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STICKING COEFFICIENTS OF NEUTRALS IN AN RF FLUOROCARBON DISCHARGE

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AGENDA

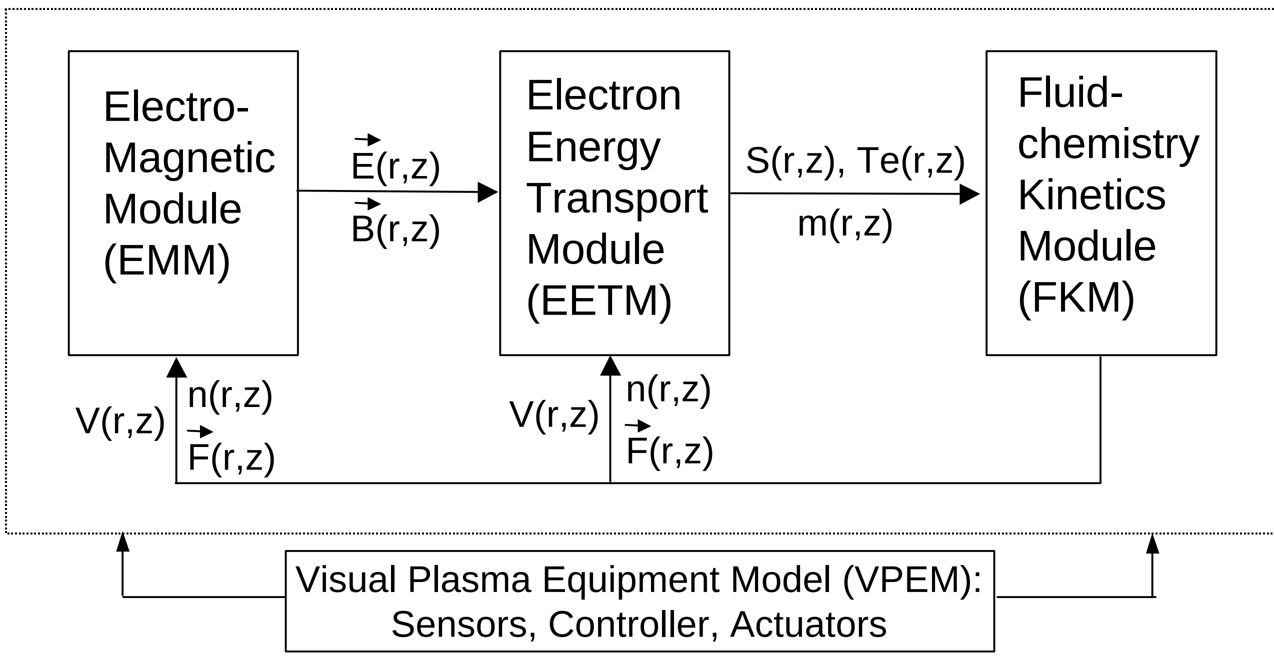
- Introduction
- Description of the Model
  - Hybrid Plasma Equipment Model (HPEM)
  - Surface Kinetics Module (SKM)
- C_mF_n Plasma Surface Reaction Mechanism
- CF_2 Density vs. Bias
- CF_2 Density vs. Pressure
- Summary

INTRODUCTION

- 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.
- Plasma-surface interactions can influence gas phase radical densities.
- A better understanding of the mechanism of the reactions occurring at the surface, and the influences on the surface reactions resulting from different processing parameters, can help optimize the process.
- Our goal: By coupling surface reaction modeling with a plasma physics-plasma chemistry simulator, we numerically investigate the mechanism of surface reactions, and characterize their influence on plasma properties and process kinetics.

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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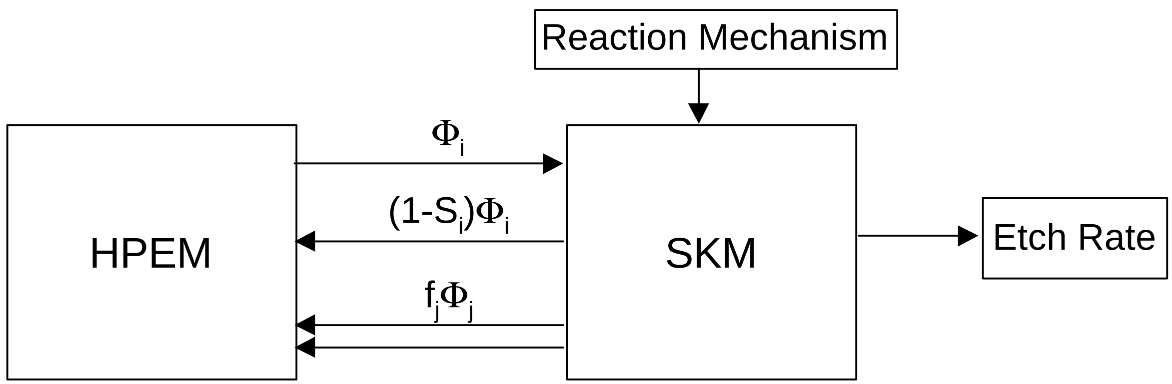
SURFACE KINETICS MODEL (SKM)

- The Surface Kinetics Model (SKM) is an integrated module of the HPEM.
- The SKM uses reactant fluxes to surfaces from the HPEM, together with a user defined reaction mechanism, as inputs for the calculation.
- The SKM updates surface sticking and product reflection coefficients used as surface boundary conditions in the HPEM, and 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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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).

- Ions with higher bombarding energy produces higher etch yield.

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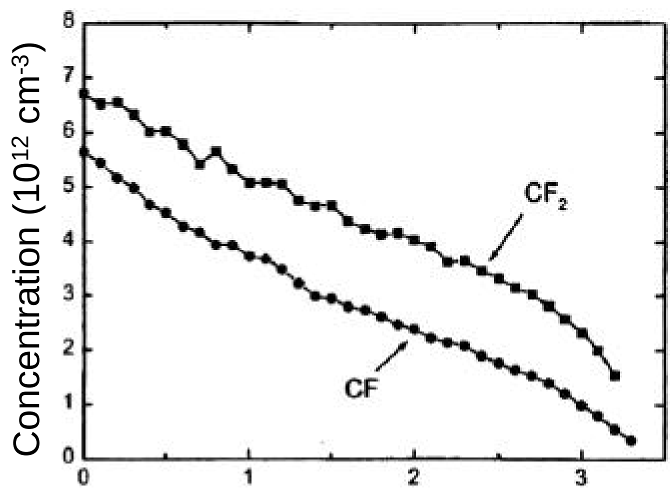
C_mF_n PLASMA: SURFACE REACTIONS

- It has been observed in C_mF_n discharge that surfaces contribute differently to the CF/CF_2 radicals under different conditions. A surface can act either as sources, or conversely a sink, for the CF/CF_2 radicals.

- The net effect of the surface to the CF/CF_2 density is due to the summation of several primary interactions:
  - C_xF_y radicals (CF, CF_2, C_2F_4, C_2F_5, etc.) sticking to the surface to polymerize, forming a passivation layer on the surface.
  - Ion sputtering of the polymer layer to release CF/CF_2 from the surface.
  - F atoms etching of the polymer layer.

- Axial radical density distribution*

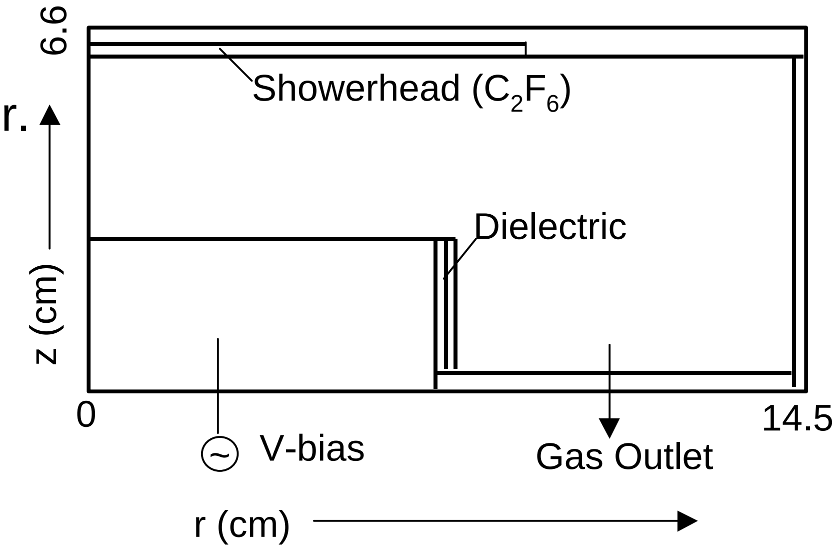


- CF_4, rf discharge
- 100 W, 200 mtorr

* J.P. Booth et. al, *J. Appl. Physics* 85 , 3097(1999)

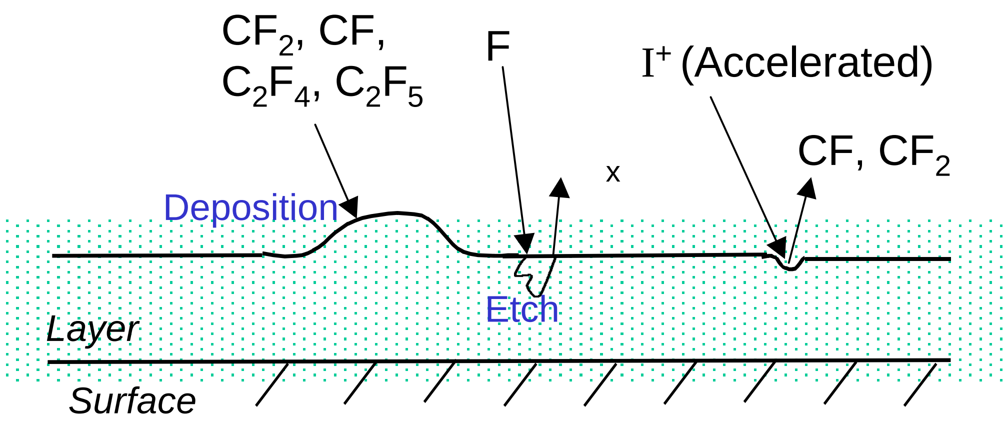
SIMULATION PARAMETERS

- Simulations of a rf C_2F_6 discharge were performed for a cylindrical reactor.



- Processing conditions:
  - C_2F_6 pressure: 30-70 mtorr.
  - Gas flow rate: 30 sccm.
  - RF bias: 30-400 Volts.

- Important surface reactions used in the SKM model:
  - CF, CF_2 deposition.
  - C_2F_4, C_2F_5 deposition.
  - I^+ sputtering to generate CF, CF_2.
  - F etching of the passivation layer.



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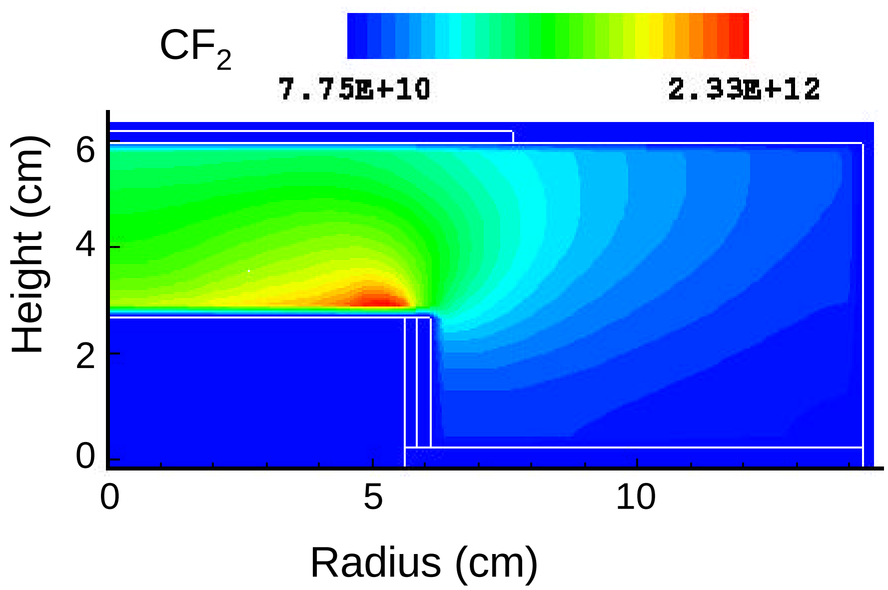
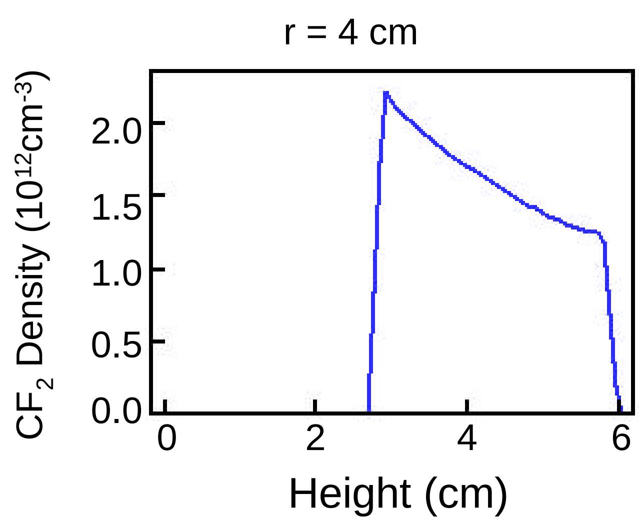
CF_2 DENSITY DISTRIBUTION

- Simulation was performed at V_{bias}=400 V, P=50 mtorr.
- The CF_2 density peaks close to the corner of the electrode because of field enhancement.
- CF_2 density decreases from the lower electrode to the upper electrode.
- The lower electrode acts as a source and the upper electrode acts as a sink for CF_2 radical.





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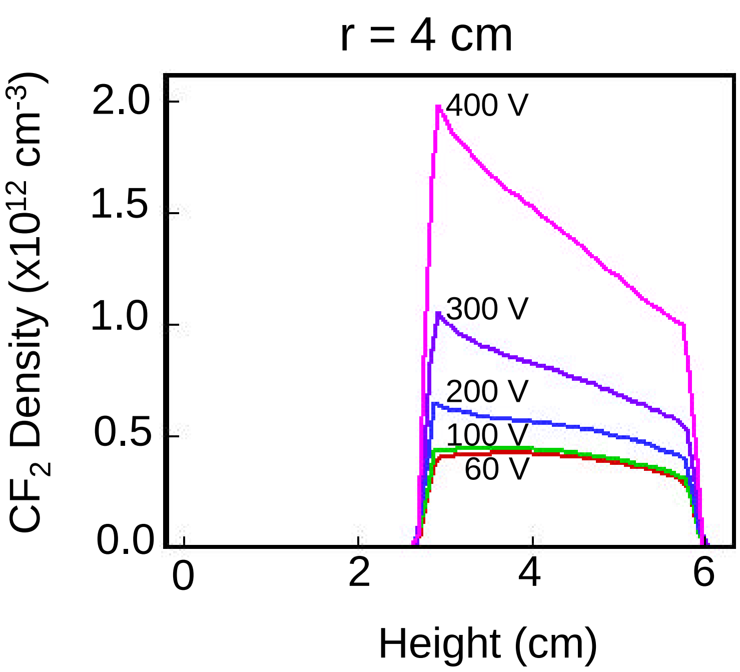
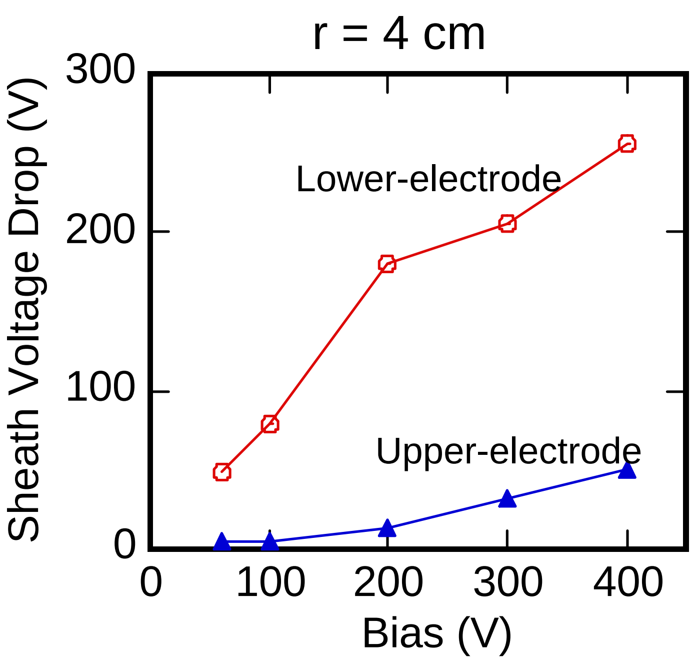
BIAS DEPENDENCE OF CF_2 DENSITY DISTRIBUITON

- Simulations were performed for different biases: 60, 100, 200, 300, 400 V.
- At the upper electrode, the sheath voltage drops are low for all conditions, so the ion sputtering yields of CF_2 are low compared with the CF_2 sticking loss rate. The net effect of the upper electrode is a sink for CF_2.
- At the lower electrode, the sheath voltage drop increases with the increase of the bias, so more CF_2 is generated. The slope of the axial distribution increases with the increase of the bias.

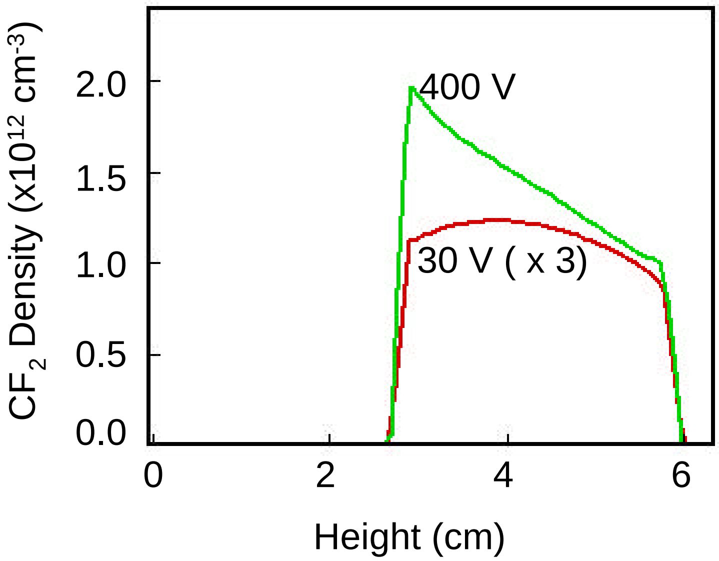




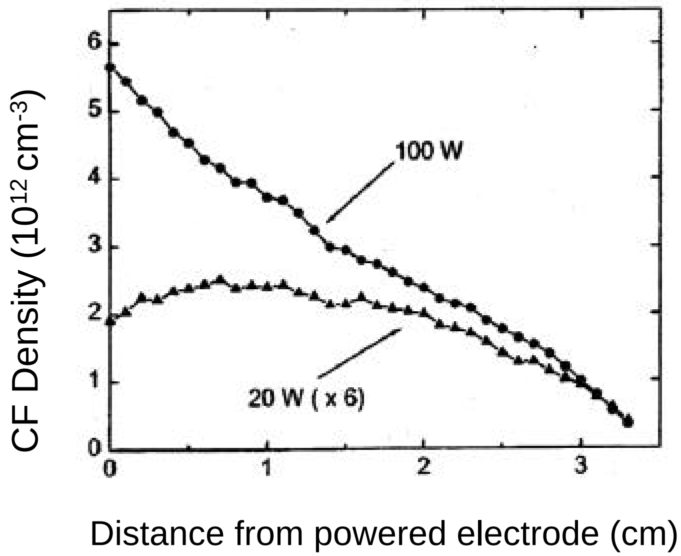
GEC99-09

CF_2 DENSITY DISTRIBUITON: LOW BIAS

- When the bias was as low as 30 V, simulation showed that the CF_2 density decreases at both electrodes due to low ion sputtering yield under low bias.
- Experiments by Booth et. al. Produced similar results.*



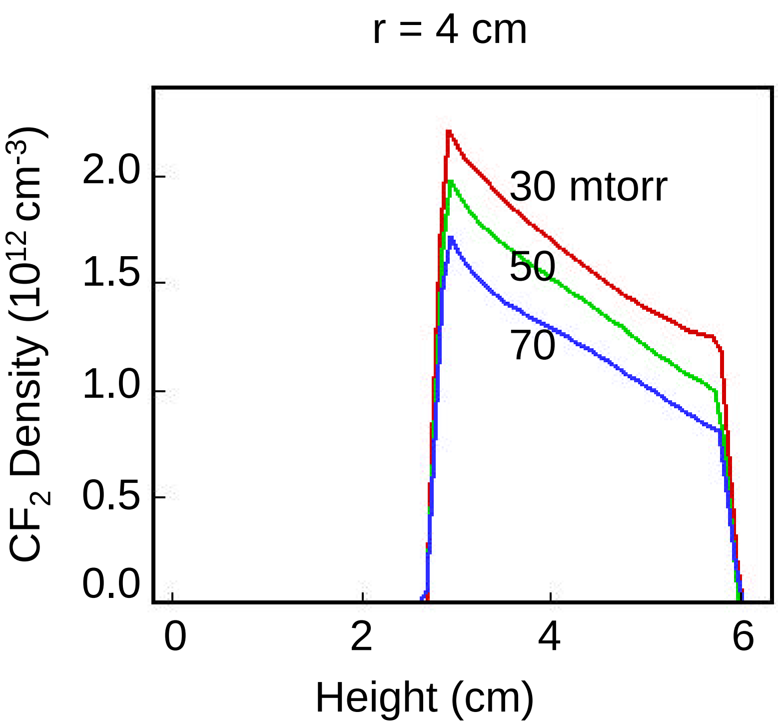
• CF_4, rf discharge

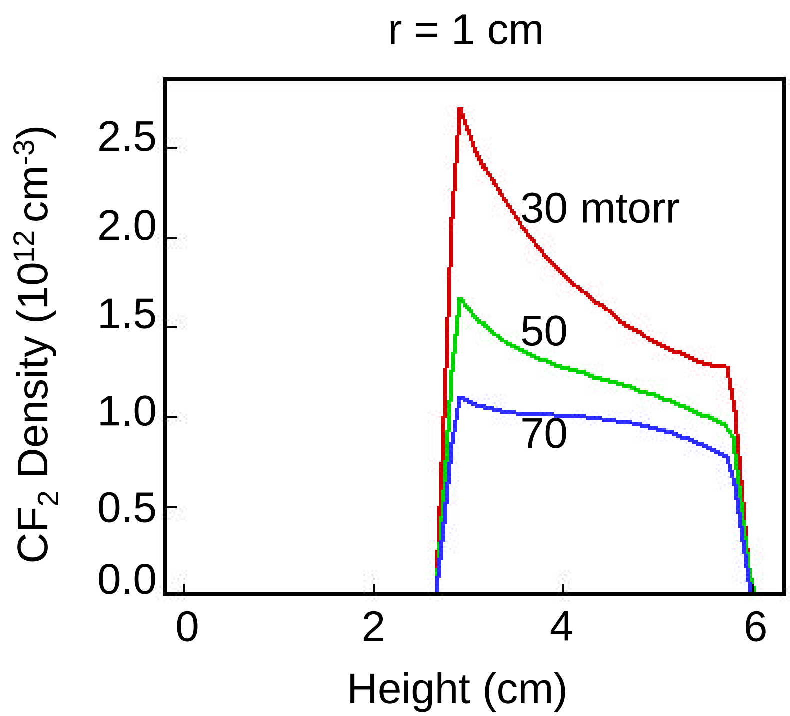


* J.P.Booth, G.Cunge, P.Chabert, and N. Sadeghi, *J. Appl. Phys.* 85, 3097 (1999)

PRESSURE DEPENDENCE OF CF_2 DENSITY DISTRIBUTION

- The axial CF_2 density distributions at r=4 cm and r=1 cm were obtained for different pressures (30, 50, 70 mtorr) with a 400 V bias.
- At r=4 cm, the slopes for different pressures are similar.
- At r=1 cm, the slopes decrease with increasing pressure.





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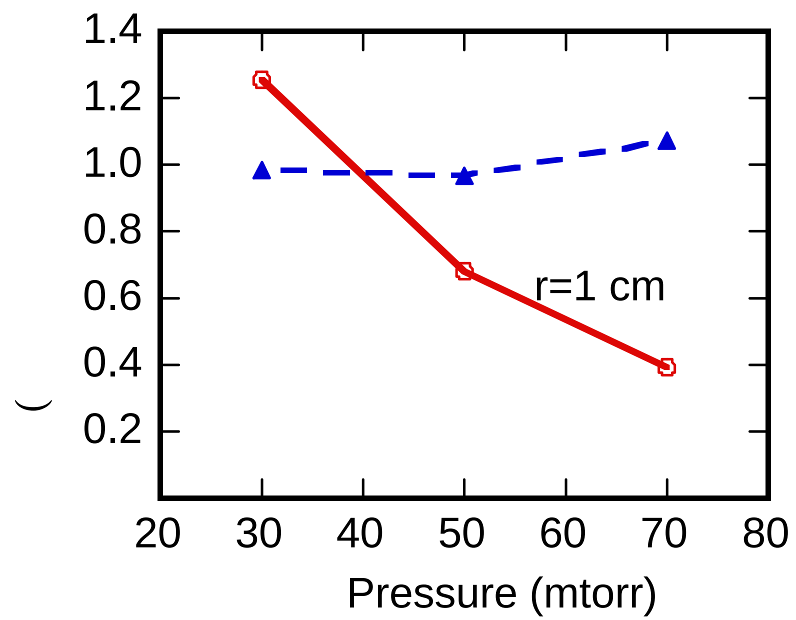
PRESSURE DEPENDENCE OF CF_2 DENSITY DISTRIBUITON (cont.)

- At r=4 cm, Φ(ion) / n(CF_2) for different pressures are similar, so the net effect of the wall to the CF_2 density is nearly the same. This leads to similar CF_2 distributions for different pressures.

- At r=1 cm, Φ(ion) / n(CF_2) decreases with increasing pressure, so the net CF_2 generation from wall reactions decreases. This leads to smaller distribution slope at higher pressure.



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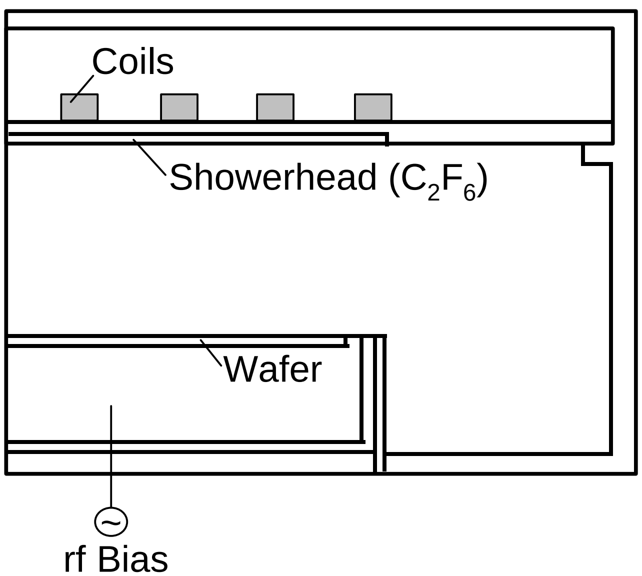
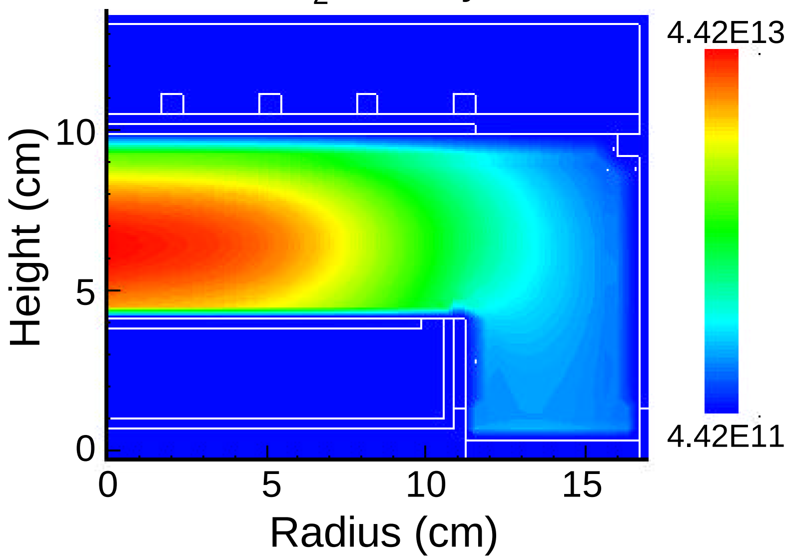
C_2F_6 ETCHING OF Si IN AN ICP REACTOR

- Simulations were performed on a C_2F_6 discharge in an ICP reactor with an rf bias.
- The CF_2 sticking coefficient at the wall was changed to simulate the variation of reactor wall temperature.
- The consequences on plasma properties and Si etch rate were investigate.



- CF_2 Density



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

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REACTION MECHANISM FOR C_2F_6 ETCHING OF Si

- The reaction mechanism for C_2F_6 etching of Si 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 balanced result of CF_x deposition, ion sputtering and F etching of the layer.
- Si etching precursor (F) needs to diffuse through the passivation layer.

2 →

CF_3^+ + P_s → CF_4

F + P_s → CF_4

F + P_s → F_t

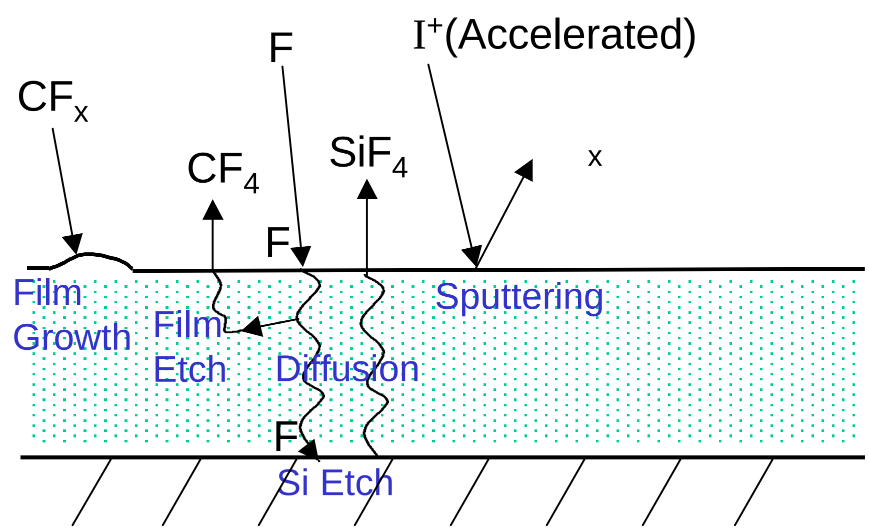
F_t → F_i

F_i + Si_s → SiF

F_i + SiF → $_2$_s

F_i + SiF → SiF_3_s

$_3$_s → SiF_4



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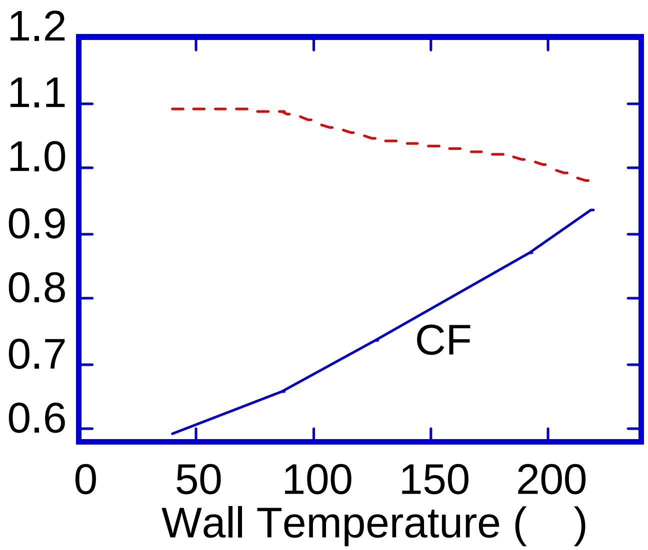
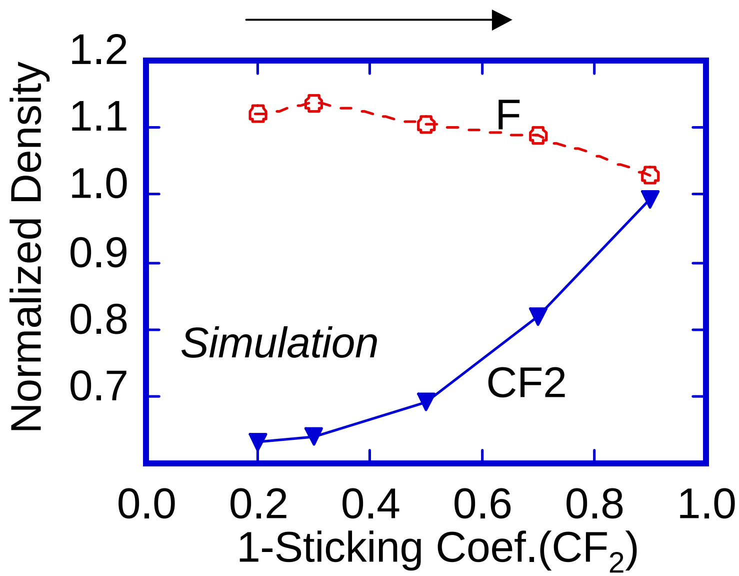
INFLUENCE OF WALL TEMPERATURE

- Experiments showed a variation of radical densities as the reactor wall temperature changes.* We simulated the consequences of wall temperature variation 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 increased CF_2 density induces decreased F density.

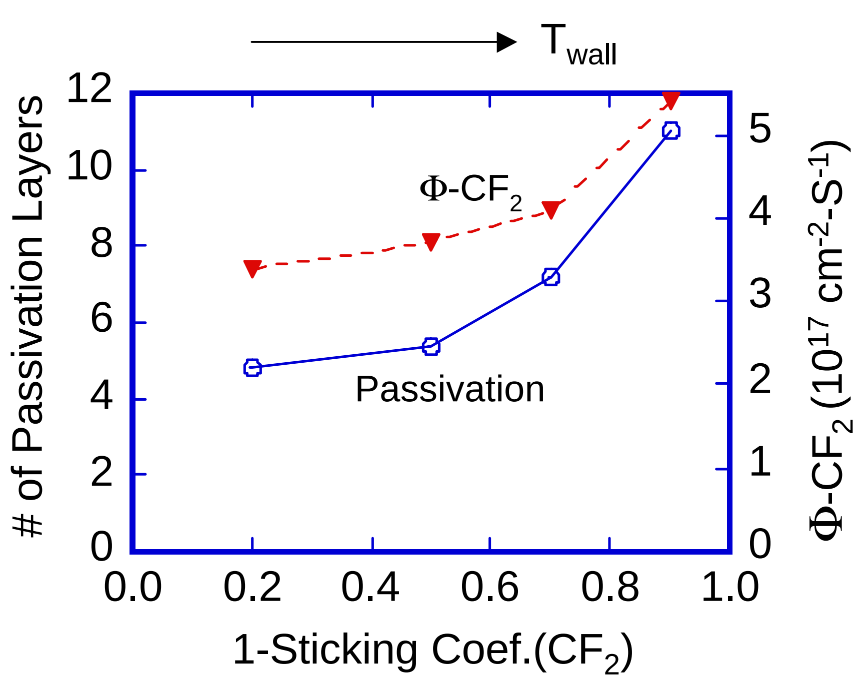


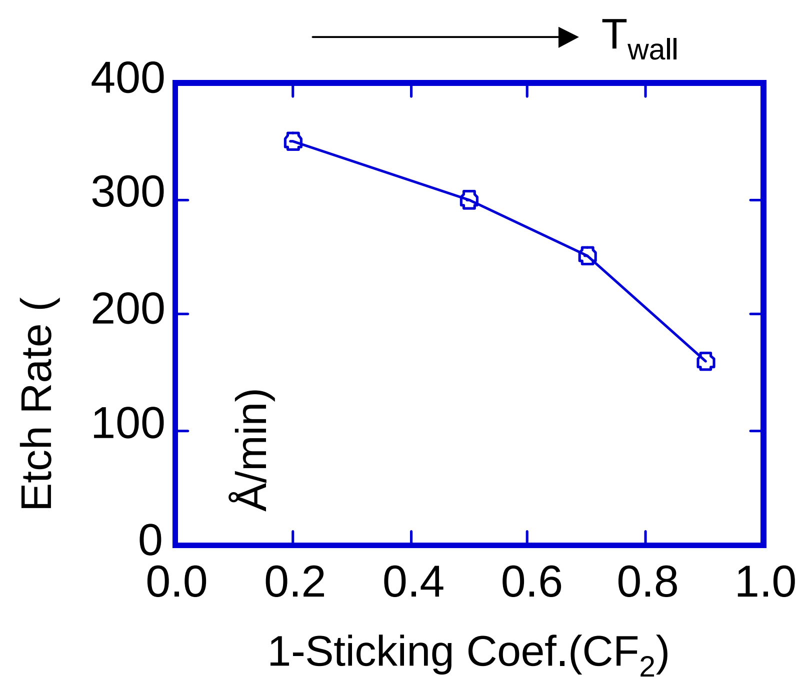


* M.Scharkens, R.C.M. Bosch, and G.S. Oehrlein, J. Vac. Sci. Technol. A 16(1), 239 (1998)

PASSIVATION LAYER AND ETCH RATE

- With the decrease of the CF_2 sticking coefficient to the wall (reactor wall temperature increases), the CF_2 radical flux to the wafer increases due to the increased CF_2 density. This leads to thicker passivation layer.
- The diffusion flux of the Si etching precursor (F) through the passivation layer decreases for thicker passivation, and so the etch rate drops.





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SUMMARY

- The Surface Kinetics Module (SKM) was developed in coupling with the Hybrid Plasma Equipment Model (HPEM) to obtain fully integrated simulation of plasma physics, plasma chemistry and surface chemistry.

- The surface reaction mechanism of C_2F_6 discharge involves C_xF_y deposition, F etching, and ion sputtering of a passivation layer.

- The net effect of a surface to CF_2 density depends on the relative strength of the deposition loss and ion sputtering generation of CF_2.

- Increasing ion energy or ion to neutral flux ratio can enhance the generation of CF_2 from a surface.