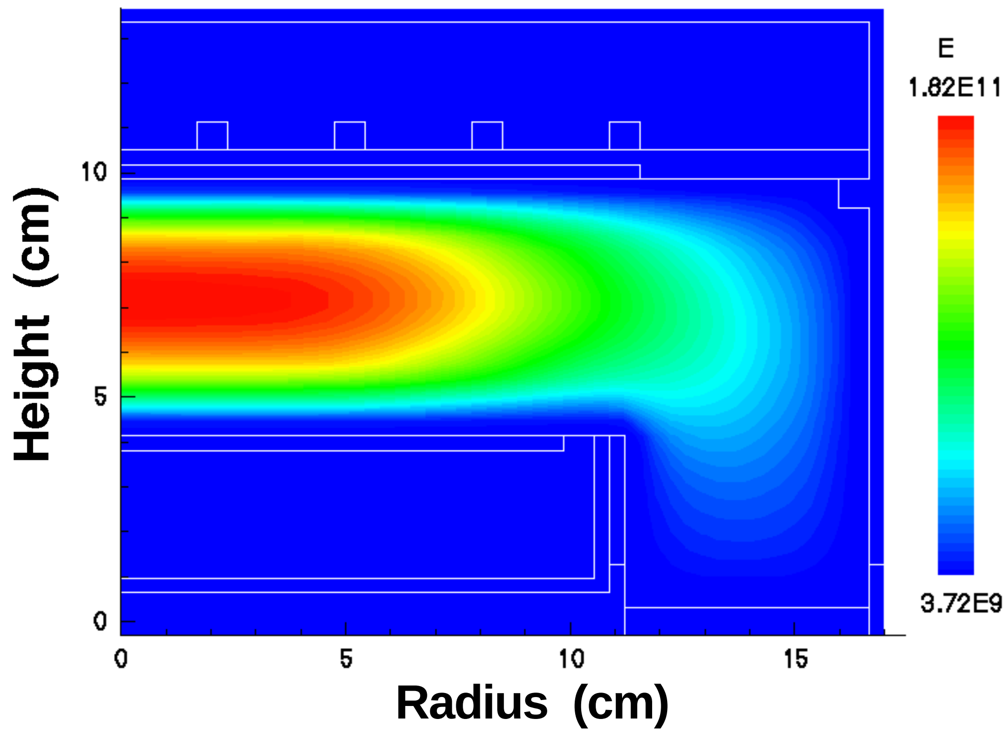
* T.E.F.M. Standert, M.Scharkens, N.R. Rueger, P.G.M. Sebel, and G.S. Oehrlein, J.Vac. Sci. Technol. A 16(1), 239 (1998)

ICP REACTOR: TYPICAL CONDITIONS

- **Simulations were performed for an ICP reactor having a substrate bias.**



- **Electron Density**



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

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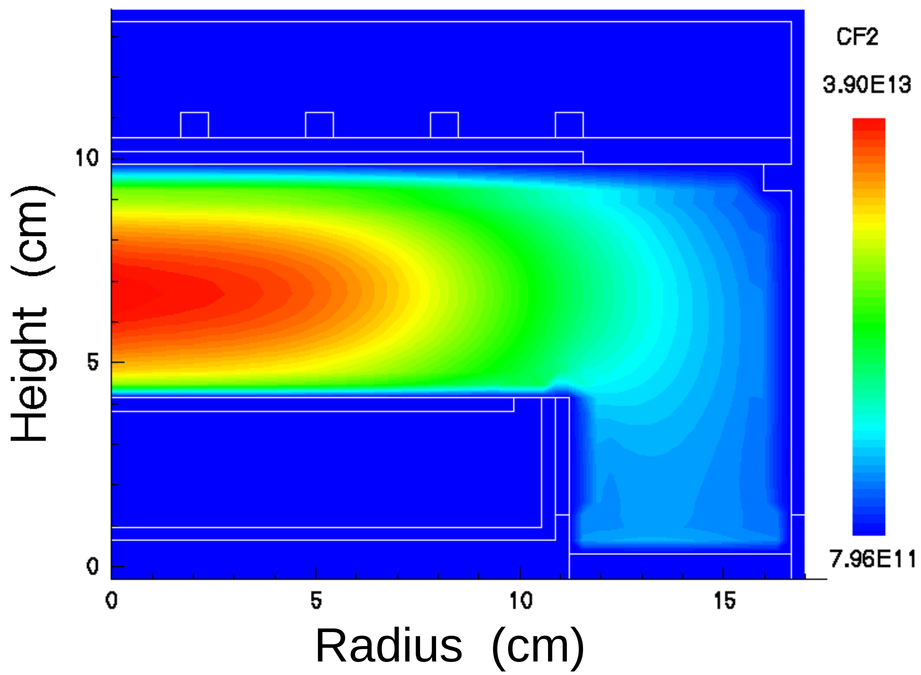
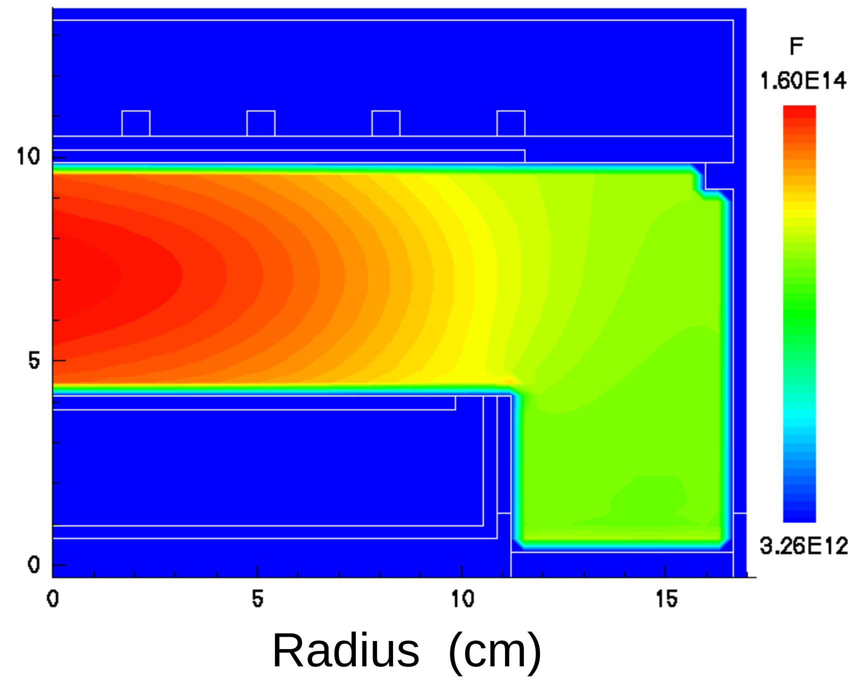
RADICAL DENSITIES: BASE CASE

- CF_2 and F radical density distributions.
- High CF_2 density will cause thick passivation layer deposited on the wafer.
- F radical contributes to the etching of Si to form SiF_4 gas.

• CF_2 Density



• F Density



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

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WALL TEMPERATURE DEPENDENCE

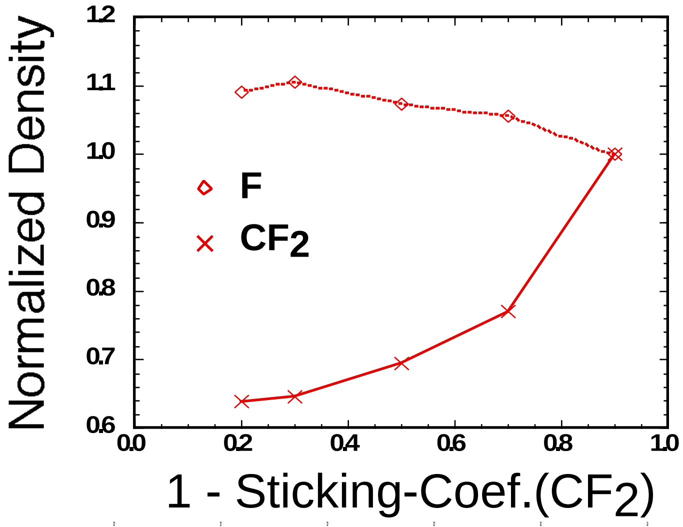
- Experiments (M. Schaepkens et. al *) have shown a variation of radical densities as the wall temperature changes.
- We simulated the consequences of wall temperature by modifying the sticking coefficient of CF_2 to the wall.
- With increasing wall temperature, the CF_2 loss rate is smaller due to the lower sticking coefficient, which produces an increase of CF_2 density in the bulk plasma region.
- The resulting gas chemistry favors consumption of F atoms:

  $CF_2 + F_2 > CF_3 + F$ *slow*

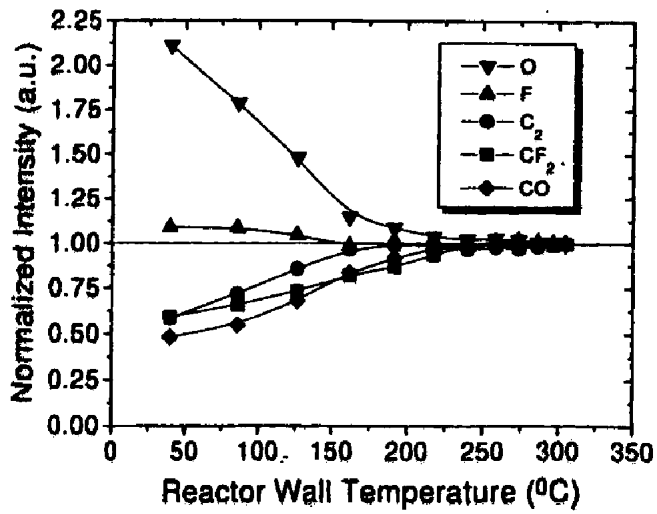
  $CF_2 + F > CF_3$ *fast*

  So increased CF_2 density will induce decreased F density.

• Simulation results



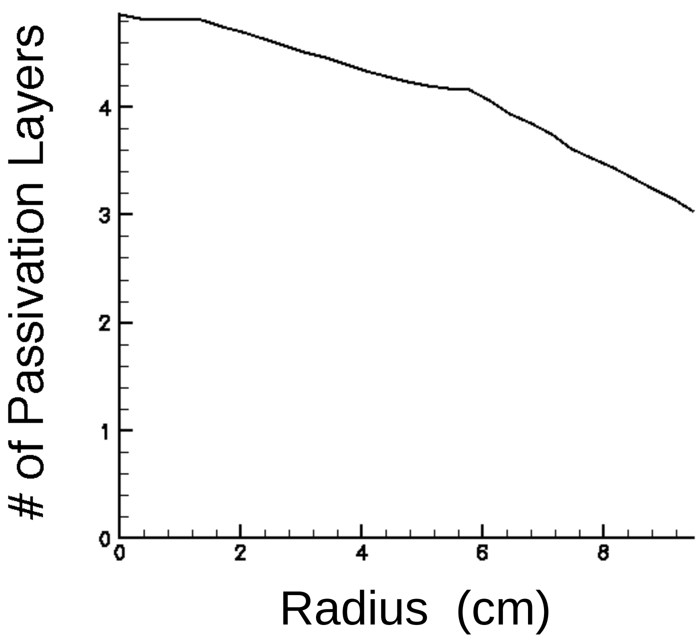
• Experimental results

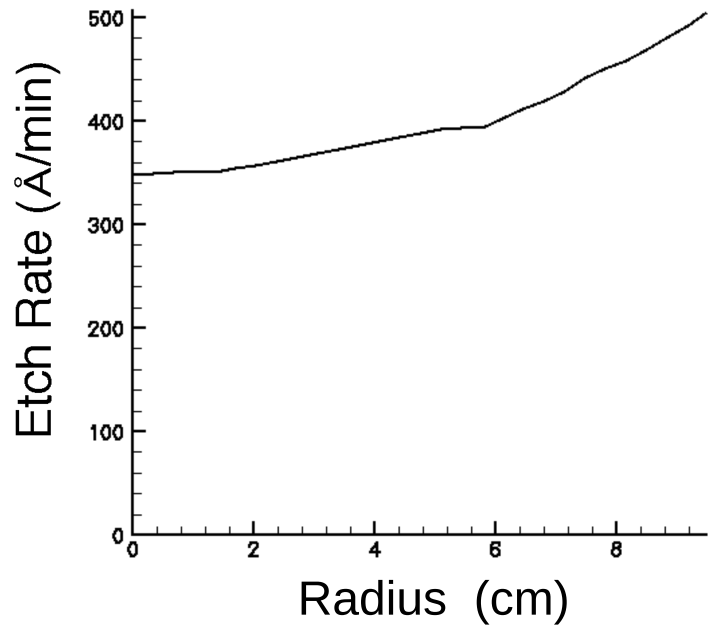


* M. Schaepkens, R.C.M. Bosch, G.S. Oehlein, J. Vac. Sci. Technol. A 16(4), 2099 (1998)

PASSIVATION LAYER AND ETCH RATE

- **Conditions were chosen which purposely produce non-uniform fluxes to demonstrate the influence of passivation layer thickness on etch rate.**
- **Higher CF_2 fluxes at the center of the substrate produce a thicker passivation layer.**
- **This in turn produces a minimum in etch rate.**





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

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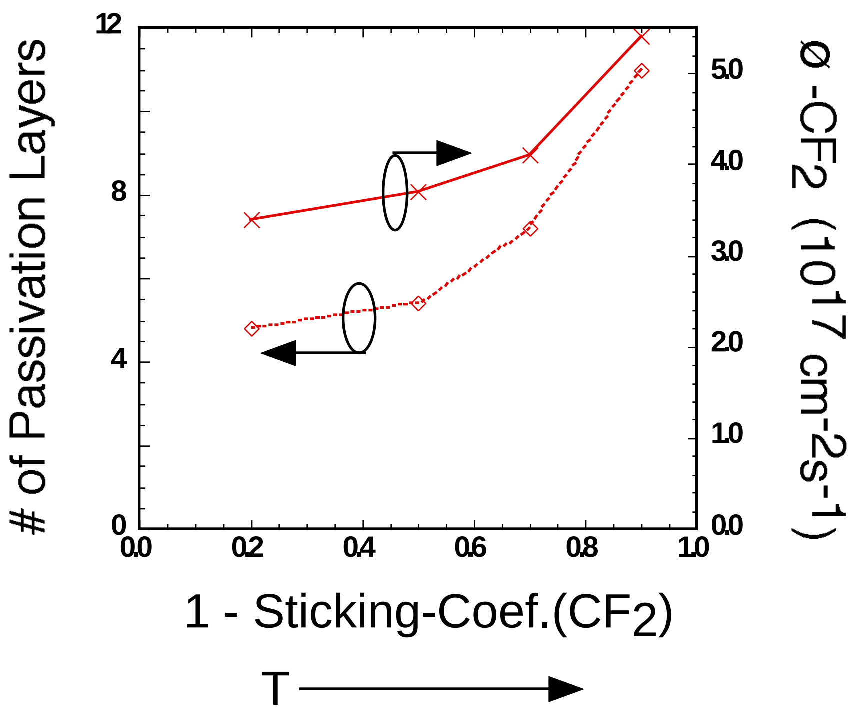
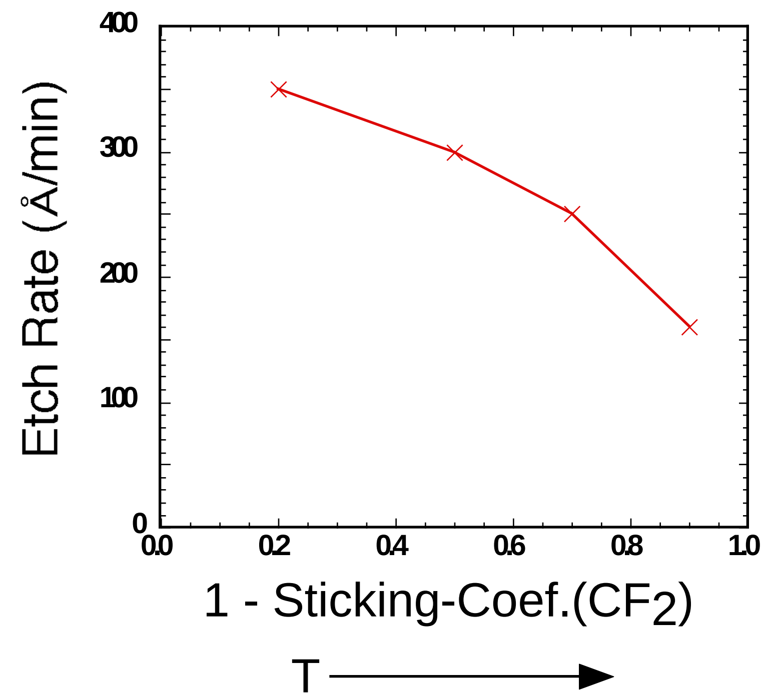
PASSIVATION LAYER AND ETCH RATE vs.WALL TEMPERATURE

- The passivation layer thickness and etch rate at the center of the wafer depend on the wall temperature due to the change in CF_2 and F densities.
- As the wall temperature increases, the increase in CF_2 density produces an increase of the passivation layer thickness, and a decrease in etch rate.





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

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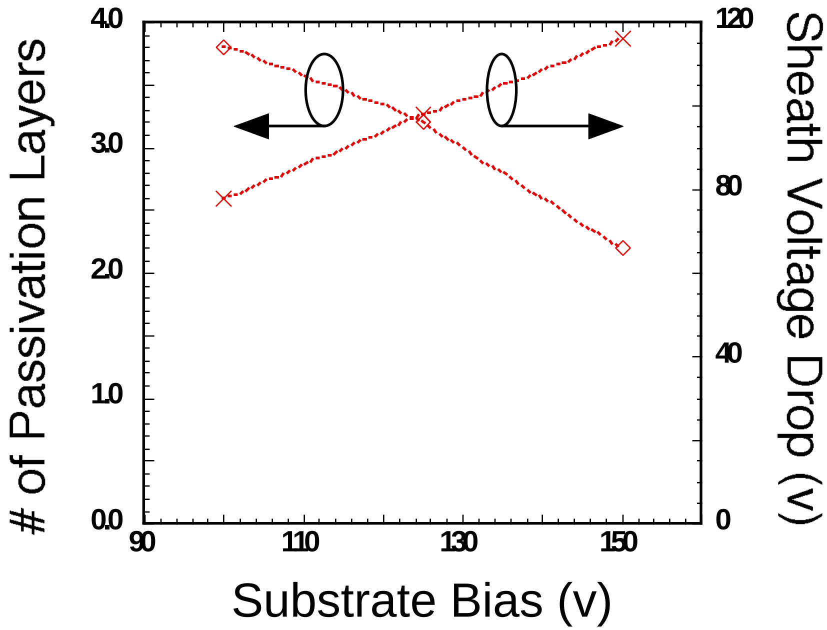
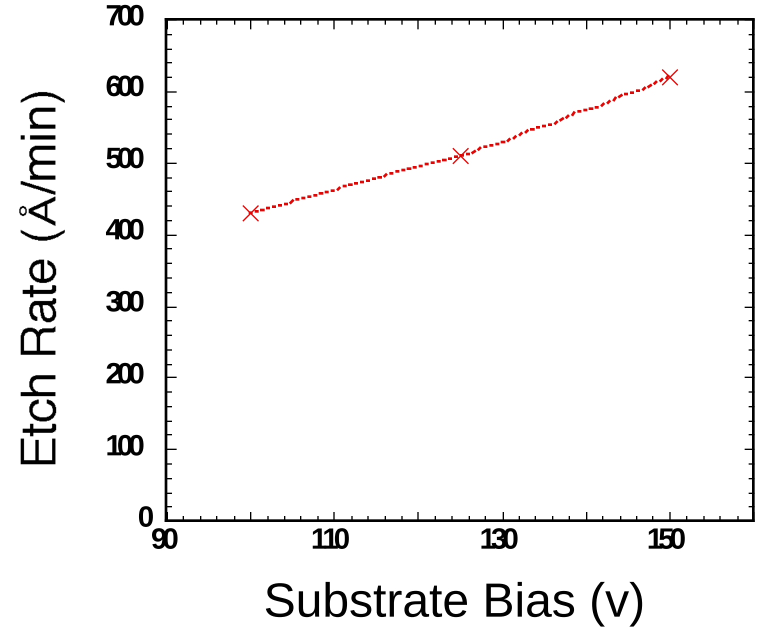
PASSIVATION LAYER AND ETCH RATE vs. BIAS

- As the bias voltage increases, the ion bombardment energy increases, leading to a decrease in the passivation layer thickness. The etch rate therefore increases due to a higher F atom diffusion flux through the passivation layer.





- C_2F_6, 6 mTorr, 200 sccm, 1000 W ICP.

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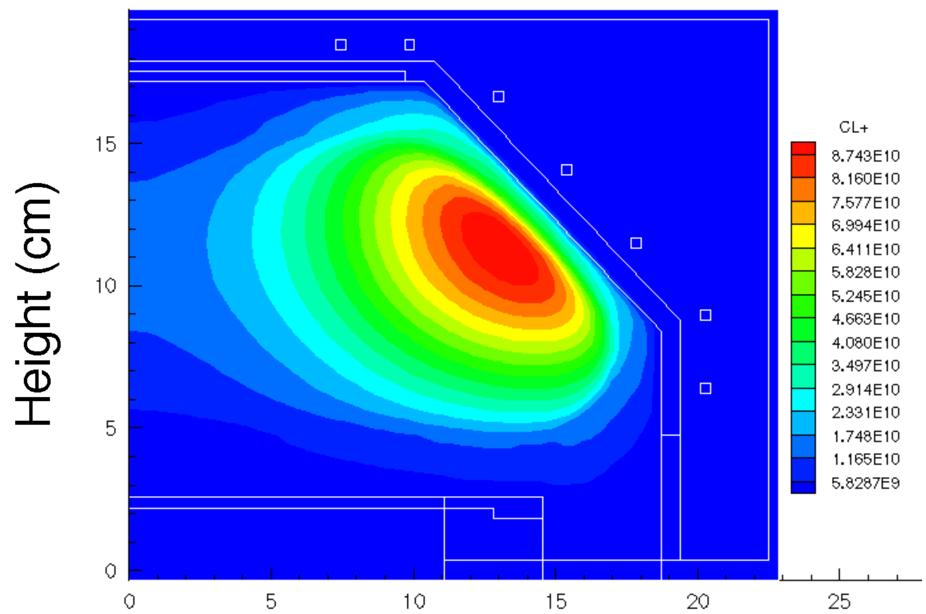
Cl_2 ETCHING OF p-Si

- **The SKM was applied to the analysis of Cl_2 etching of p-Si.**
- **Representative surface reactions ("_s" denotes surface species)**

Cl + Si_s	**--> SiCl_s**
Cl + SiCl_s	**--> $SiCl_2$_s**
Cl + $SiCl_2$_s	**--> $SiCl_3$_s**
Cl* + SiCl_s	**--> $SiCl_2$ + Si_s**
Cl* + $SiCl_3$_s	**--> $SiCl_4$ + Si_s**
Cl^+ + SiCl_s	**--> $SiCl_2$ + Si_s**
Cl^+ + $SiCl_2$_s	**--> $SiCl_2$ + Cl + Si_s**
Cl^+ + $SiCl_3$_s	**--> $SiCl_4$ + Si_s**
Cl_2^+ + $SiCl_2$_s	**--> $SiCl_4$ + Si_s**
Ar^+ + $SiCl_2$_s	**--> $SiCl_2$ + Ar + Si_s**
Cl + W_s	**--> WCl_s**
Cl^+ + WCl_s	**--> W_s + Cl_2**

- Cl^+ Density

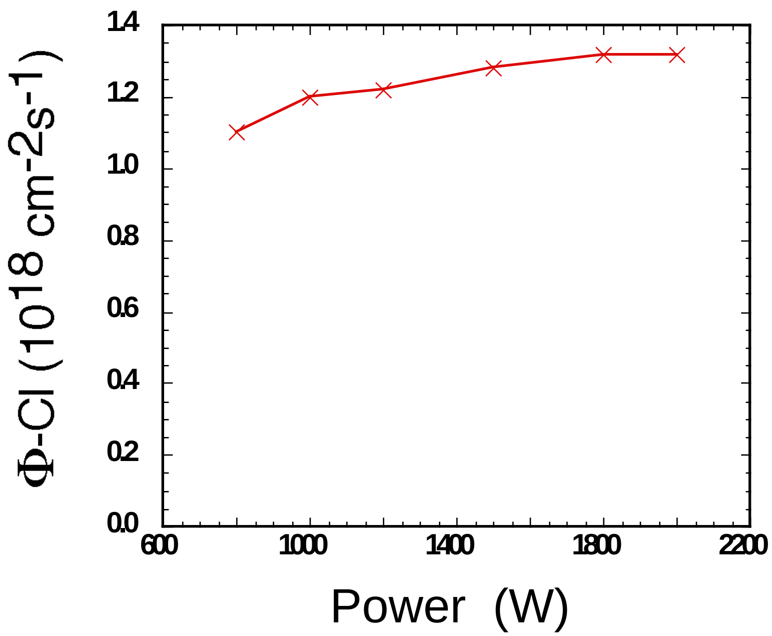


- **Ar/Cl_2 = 70/30, 10 mTorr, 100 sccm, 800 W ICP**

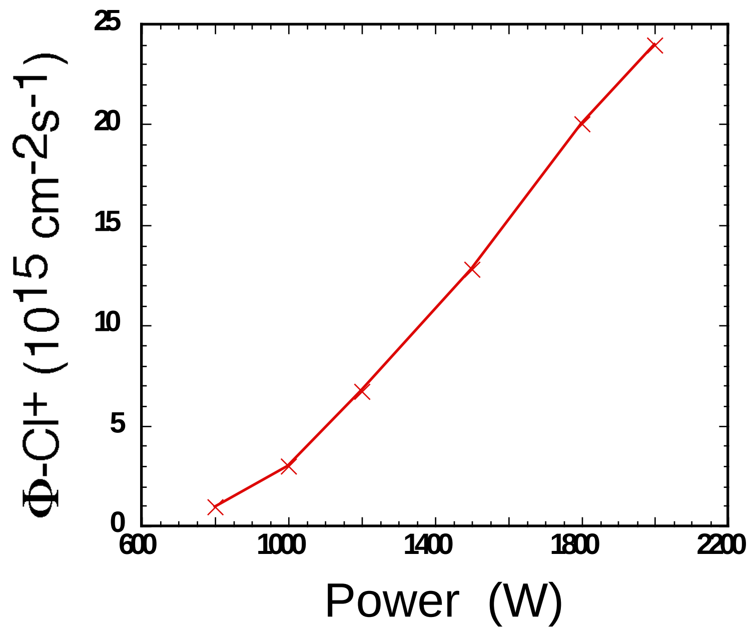
RADICAL AND ION FLUXES

- Since Cl_2 is almost totally dissociated for the conditions of interests, the Cl atom flux to the substrate is nearly constant with power.
- The ion flux increases nearly linearly with power.

Cl Flux



Cl^+ Flux



- Ar/Cl_2 = 70/30, 10 mTorr, 100 sccm

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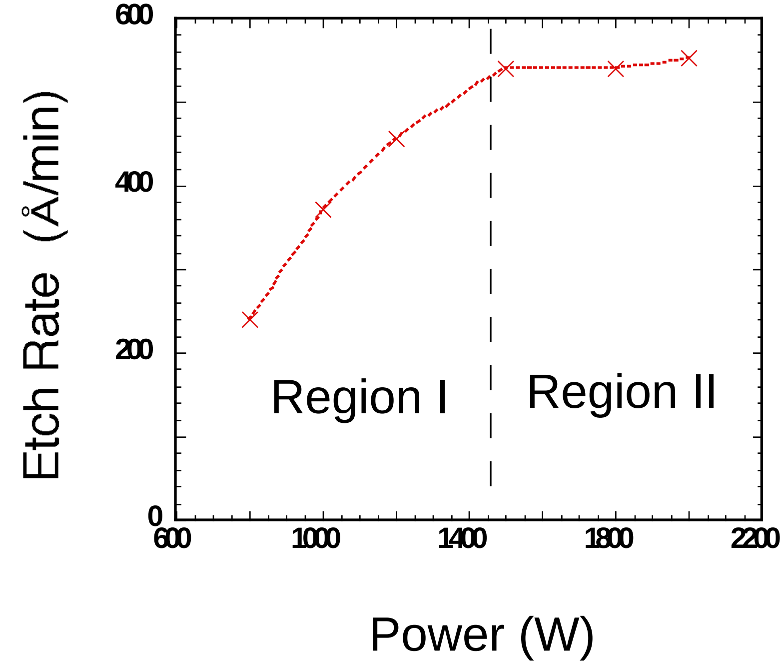
p-Si ETCH RATE

- **Predictions for etch rate correlate well with the semi-emperical model of D. Dane and T. D. Mantei *:**

$$R = \left(\frac{1}{a\Gamma_{Cl}} + \frac{1}{b[J_i V_s - (JV)_{th}]} \right)^{-1}$$

- **Region I: Etching is in the ion-starved region, so the increased ion flux at higher power produces an increase of etch rate.**

- **Region II: Etching is in the Cl radical-starved region, so further increase of the ion flux does not increase the etch rate.**



- **Ar/Cl_2 = 70/30, 10 mTorr, 100 sccm**

* D. Dane and T. D. Mantei, Appl. Phys. Lett. 65 (4), 478 (1994)

CONCLUSIONS

- A Surface Kinetics Module (SKM) has been developed and integrated into the Hybrid Plasma Equipment Model (HPEM).
- The SKM applies a surface reaction mechanism and uses fluxes from the HPEM to update sticking coefficients and surface species coverage. It also yields etching/deposition rate.
- The SKM was used to study the C_2F_6 etching of Si and Cl_2 etching of p-Si.
- Results indicate that for C_2F_6 etching of Si, the decrease of CF_2 sticking to the wall with increasing temperature increases the CF_2 density in the plasma. As a result the passivation layer thickness increases, and the etch rate drops.
- Higher bias voltages on the substrate decrease the passivation layer thickness and so allow the etch rate to increase through higher F atom diffusion flux.
- For Cl_2 etching of p-Si, the simulation demonstrates the ion-starved and the Cl radical-starved regions for processing.